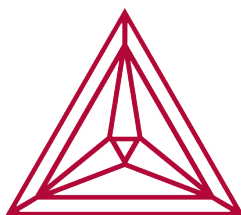


Thermo-Calc Console Mode Example Macros

Thermo-Calc Version 2025b



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Note the following examples are deprecated:
○ *tcex45, tcex46, tcex47, and tcex50 are deprecated as of Thermo-Calc version 2019b*
○ *tcex25 and tcex40d are deprecated as of Thermo-Calc version 2022a*

Pitting Resistance Equivalence (PRE) for a duplex stainless steel.

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Scheil calculation for an Al-4Mg-2Si-2Cu alloy

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Calculate volumetric thermal expansion coefficients of the L12-type Al₃Sc.

tcex59

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tcex60

Calculate the electrical resistivity (ELRS) and thermal conductivity (THCD) from FCC_A1 to liquid.

Results

tcex01

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex01\tcex01.TCM"

SYS: set-echo

SYS:

SYS: @@ Calculation of the Fe-C binary phase diagram.

SYS:

SYS: @@ This example calculates the binary Fe-C phase

SYS: @@ diagram using the Binary module.

SYS:

SYS: set-log ex01,,,

SYS:

SYS: @@ The log file is set to get command echo.

SYS: @@ The menu is shown by typing a question mark "?"

SYS: ?

... the command in full is HELP

ABOUT	HP_CALCULATOR	SET_INTERACTIVE_MODE
BACK	INFORMATION	SET_LOG_FILE
CLOSE_FILE	MACRO_FILE_OPEN	SET_PLOT_ENVIRONMENT
DISPLAY_LICENSE_INFO	OPEN_FILE	SET_TC_OPTIONS
EXIT	SET_COMMAND_UNITS	SET_TERMINAL
GOTO_MODULE	SET_ECHO	STOP_ON_ERROR
HELP	SET_GES_VERSION	

SYS: @@ When you give a command the program may ask questions.

SYS: @@ You may obtain help for each question by typing a ? .

SYS: @@ If you accept the default answer suggested /within slashes/

SYS: @@ just press "return"

SYS: info

... the command in full is INFORMATION

FILE SYSTEM ERROR 37

*** ERROR 1717 IN MOPEN: FILE DOES NOT EXIST: c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\help\sysmon.hlp

ERROR 1717 RESET

SYS: ?

... the command in full is HELP

ABOUT	HP_CALCULATOR	SET_INTERACTIVE_MODE
BACK	INFORMATION	SET_LOG_FILE
CLOSE_FILE	MACRO_FILE_OPEN	SET_PLOT_ENVIRONMENT
DISPLAY_LICENSE_INFO	OPEN_FILE	SET_TC_OPTIONS
EXIT	SET_COMMAND_UNITS	SET_TERMINAL
GOTO_MODULE	SET_ECHO	STOP_ON_ERROR
HELP	SET_GES_VERSION	

SYS:

SYS:

SYS:Hit RETURN to continue

SYS: @@ For a binary phase diagram calculation we use the binary module

SYS: go

... the command in full is GOTO_MODULE

MODULE NAME: ?

NO SUCH MODULE, USE ANY OF THESE:

SYSTEM UTILITIES
GIBBS_ENERGY_SYSTEM
TABULATION_REACTION
POLY_3
DICTRA_MONITOR
BINARY_DIAGRAM_EASY
DATABASE_RETRIEVAL
DIC_PARROT
REACTOR_SIMULATOR_3
PARROT
POTENTIAL_DIAGRAM
SCHEIL_SIMULATION
OLD_SCHEIL_SIM
POURBAIX_DIAGRAM
TERNARY_DIAGRAM

MODULE NAME: BIN

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

VA /- DEFINED

BCC_B2 FCC_L12 FCC_L102

D021_HCP REJECTED

First element: fe

Second element: c

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase-Diagram

```
... the command in full is REJECT
VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021 HCP REJECTED
REINITIATING GES .....
... the command in full is DEFINE_ELEMENTS
C FE DEFINED
LIQUID:L IONIC_LIQUID:Y FCC_A1
BCC_A2 A2_BCC HCP_A3
HCP_ZN DIAMOND_A4 GRAPHITE_A9
CBCC_A12 CUB_A13 B2_FEPD
C14_LAVES C15_LAVES D011_CEMENTITE
D82_FEZN_GAMMA L12_FEPD3 AL5FE4
FE3AS2 FEZN4 FEZN_DELTA
FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
BCC_A2 RESTORED
D011_CEMENTITE RESTORED
GRAPHITE_A9 RESTORED
DIAMOND_A4 RESTORED
... the command in full is GET_DATA
08:34:41,882 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST_REFERENCES to see the list of references for assessed data

```
-OK-
... the command in full is SET_CONDITION
... the command in full is SET_AXIS_VARIABLE
The condition X(Fe)=.1234 created
... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08 created
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
... the command in full is SET_CONDITION
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
... the command in full is SAVE_WORKSPACES
Version S mapping is selected
```

Organizing start points

```
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 9.944E-01 1.100E+03
BCC_A2
** FCC_A1
Calculated. 5 equilibria

Phase region boundary 2 at: 9.838E-01 1.011E+03
BCC_A2
** FCC_A1
** GRAPHITE_A9

Phase region boundary 3 at: 4.996E-01 1.011E+03
BCC_A2
** GRAPHITE_A9
Calculated.. 30 equilibria
Terminating at axis limit.

Phase region boundary 4 at: 4.845E-01 1.011E+03
FCC_A1
** GRAPHITE_A9
Calculated. 18 equilibria

Phase region boundary 5 at: 4.561E-01 1.427E+03
** LIQUID
FCC_A1
** GRAPHITE_A9

Phase region boundary 6 at: 8.690E-01 1.427E+03
** LIQUID
FCC_A1
Calculated. 15 equilibria

Phase region boundary 7 at: 9.840E-01 1.768E+03
** LIQUID
** BCC_A2
FCC_A1

Phase region boundary 8 at: 9.939E-01 1.768E+03
** BCC_A2
FCC_A1
Calculated 25 equilibria

Phase region boundary 9 at: 9.858E-01 1.768E+03
LIQUID
** BCC_A2
Calculated 20 equilibria

Phase region boundary 10 at: 4.129E-01 1.427E+03
** LIQUID
GRAPHITE_A9
Calculated.. 44 equilibria
Terminating at axis limit.

Phase region boundary 11 at: 9.841E-01 1.011E+03
BCC_A2
** FCC_A1
Calculated 25 equilibria

Phase region boundary 12 at: 9.944E-01 1.100E+03
```

```

      BCC_A2
** FCC_A1
Calculated          16 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping      4 seconds
POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

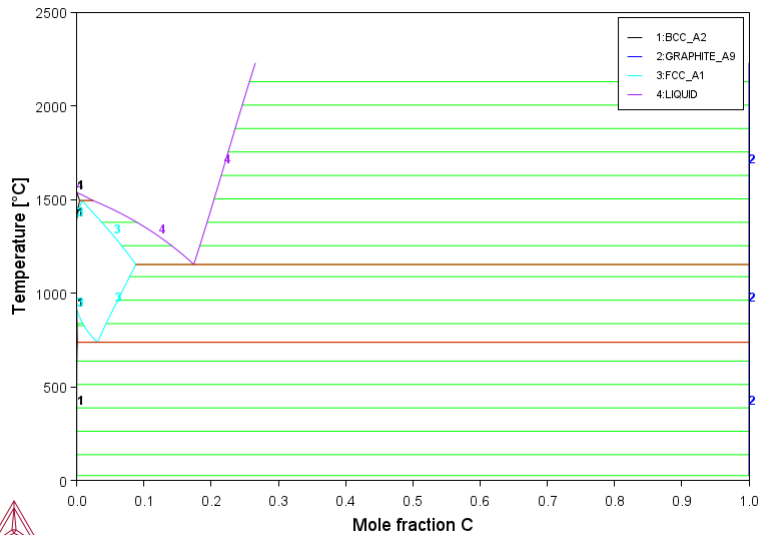
Setting automatic diagram axes

```

... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

```

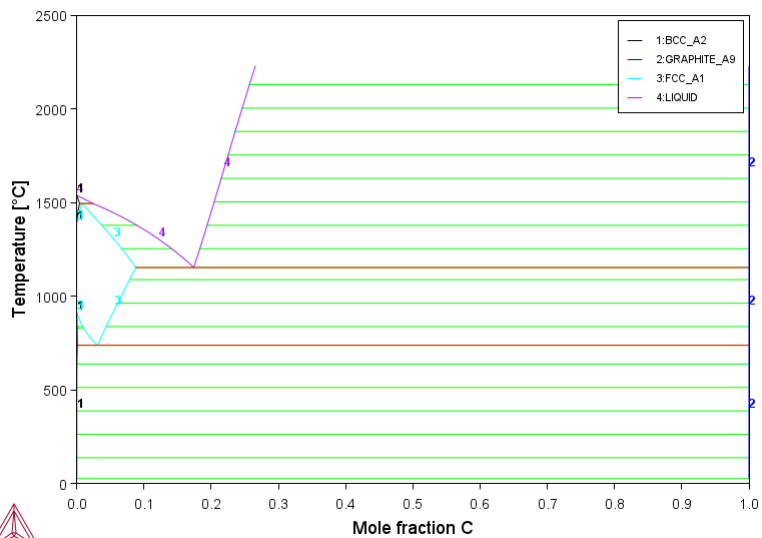
C FE



```

POST:
POST:Hit RETURN to continue
POST:
POST: set-title example 1a
POST: plot
... the command in full is PLOT_DIAGRAM
example 1a

```

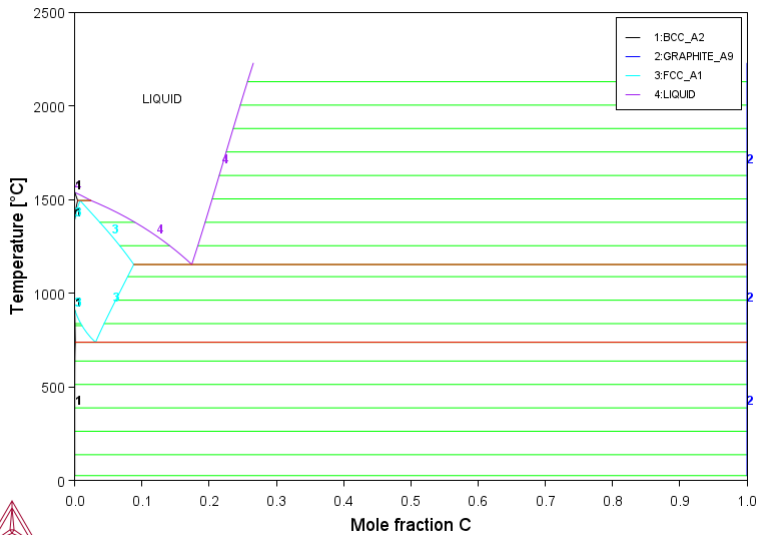


```

POST:
POST:Hit RETURN to continue
POST: @@ By default labels is given for phase boundaries lines.
POST: @@ If you want to label areas the user must supply a coordinate for the
POST: @@ label, for example
POST: ADD
... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .1
Give Y coordinate in axis units: 2000
Automatic phase labels? /Y/: Y
Automatic labelling not always possible
Using global minimization procedure
Calculated          630 grid points in      0.011 s
Found the set of lowest grid points in      0.001 s
Calculated POLY solution      0.011 s, total time      0.023 s
Stable phases are: LIQUID
Text size: /.36/:
POST: set-title example 1b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1b

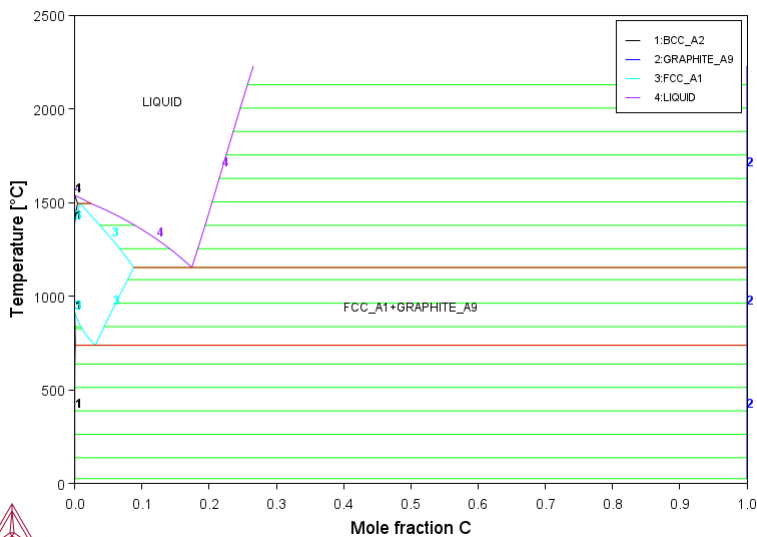


```

POST:
POST:
POST:Hit RETURN to continue
POST: add .4 900
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/: Y
Automatic labelling not always possible
Using global minimization procedure
Calculated      630 grid points in      0.020 s
Found the set of lowest grid points in      0.004 s
Calculated POLY solution      0.014 s, total time      0.038 s
Stable phases are: FCC_A1+GRAPHITE_A9
Text size: /.36/:
POST: set-title example 1c
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1c



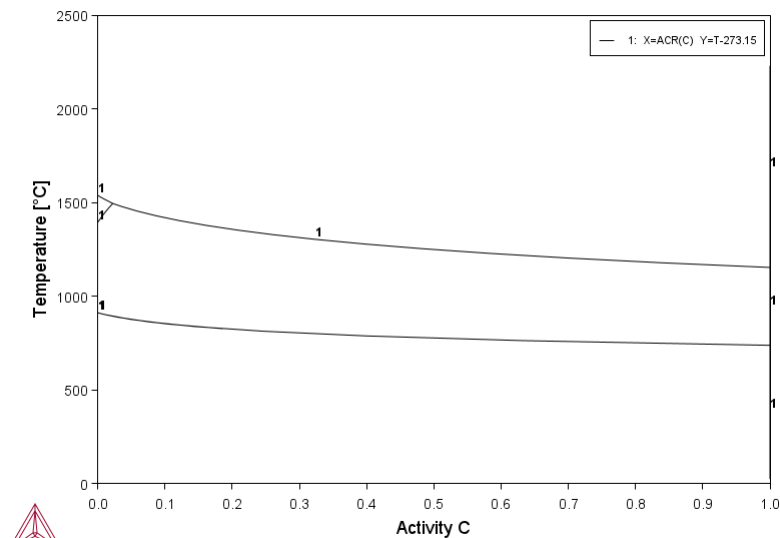
```

POST:
POST:
POST:
POST: @@ This is the stable phase diagram with graphite and no cementite.
POST: @@ In Thermo-Calc all relevant data from the calculation of the diagram is saved
POST: @@ and it is possible to plot the same diagram using other thermodynamic
POST: @@ quantities, for example replace the carbon composition with its activity
POST: @@ Find out the commands in the post processor by entering ?
POST:Hit RETURN to continue
POST: ?
... the command in full is HELP
ADD_LABEL_TEXT      PLOT_DIAGRAM      SET_INTERACTIVE_MODE
APPEND_EXPERIMENTAL_DATA  PRINT_DIAGRAM      SET_LABEL_CURVE_OPTION
BACK      QUICK_EXPERIMENTAL_PLOT  SET_PLOT_FORMAT
CHANGE_LEGEND      REINITIATE_PLOT_SETTINGS  SET_PLOT_OPTIONS
CREATE_3D_PLOTFILE  RESTORE_PHASE_IN_PLOT  SET_PLOT_SIZE
DUMP_DIAGRAM      SELECT_PLOT      SET_PREFIX_SCALING
ENTER_SYMBOL      SET_AXIS_LENGTH      SET_RASTER_STATUS
EXIT      SET_AXIS_PLOT_STATUS      SET_REFERENCE_STATE
FIND_LINE      SET_AXIS_TEXT_STATUS      SET_SCALING_STATUS
HELP      SET_AXIS_TYPE      SET_TIC_TYPE
LIST_DATA_TABLE      SET_COLOR      SET_TIELINE_STATUS
LIST_PLOT_SETTINGS      SET_CORNER_TEXT      SET_TITLE
LIST_SYMBOLS      SET_DIAGRAM_AXIS      SET_TRUE_MANUAL_SCALING
MAKE_EXPERIMENTAL_DATAFI  SET_DIAGRAM_TYPE  SUSPEND_PHASE_IN_PLOT
MODIFY_LABEL_TEXT      SET_FONT      TABULATE
POST: @@ The command to set axis for the diagram is SET-DIAGRAM-AXIS
POST: s-d-a x
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
FILE SYSTEM ERROR IN FILHLP

```

ERROR 1717 READING HELP FILE

```
VARIABLE : ac
FOR COMPONENT : c
POST: set-title example 1d
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 1d
```



```
POST:
POST:
POST:
POST: @@ The diagram stops at unit activity which represent graphite.
POST: @@ The area labels disappear when one sets a new diagram axis because they
POST: @@ are relative to the axis values, not the axis quantities.
POST: @@
POST:Hit RETURN to continue
POST:
POST: @@ The metastable diagram, with cementite, can also be calculated but then
POST: @@ one must do some manipulations in POLY. We can use the data
POST: @@ we already retrieved from the database.
POST: back
Current database: Steels/Fe-Alloys v11.0
```

```
VA /- DEFINED
DICTRA_FCC_A1 REJECTED
SYS: go p-3
... the command in full is GOTO_MODULE
POLY:
POLY: @@ The BIN module has used the poly-3 workspace to calculate the
POLY: @@ diagram. We have all data available here. The workspace has been
POLY: @@ saved on a file and we can read this back with the command READ.
POLY:
POLY: read,,,
... the command in full is READ_WORKSPACES
POLY:
POLY: @@ There are many commands in the POLY module. This enables you
POLY: @@ to calculate almost any kind of equilibrium and diagram.
POLY: @@ With the ? you can list all commands
POLY:Hit RETURN to continue
POLY: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM GOTO_MODULE REINITIATE_MODULE
ADVANCED_OPTIONS HELP SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA INFORMATION SELECT_EQUILIBRIUM
BACK LIST_AXIS_VARIABLE SET_ALL_START_VALUES
CHANGE_STATUS LIST_CONDITIONS SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM LIST_EQUILIBRIUM SET_CONDITION
COMPUTE_TRANSITION LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_STATUS SET_INTERACTIVE
DEFINE_COMPONENTS LIST_SYMBOLS SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
DEFINE_MATERIAL MACRO_FILE_OPEN SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB LIB MAKE_COMPONENT_ENTERED SET_START_VALUE
DELETE_SYMBOL MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL MAP STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS POST TABULATE
EXIT READ_WORKSPACES
POLY:
POLY:Hit RETURN to continue
POLY: @@ Get more command information with the HELP command
POLY: help
COMMAND: list-status
*** ERROR 37 IN FILDOC: FILE SYSTEM ERROR
POLY:Hit RETURN to continue
POLY: @@ General information can be obtained using the INFORMATION command
POLY: INFO
... the command in full is INFORMATION
FILE SYSTEM ERROR 37
POLY:
POLY: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM GOTO_MODULE REINITIATE_MODULE
ADVANCED_OPTIONS HELP SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA INFORMATION SELECT_EQUILIBRIUM
BACK LIST_AXIS_VARIABLE SET_ALL_START_VALUES
CHANGE_STATUS LIST_CONDITIONS SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM LIST_EQUILIBRIUM SET_CONDITION
COMPUTE_TRANSITION LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_STATUS SET_INTERACTIVE
DEFINE_COMPONENTS LIST_SYMBOLS SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
```

```

DEFINE_MATERIAL      MACRO_FILE_OPEN      SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB MAKE_COMPONENT_ENTERED SET_START_VALUE
DELETE_SYMBOL        MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL         MAP                   STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS   POST                 TABULATE
EXIT                 READ_WORKSPACES

POLY: state
No such command: state. Use ? for list of available commands
POLY:
POLY:Hit RETURN to continue
POLY: @@ List the current equilibrium by
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: ?
FILE SYSTEM ERROR IN FILHLP
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0  , database: TCBIN

Conditions:
N=1, P=100000, X(Fe)=0.99, T=1100
DEGREES OF FREEDOM 0

Temperature 1100.00 K ( 826.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.54086E+01
Total Gibbs energy -4.90502E+04, Enthalpy 3.18534E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
C               1.0000E-02  2.1677E-03 1.8555E-01 -1.5406E+04 GRAPHITE
FE              9.9000E-01  9.9783E-01 9.9957E-01 -3.9762E+00 BCC_A2

FCC_A1          Status ENTERED      Driving force 0.0000E+00
Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.97662E-01 C 2.33819E-03

BCC_A2          Status ENTERED      Driving force 0.0000E+00
Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99907E-01 C 9.33835E-05
POLY:Hit RETURN to continue
POLY: @@ The actual conditions are listed by the list-equil command but
POLY: @@ can be obtained also by
POLY: l-c
... the command in full is LIST_CONDITIONS
N=1, P=100000, X(Fe)=0.99, T=1100
DEGREES OF FREEDOM 0
POLY:
POLY:Hit RETURN to continue
POLY: @@ The meaning of the state variables T, P, X, N and many others
POLY: @@ are explained by the INFO command
POLY: INFO
... the command in full is INFORMATION
FILE SYSTEM ERROR 37
POLY: state
No such command: state. Use ? for list of available commands
POLY:
POLY:Hit RETURN to continue
POLY: @@ The use of state variables as conditions is the key to the
POLY: @@ flexibility of Thermo-Calc. Each condition is set independently and
POLY: @@ any condition can be set as an axis variable.
POLY: @@
POLY: @@ Now we just want to take away the graphite in order to calculate the
POLY: @@ metastable Fe-C diagram with cementite. We can list all phases with the
POLY: @@ LIST_STATUS command
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)      P(Pa)
VA             ENTERED      SER
C              ENTERED      GRAPHITE_A9     *          100000
FE             ENTERED      BCC_A2          *          100000
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
FCC_A1         ENTERED      0.000000E+00      9.246266E-01
BCC_A2         ENTERED      0.000000E+00      7.537335E-02
D011_CEMENTITE ENTERED      -4.153716E-01      0.000000E+00
LIQUID         ENTERED      -4.668963E-01      0.000000E+00
GRAPHITE_A9    ENTERED      -1.684424E+00      0.000000E+00
DIAMOND_A4     ENTERED      -2.386932E+00      0.000000E+00
*** STATUS FOR ALL SPECIES
C      ENTERED      C3      ENTERED      FE      ENTERED      VA      ENTERED
C1     ENTERED      C4     ENTERED      FE+2   ENTERED      VA-2   ENTERED
C2     ENTERED      C5     ENTERED      FE+3   ENTERED      VA-4   ENTERED
POLY:Hit RETURN to continue
POLY: @@ The status is changed with the CHANGE_STATUS command
POLY: ch-st
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): ?
FILE SYSTEM ERROR IN FILHLP
Phase name(s): gra
Status: /ENTERED/: sus
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)      P(Pa)
VA             ENTERED      SER
C              ENTERED      GRAPHITE_A9     *          100000
FE             ENTERED      BCC_A2          *          100000
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
FCC_A1         ENTERED      0.000000E+00      9.246266E-01
BCC_A2         ENTERED      0.000000E+00      7.537335E-02
D011_CEMENTITE ENTERED      -4.153716E-01      0.000000E+00
LIQUID         ENTERED      -4.668963E-01      0.000000E+00
DIAMOND_A4     ENTERED      -2.386932E+00      0.000000E+00
SUSPENDED PHASES:
GRAPHITE_A9
*** STATUS FOR ALL SPECIES
C      ENTERED      C3      ENTERED      FE      ENTERED      VA      ENTERED
C1     ENTERED      C4     ENTERED      FE+2   ENTERED      VA-2   ENTERED
C2     ENTERED      C5     ENTERED      FE+3   ENTERED      VA-4   ENTERED
POLY:Hit RETURN to continue

```

```

POLY: @@ Note that the graphite is listed as suspended this time.
POLY: @@ Now try to calculate the equilibrium without graphite.
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      629 grid points in      0.015 s
Found the set of lowest grid points in      0.003 s
Calculated POLY solution      0.015 s, total time      0.033 s
POLY: @@ A number of ,,, after a command means to accept default values.
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCBIN

Conditions:
N=1, P=100000, X(Fe)=0.99, T=1100
DEGREES OF FREEDOM 0

Temperature 1100.00 K ( 826.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.54086E+01
Total Gibbs energy -4.90502E+04, Enthalpy 3.18534E+04, Volume 0.00000E+00

Component      Moles      W-Fraction      Activity      Potential      Ref.stat
C                1.0000E-02      2.1677E-03      1.8555E-01      -1.5406E+04      GRAPHITE
FE               9.9000E-01      9.9783E-01      9.9957E-01      -3.9762E+00      BCC_A2

FCC_A1          Status ENTERED      Driving force 0.0000E+00
Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.97662E-01 C 2.33819E-03

BCC_A2          Status ENTERED      Driving force 0.0000E+00
Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99907E-01 C 9.33835E-05
POLY:Hit RETURN to continue
POLY: @@ It may seem surprising that diamond is stable but the total mole fraction
POLY: @@ of iron is less than 0.5, so we are on the carbon rich side
POLY: @@ of cementite, and it is reasonable.
POLY:
POLY: @@ Now try to map the metastable diagram
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32

Phase region boundary 1 at: 5.000E-01 3.100E+02
BCC_A2
** DIAMOND_A4
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 5.000E-01 3.000E+02
BCC_A2
** DIAMOND_A4
Calculated.. 24 equilibria

Phase region boundary 3 at: 4.999E-01 8.605E+02
BCC_A2
** D011_CEMENTITE
** DIAMOND_A4

Phase region boundary 4 at: 8.749E-01 8.605E+02
BCC_A2
** D011_CEMENTITE
Calculated.. 7 equilibria

Phase region boundary 5 at: 8.746E-01 9.998E+02

```

```

    BCC_A2
    ** D011_CEMENTITE
    ** FCC_A1

Phase region boundary 6 at: 9.823E-01 9.998E+02
    BCC_A2
    ** FCC_A1
Calculated. 23 equilibria

Phase region boundary 7 at: 8.578E-01 9.998E+02
    D011_CEMENTITE
    ** FCC_A1
Calculated. 18 equilibria

Phase region boundary 8 at: 8.354E-01 1.422E+03
    ** LIQUID
    D011_CEMENTITE
    ** FCC_A1

Phase region boundary 9 at: 7.872E-01 1.422E+03
    ** LIQUID
    D011_CEMENTITE
Calculated. 5 equilibria

Phase region boundary 10 at: 7.657E-01 1.484E+03
    ** LIQUID
    D011_CEMENTITE
    ** DIAMOND_A4

Phase region boundary 11 at: 3.750E-01 1.484E+03
    D011_CEMENTITE
    ** DIAMOND_A4
Calculated. 26 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 3.907E-01 1.484E+03
    LIQUID
    ** DIAMOND_A4
Calculated. 42 equilibria
Terminating at axis limit.

Phase region boundary 13 at: 8.678E-01 1.422E+03
    ** LIQUID
    FCC_A1
Calculated. 15 equilibria

Phase region boundary 14 at: 9.840E-01 1.768E+03
    ** LIQUID
    ** BCC_A2
    FCC_A1

Phase region boundary 15 at: 9.939E-01 1.768E+03
    ** BCC_A2
    FCC_A1
Calculated. 25 equilibria

Phase region boundary 16 at: 9.858E-01 1.768E+03
    LIQUID
    ** BCC_A2
Calculated. 20 equilibria

Phase region boundary 17 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 19 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 23 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 24 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4
Calculated. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 25 at: 5.000E-01 3.100E+02
    BCC_A2
    ** DIAMOND_A4

```


Calculated. 24 equilibria
 Terminating at known equilibrium

 Phase region boundary 26 at: 5.000E-01 3.100E+02
 BCC_A2
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 27 at: 5.000E-01 3.100E+02
 BCC_A2
 ** DIAMOND_A4
 Calculated. 24 equilibria
 Terminating at known equilibrium

 Phase region boundary 28 at: 3.750E-01 1.037E+03
 ** D011_CEMENTITE
 DIAMOND_A4
 Calculated. 9 equilibria
 Terminating at known equilibrium

 Phase region boundary 29 at: 3.750E-01 1.037E+03
 ** D011_CEMENTITE
 DIAMOND_A4
 Calculated. 19 equilibria
 Terminating at known equilibrium

 Phase region boundary 30 at: 9.877E-01 1.037E+03
 BCC_A2
 ** FCC_A1
 Calculated. 3 equilibria
 Terminating at known equilibrium

 Phase region boundary 31 at: 9.877E-01 1.037E+03
 BCC_A2
 ** FCC_A1
 Calculated 23 equilibria

 Phase region boundary 32 at: 3.754E-01 1.763E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 13 equilibria
 Terminating at known equilibrium

 Phase region boundary 33 at: 3.754E-01 1.763E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 31 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 34 at: 9.820E-01 1.763E+03
 LIQUID
 ** FCC_A1
 Calculated. 15 equilibria
 Terminating at known equilibrium

 Phase region boundary 35 at: 9.820E-01 1.763E+03
 LIQUID
 ** FCC_A1
 Calculated. 2 equilibria
 Terminating at known equilibrium

 Phase region boundary 36 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 42 equilibria
 Terminating at known equilibrium

 Phase region boundary 37 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 38 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 42 equilibria
 Terminating at known equilibrium

 Phase region boundary 39 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 40 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 42 equilibria
 Terminating at known equilibrium

 Phase region boundary 41 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 42 at: 3.317E-01 2.475E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 43 at: 3.317E-01 2.475E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 41 equilibria
 Terminating at known equilibrium

```

Phase region boundary 44 at: 3.306E-01 2.490E+03
LIQUID
** DIAMOND_A4
Calculated. 42 equilibria
Terminating at known equilibrium

Phase region boundary 45 at: 3.306E-01 2.490E+03
LIQUID
** DIAMOND_A4
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 46 at: 9.941E-01 1.794E+03
LIQUID
** BCC_A2
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 47 at: 9.941E-01 1.794E+03
LIQUID
** BCC_A2
Calculated 12 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping 3 seconds

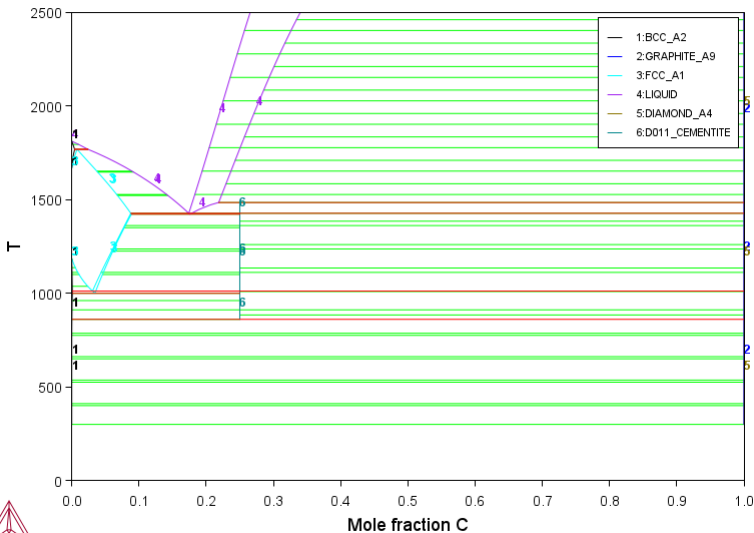
```

```

POLY:
POST: post
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x m-f C
... the command in full is SET_DIAGRAM_AXIS
POST: set-tieline
... the command in full is SET_TIELINE_STATUS
PLOTING EVERY TIE-LINE NO /5/: 5
POST:
POST: set-title example 1e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1e

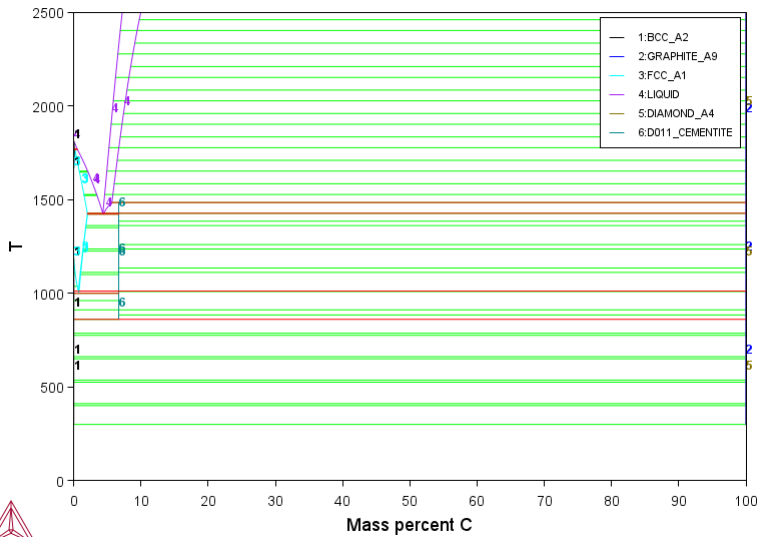


```

POST:
POST:
POST: Hit RETURN to continue
POST: @@ The previous stable diagram is also plotted. The reason is that
POST: @@ we never removed it from the workspace. (It can be done with a SAVE
POST: @@ command. Search the online help to read more about this command).
POST:
POST: @@ It may be surprising to find that diamond is more stable than
POST: @@ cementite at low temperatures. However, diamonds are never
POST: @@ found in steel as graphite forms first.
POST:
POST: @@ Now change the axis to composition, use weight-percent of carbon
POST: s-d-a x
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
FILE SYSTEM ERROR IN FILHLP
ERROR 1717 READING HELP FILE
VARIABLE : w-p
FOR COMPONENT : c
POST: set-title example 1f
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1f

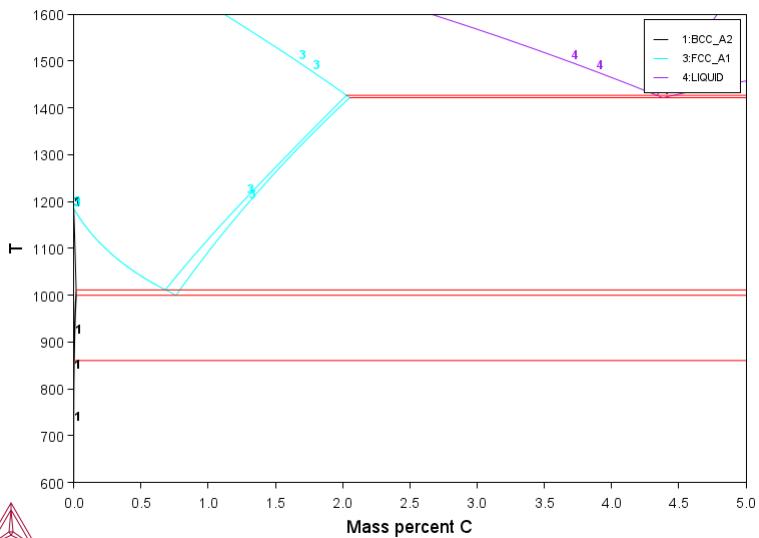


```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ The tie-lines now obscure the diagram. Remove these and
POST: @@ also change the scale of the x and y axis
POST: s-t-s 0
... the command in full is SET_TIELINE_STATUS
POST: s-s x n 0 5
... the command in full is SET_SCALING_STATUS
POST: s-s y n 600 1600
... the command in full is SET_SCALING_STATUS
POST: set-title example 1g
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
1

```

example 1g

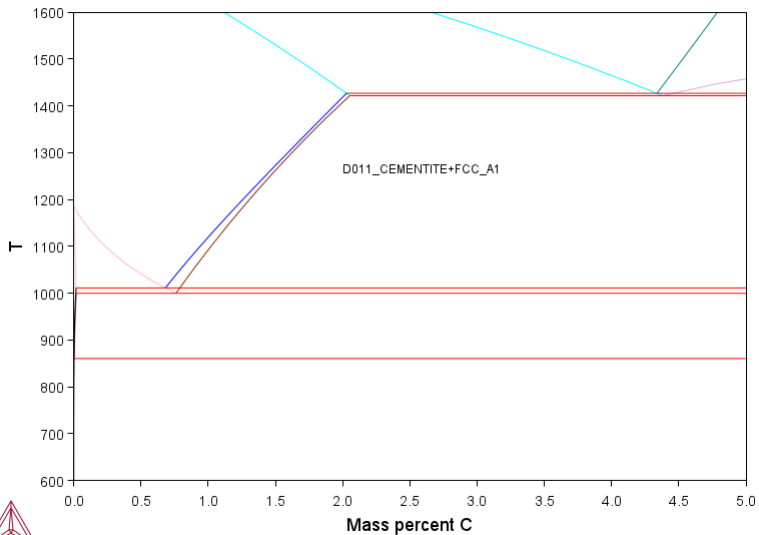


```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Finally add some labels
POST: set-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: add 2 1250
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 629 grid points in 0.009 s
Found the set of lowest grid points in 0.005 s
Calculated POLY solution 0.012 s, total time 0.026 s
Stable phases are: D011_CEMENTITE+FCC_A1
Text size: /.36/:
POST: set-title example 1h
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1h

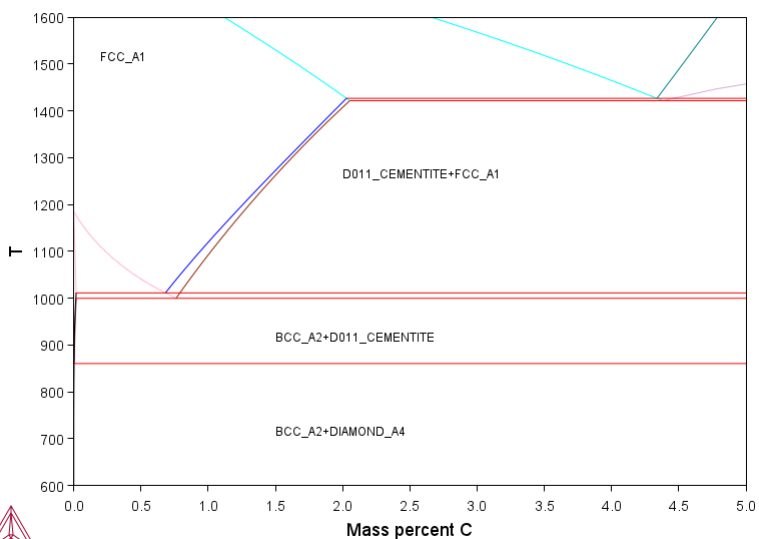


```

POST:
POST:
POST:Hit RETURN to continue
POST: add 1.5 900
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      629 grid points in      0.010 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.009 s, total time      0.019 s
Stable phases are: BCC_A2+D011_CEMENTITE
Text size: /.36/:
POST: add 1.5 700
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      629 grid points in      0.006 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.008 s, total time      0.014 s
Stable phases are: BCC_A2+DIAMOND_A4
Text size: /.36/:
POST: add .2 1500
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      629 grid points in      0.005 s
Found the set of lowest grid points in      0.005 s
Calculated POLY solution      0.010 s, total time      0.020 s
Stable phases are: FCC_A1
Text size: /.36/:
POST: set-title example 1i
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1i



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ As graphite is suspended, cementite is the stable carbide
POST: @@ so that is the phase that is listed in the two-phase regions.
POST: @@ The label for the FCC region is a bit too high, move it down
POST: modify
... the command in full is MODIFY_LABEL_TEXT
These labels are defined
No 1 at 2.00000E+00 1.25000E+03 : D011_CEMENTITE+FCC_A1
No 2 at 1.50000E+00 9.00000E+02 : BCC_A2+D011_CEMENTITE

```

example 1j



```
POST:
POST: set-inter
    ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex02

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex02\tcex02.TCM.test"

SYS: set-echo

SYS: @@

SYS: @@ Plotting thermodynamic functions

SYS:

SYS: @@ This example shows how to plot thermodynamic

SYS: @@ functions in unary, binary and ternary systems.

SYS: @@ It also involves working with partial derivatives

SYS: @@ and partial quantities.

SYS:

SYS: set-log ex02,,

SYS:

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw ssol6

... the command in full is SWITCH_DATABASE

Current database: SGTE Alloy Solutions v6.0

VA DEFINED

BCC_B2

FCC_L12

FCC_COV

FCC_AUCU

HCP_ORD

REJECTED

GAS;G REJECTED

TDB_SSOL6: @@ Pure Fe is selected as a unary system

TDB_SSOL6: d-sys fe

... the command in full is DEFINE_SYSTEM

FE DEFINED

TDB_SSOL6: get

... the command in full is GET_DATA

08:35:59,039 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_SSOL6:

TDB_SSOL6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ In POLY-3 first define a single equilibrium

POLY: s-c t=300,p=1e5,n=1

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 21 grid points in 0.403 s

POLY: l-e,,,

... the command in full is LIST_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: SSOL6

Conditions:

T=300, P=100000, N=1

DEGREES OF FREEDOM 0

Temperature 300.00 K (26.85 C), Pressure 1.000000E+05

Number of moles of components 1.000000E+00, Mass in grams 5.58470E+01

Total Gibbs energy -8.18407E+03, Enthalpy 4.59751E+01, Volume 0.000000E+00

Component

Moles

W-Fraction

Activity

Potential

Ref.stat

FE

1.0000E+00

1.0000E+00

3.7589E-02

-8.1841E+03

SER

BCC A2

Status ENTERED

Driving force

0.0000E+00

Moles 1.0000E+00, Mass 5.5847E+01, Volume fraction 0.0000E+00 Mass fractions:

FE 1.000000E+00

POLY:

POLY:Hit RETURN to continue

POLY: @@ Set T as an axis variable

POLY: s-a-v

... the command in full is SET_AXIS_VARIABLE

Axis number: /1/: 1

Condition /NONE/: t

Min value /0/: 300

Max value /1/: 2000

Increment /42.5/: 42.5

POLY: @@ Save the macro to be able to come back to this point

POLY: save tcex02a y

... the command in full is SAVE_WORKSPACES

POLY: @@ Step along the axis

```

POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value      300.000
...OK

Phase Region from      300.000      for:
  BCC_A2
Global test at 3.80000E+02 .... OK
Global test at 4.80000E+02 .... OK
Global test at 5.80000E+02 .... OK
Global test at 6.80000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 9.80000E+02 .... OK
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global check of adding phase at 1.18481E+03
Calculated      91 equilibria

Phase Region from      1184.81      for:
  BCC_A2
  FCC_A1
Calculated      2 equilibria

Phase Region from      1184.81      for:
  FCC_A1
Global test at 1.26000E+03 .... OK
Global test at 1.36000E+03 .... OK
Global test at 1.46000E+03 .... OK
Global test at 1.56000E+03 .... OK
Global test at 1.66000E+03 .... OK
Global check of adding phase at 1.66747E+03
Calculated      51 equilibria

Phase Region from      1667.47      for:
  BCC_A2
  FCC_A1
Calculated      2 equilibria

Phase Region from      1667.47      for:
  BCC_A2
Global test at 1.74000E+03 .... OK
Global check of adding phase at 1.81095E+03
Calculated      18 equilibria

Phase Region from      1810.95      for:
  LIQUID
  BCC_A2
Calculated      2 equilibria

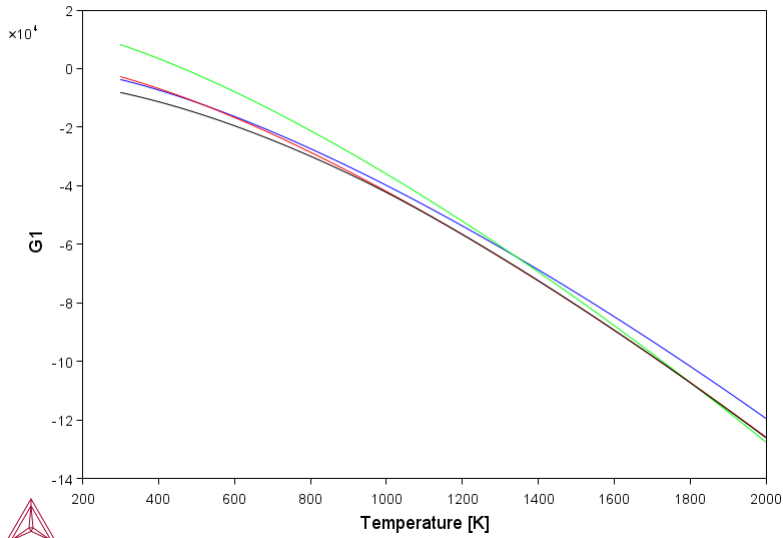
Phase Region from      1810.95      for:
  LIQUID
Global test at 1.89000E+03 .... OK
Global test at 1.99000E+03 .... OK
Terminating at      2000.00
Calculated      22 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex02\tcex02a.POLY3
POLY: @@ Post processing (plotting) is the essential part of this example
POLY: @@ We will plot Gm, Hm and Cp for some phases
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: @@ The x-axis is the temperature in Kelvin
POST: s-d-a x
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
FILE SYSTEM ERROR IN FILHLP
ERROR      1717  READING HELP FILE
VARIABLE : t-k
POST: @@ The phases for which Gm shall be plotted must be defined
POST: @@ in a table
POST: ent tab
... the command in full is ENTER_SYMBOL
Name: g1
Variable(s): gm(bcc_a2) gm(fcc_a1) gm(liq) gm(hcp_a3)
&
POST:
POST: @@ The table is set as the y-axis and all columns are included
POST: @@ by using *
POST: s-d-a y g1
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2a

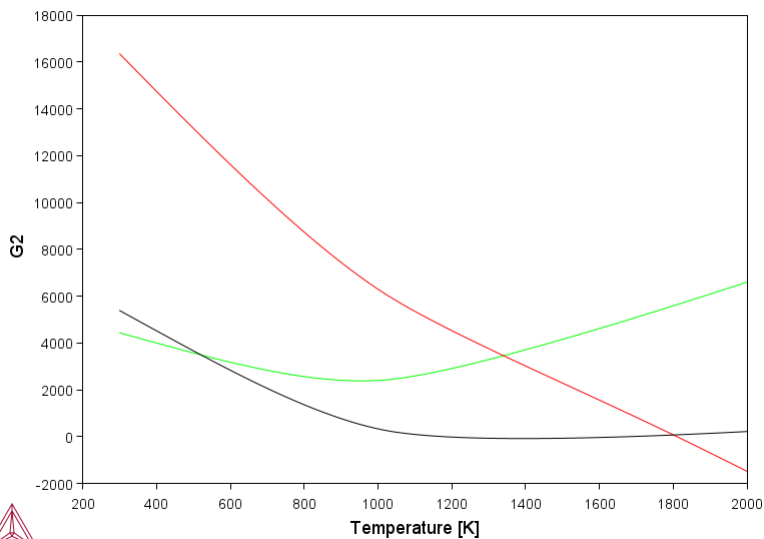


```

POST:
POST:Hit RETURN to continue
POST: @@
POST:
POST:
POST: @@ The magnitude makes it difficult to see anything. Enter
POST: @@ functions for the differences with respect to bcc
POST: ent fun dgf=gm(fcc_a1)-gm(bcc_a2);
... the command in full is ENTER_SYMBOL
POST: ent fun dgl=gm(liq)-gm(bcc_a2);
... the command in full is ENTER_SYMBOL
POST: ent fun dgh=gm(hcp_a3)-gm(bcc_a2);
... the command in full is ENTER_SYMBOL
POST: @@ and enter a new table and set it as the y-axis
POST: ent tab g2
... the command in full is ENTER_SYMBOL
Variable(s): dgf dgl dgh;
POST: s-d-a y g2
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2b

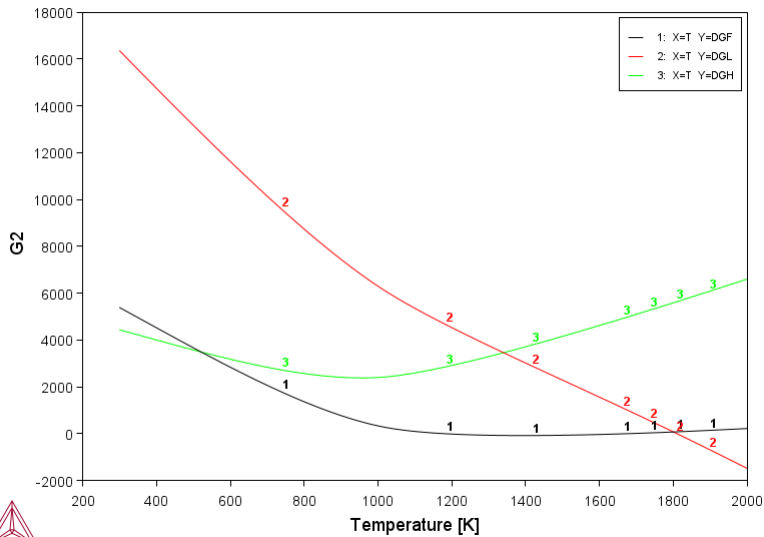


```

POST:
POST:Hit RETURN to continue
POST: @@ In order to have some identification on the lines
POST: @@ use the command Set_Label
POST: s-lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: D
POST: set-title example 2c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```


example 2c

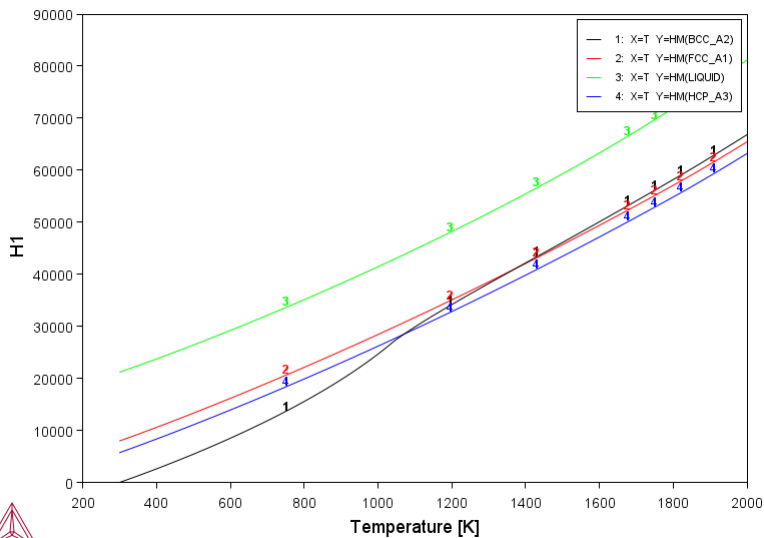


```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot enthalpies
POST: ent tab h1
... the command in full is ENTER_SYMBOL
Variable(s): hm(bcc_a2) hm(fcc_a1) hm(liq) hm(hcp_a3);
POST: s-d-a y h1
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2d

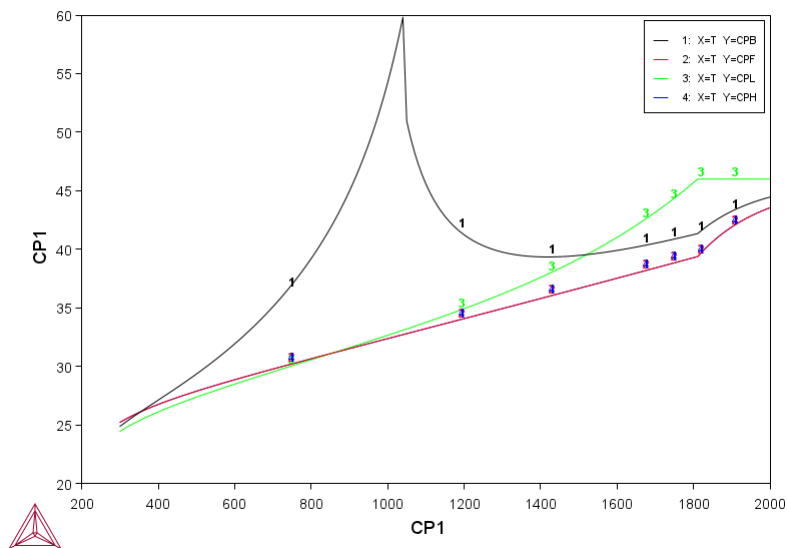


```

POST:
POST:Hit RETURN to continue
POST: @@ And finally plot heat capacities
POST: ent fun cpb=hm(bcc_a2).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cpf=hm(fcc_a1).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cpl=hm(liq).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cph=hm(hcp_a3).t;
... the command in full is ENTER_SYMBOL
POST: ent tab cpl
... the command in full is ENTER_SYMBOL
Variable(s): t cpb cpf cpl cph;
POST: s-d-a y
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : cpl
COLUMN NUMBER /*/: 2-5
POST: s-d-a x cpl 1
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 2e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:

```

POST: plot
 ... the command in full is PLOT_DIAGRAM
 example 2e



POST:
 POST:Hit RETURN to continue
 POST:
 POST: @@ The next example plots functions for a binary system
 POST:
 POST: ba
 ... the command in full is BACK
 POLY: go da
 ... the command in full is GOTO_MODULE
 TDB_SSOL6: rej sys
 ... the command in full is REJECT
 VA DEFINED
 BCC_B2 FCC_L12 FCC_COV
 FCC_AUCU HCP_ORD REJECTED
 GAS:G REJECTED
 REINITIATING GES
 TDB_SSOL6: @@ Select the Cu-Fe system and only
 TDB_SSOL6: @@ the fcc, bcc, liquid and hcp phases
 TDB_SSOL6: d-sys fe cu
 ... the command in full is DEFINE_SYSTEM
 FE CU DEFINED
 TDB_SSOL6: rej ph /all
 ... the command in full is REJECT
 LIQUID:L FCC_A1 BCC_A2
 HCP_A3 HCP_ZN TETRAGONAL_U
 CBCC_A12 CUB_A13 ORTHORHOMBIC_A20
 LAVES_C14 LAVES_C15 LAVES_C36
 M4N ALCU_ETA ALCU_EPSILON
 ALCUZN_GAMMA_H AL5FE4 CUPD_B2
 CUTI CU4TI CU6Y
 CUZN_GAMMA D_GAMMA FEPD
 FEPD3 FESB FEU6
 FE2U FEUZR_DELTA FEZR2
 FEZR3 REJECTED
 TDB_SSOL6: rest ph fcc_a1 bcc_a2 liq hcp_a3
 ... the command in full is RESTORE
 FCC_A1 BCC_A2 LIQUID:L
 HCP_A3 RESTORED
 TDB_SSOL6: l-sys
 ... the command in full is LIST_SYSTEM
 ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 LIQUID:L :CU FE:
 FCC_A1 :CU FE:VA:
 BCC_A2 :CU FE:VA:
 HCP_A3 :CU FE:VA:
 TDB_SSOL6: get
 ... the command in full is GET_DATA
 REINITIATING GES
 ELEMENTS
 SPECIES
 PHASES
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS
 Use the command LIST_REFERENCES to see the list of references for assessed data
 -OK-
 TDB_SSOL6: go p-3
 ... the command in full is GOTO_MODULE
 POLY version 3.32
 POLY: @@ Set conditions for a single equilibrium
 POLY: s-c t=1000,p=1e5,n=1,w(cu)=.01
 ... the command in full is SET_CONDITION
 POLY: c-e
 ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated 836 grid points in 0.059 s
 Found the set of lowest grid points in 0.004 s
 Calculated POLY solution 0.972 s, total time 1.035 s
 POLY: @@ Select the fraction of Cu as the axis variable
 POLY: s-a-v 1
 ... the command in full is SET_AXIS_VARIABLE
 Condition /NONE/: w(cu)
 Min value /0/: 0
 Max value /1/: 1

```

Increment /.025/ : .025
POLY: @@ Remember to Save
POLY: save tcex02b y
... the command in full is SAVE_WORKSPACES
POLY: @@ Now a special STEP option is selected because the NORMAL
POLY: @@ option only calculates the stable phases. The option
POLY: @@ SEPARATE means that all entered phases are calculated
POLY: @@ separately.
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/ : ?
The following options are available:
NORMAL          Stepping with given conditions
INITIAL_EQUILIBRIA An initial equilibrium stored at every step
EVALUATE         Specified variables evaluated after each step
SEPARATE_PHASES  Each phase calculated separately
T-ZERO          T0 line calculation
PARAEQUILIBRIUM Paraequilibrium diagram
MIXED_SCHEIL    Scheil with fast diffusing elements
ONE_PHASE_AT_TIME One phase at a time
Option? /NORMAL/ : sep

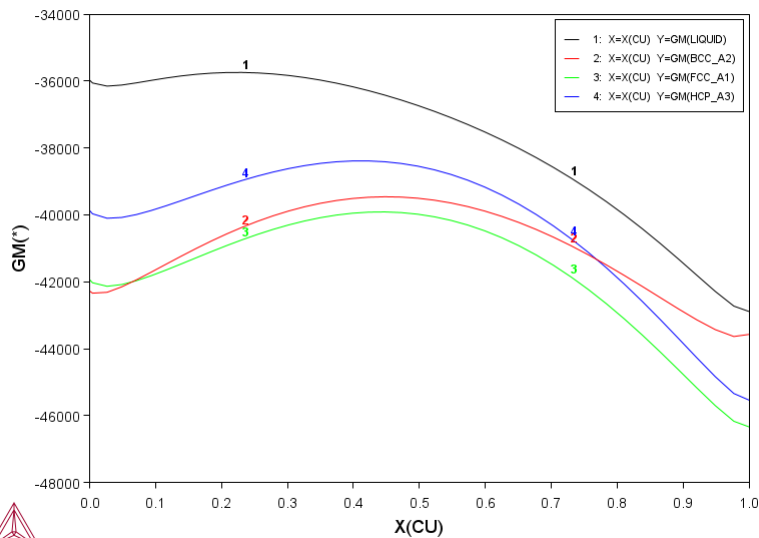
Phase Region from 0.529789 for:
LIQUID
BCC_A2
FCC_A1
HCP_A3

Phase Region from 0.529789 for:
LIQUID
BCC_A2
FCC_A1
HCP_A3

*** Buffer saved on file *** c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex02\tcex02b.POLY3
POLY: @@ Now plot the results in various ways
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: @@ Set the Gm of all phases on the y-axis
POST: s-d-a y gm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: @@ and the mole percent of Cu on the x-axis
POST: s-d-a x x(cu)
... the command in full is SET_DIAGRAM_AXIS
POST: set-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 2f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2f

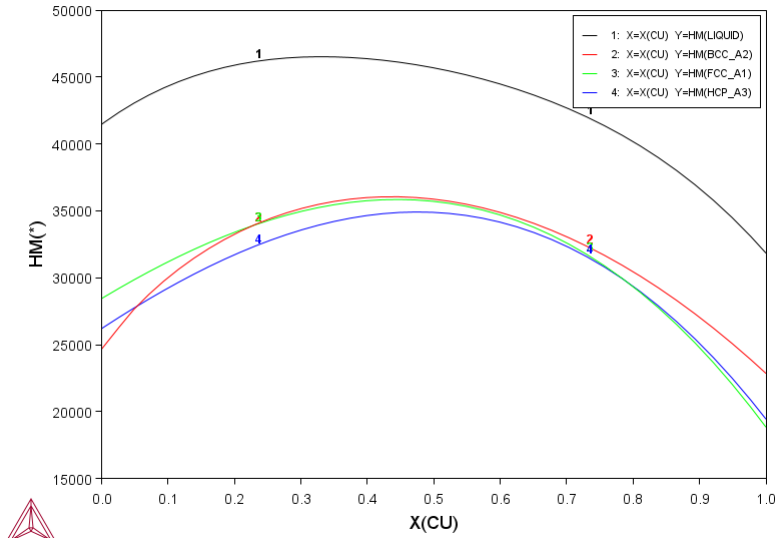


```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot the enthalpy
POST: s-d-a y hm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2g
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2g

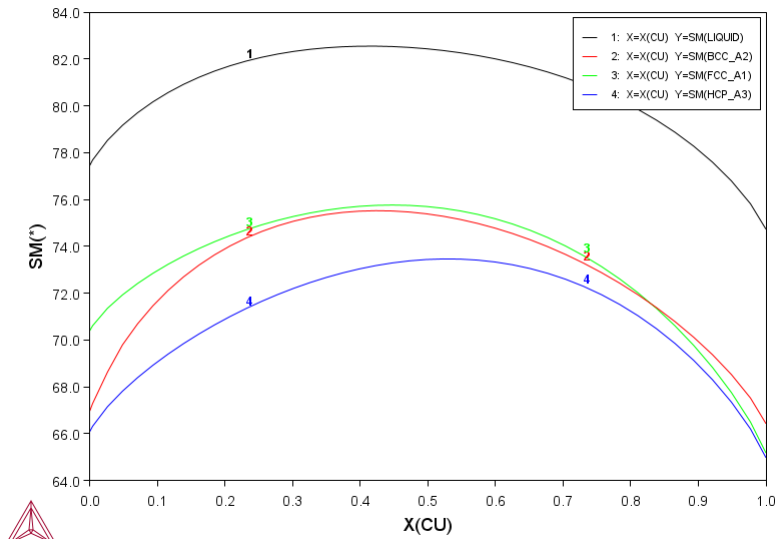


```

POST:
POST:Hit RETURN to continue
POST: @@ and finally the entropy
POST: s-d-a y sm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2h



```

POST:
POST:Hit RETURN to continue
POST: @@ The last example plots the Fe-V-C ternary system.
POST: @@ Calculate and plot Gm from the iron corner to VC
POST: ba
... the command in full is BACK
POLY: go da
... the command in full is GOTO_MODULE
TDB_SSOL6: rej sys
... the command in full is REJECT
VA DEFINED
BCC_B2          FCC_L12          FCC_COV
FCC_AUCU        HCP_ORD  REJECTED
GAS:G  REJECTED
REINITIATING GES .....
TDB_SSOL6: d-sys fe v c
... the command in full is DEFINE_SYSTEM
FE              V              C
DEFINED
TDB_SSOL6: rej ph / all
... the command in full is REJECT
LIQUID:L        FCC_A1          BCC_A2
HCP_A3          HCP_ZN          DIAMOND_A4
TETRAGONAL_U    CBCC_A12        CUB_A13
ORTHORHOMBIC_A20 SIGMA          GRAPHITE
LAVES_C14        LAVES_C15        LAVES_C36
CEMENTITE        KSI_CARBIDE      M23C6
M7C3             M3C2             V3C2
M5C2             MC_ETA           M4N
FECN_CHI         ALM_D019         AL5FE4
ALTA_SIGMA       ALTI             FEPD
FEPD3            FESB             FEU6

```

```

FE2U                      FEUZR_DELTA          FEZR2
FEZR3                      V3SI  REJECTED
TDB_SSOL6: rest ph fcc_a1 bcc_a2 hcp_a3 liq
... the command in full is RESTORE
FCC_A1                      BCC_A2              HCP_A3
LIQUID:L  RESTORED
TDB_SSOL6: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_SSOL6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ Set conditions for a single equilibrium
POLY: s-c t=1000,p=1e5,n=1,w(v)=.0015,x(c)=.001
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 7821 grid points in 0.082 s
Found the set of lowest grid points in 0.002 s
Calculated POLY solution 0.029 s, total time 0.113 s
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL6

Conditions:
T=1000, P=100000, N=1, W(V)=1.5E-3, X(C)=1E-3
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.57951E+01
Total Gibbs energy -4.23963E+04, Enthalpy 2.45646E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
C                1.0000E-03  2.1527E-04  3.4515E-02 -2.7990E+04 SER
FE               9.9736E-01  9.9828E-01  6.1891E-03 -4.2279E+04 SER
V               1.6429E-03  1.5000E-03  4.0605E-07 -1.2236E+05 SER

BCC_A2                      Status ENTERED      Driving force 0.0000E+00
Moles 9.9814E-01, Mass 5.5735E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99368E-01 V 6.07213E-04 C 2.49276E-05

FCC_A1#2                      Status ENTERED      Driving force 0.0000E+00
Moles 1.8638E-03, Mass 6.0520E-02, Volume fraction 0.0000E+00 Mass fractions:
V 8.23694E-01 C 1.75507E-01 FE 7.99487E-04
POLY:Hit RETURN to continue
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
FCC_A1#2    ENTERED      0.000000E+00      1.863776E-03
BCC_A2      ENTERED      0.000000E+00      9.981362E-01
FCC_A1#1    ENTERED      -3.462152E-02      0.000000E+00
HCP_A3#2    ENTERED      -2.875358E-01      0.000000E+00
HCP_A3#1    ENTERED      -2.875358E-01      0.000000E+00
LIQUID      ENTERED      -6.510578E-01      0.000000E+00
POLY:Hit RETURN to continue
POLY: @@ Note we have several composition sets because fcc
POLY: @@ (and possibly hcp) can exist both as metallic and
POLY: @@ as carbide. However, in this case it is unnecessary
POLY: @@ as we are only interested in the value of the
POLY: @@ thermodynamic functions, not the equilibrium, and therefore
POLY: @@ we suspend them
POLY:
POLY: c-s p hcp_a3#2
... the command in full is CHANGE_STATUS
Status: /ENTERED/: sus
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1000, P=100000, N=1, W(V)=1.5E-3, X(C)=1E-3
DEGREES OF FREEDOM 0
POLY: @@ We would like to calculate the Gibbs energy from
POLY: @@ pure Fe to the corner VC. Select a line with equal
POLY: @@ fraction of V and C
POLY: s-c x(v)-x(c)=0
... the command in full is SET_CONDITION
POLY: s-c w(v)=none
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1000, P=100000, N=1, X(C)=1E-3, X(V)-X(C)=0
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
10 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL6

Conditions:
T=1000, P=100000, N=1, X(C)=1E-3, X(V)-X(C)=0
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.57983E+01

```

Total Gibbs energy -4.23424E+04, Enthalpy 2.46245E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	1.0000E-03	2.1526E-04	9.5381E-02	-1.9538E+04	SER
FE	9.9800E-01	9.9887E-01	6.1904E-03	-4.2277E+04	SER
V	1.0000E-03	9.1295E-04	1.6021E-07	-1.3010E+05	SER

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 9.9858E-01, Mass 5.5752E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99691E-01 V 2.40126E-04 C 6.83917E-05

FCC_A1#2 Status ENTERED Driving force 0.0000E+00
Moles 1.4208E-03, Mass 4.5810E-02, Volume fraction 0.0000E+00 Mass fractions:
V 8.19759E-01 C 1.78955E-01 FE 1.28625E-03

POLY:Hit RETURN to continue

POLY: @@ Set the fraction of C as the axis

POLY: @@ The fraction of V will be the same

POLY: s-a-v

... the command in full is SET_AXIS_VARIABLE

Axis number: /1/: 1

Condition /NONE/: x(c)

Min value /0/: 0

Max value /1/: .5

Increment /.0125/: .0125

POLY: save tcex02c y

... the command in full is SAVE_WORKSPACES

POLY: @@ step along the axis

POLY: step

... the command in full is STEP_WITH_OPTIONS

Option? /NORMAL/: sep

Phase Region from 0.330065 for:

LIQUID

BCC_A2

FCC_A1#1

FCC_A1#2

Phase Region from 0.330065 for:

LIQUID

BCC_A2

FCC_A1#1

FCC_A1#2

Phase Region from 0.480604E-02 for:

HCP_A3#1

Phase Region from 0.480604E-02 for:

HCP_A3#1

*** Buffer saved on file *** c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex02\tcex02c.POLY3

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST: @@ plot the Gm versus carbon content

POST: l-p-s

... the command in full is LIST_PLOT_SETTINGS

GRAPHIC DEVICE: TC-UNITE Driver (#22) PLOTFILE: SCREEN

FONT: (# 1) Arial Bold

AXIS PLOT YES

RASTER PLOT : NO

TRIANGULAR PLOT : NO

AUTOMATIC SCALING

AUTOMATIC AXIS TEXT

AXIS VARIABLES

POST: s-d-a x x(c)

... the command in full is SET_DIAGRAM_AXIS

POST: s-d-a y gm(*)

... the command in full is SET_DIAGRAM_AXIS

COLUMN NUMBER /*/: *

POST:

POST: set-lab d

... the command in full is SET_LABEL_CURVE_OPTION

POST: set-title example 2i

POST:

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

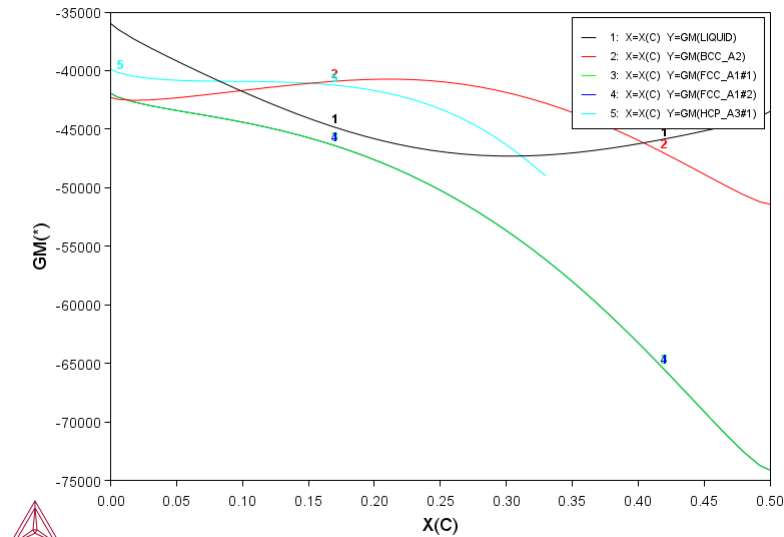
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 2i



```

POST:
POST:Hit RETURN to continue
POST: @@ This example is about more partial derivatives
POST: back
POLY: go da
... the command in full is GOTO_MODULE
TDB_SSOL6: rej sys
... the command in full is REJECT
VA DEFINED
BCC_B2          FCC_L12          FCC_COV
FCC_AUCU          HCP_ORD  REJECTED
GAS:G  REJECTED
REINITIATING GES .....
TDB_SSOL6: def-sys al cu
... the command in full is DEFINE_SYSTEM
AL              CU  DEFINED
TDB_SSOL6: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_SSOL6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: s-c t=1400 p=1e5 n=1 x(al)=.1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 11669 grid points in 0.234 s
Found the set of lowest grid points in 0.002 s
Calculated POLY solution 0.012 s, total time 0.248 s
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL6

Conditions:
T=1400, P=100000, N=1, X(AL)=0.1
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.98896E+01
Total Gibbs energy -8.53069E+04, Enthalpy 3.62263E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
AL              1.0000E-01  4.5053E-02  1.3593E-06  -1.5724E+05  SER
CU              9.0000E-01  9.5495E-01  1.3045E-03  -7.7314E+04  SER

LIQUID          Status ENTERED    Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.9890E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 9.54947E-01 AL 4.50529E-02
POLY:Hit RETURN to continue
POLY: @@ Check the activity of aluminum
POLY: show acr(al)
... the command in full is SHOW_VALUE
ACR(AL)=1.359263E-6
POLY: @@ This activity value is referred to fcc Al at 298.15 K.
POLY: @@ Set the proper reference state for activities
POLY: set-ref-state al
... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:
Pressure /1E5/:
POLY:
POLY: set-ref-state cu
... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:

```

```

Pressure /1E5/:
POLY:
POLY: show acr(al)
... the command in full is SHOW_VALUE
ACR(AL)=8.0990275E-4
POLY: @@ This value is better. The corresponding chemical potential is
POLY: show mur(al)
... the command in full is SHOW_VALUE
MUR(AL)=-82862.697
POLY: @@ The relation is simply that  $\text{acr}(al) = \exp(\text{mur}(al)/RT)$ . Check that
POLY: enter fun test
... the command in full is ENTER_SYMBOL
Function:  $\exp(\text{mur}(al)/8.31451/T)$ ;
POLY: show test
... the command in full is SHOW_VALUE
TEST=8.0990275E-4
POLY: Hit RETURN to continue
POLY: @@ POLY allows the calculation of partial derivatives of thermodynamic
POLY: @@ quantities of original reference state with respect to fractions
POLY: @@ that are conditions. For example
POLY: show gm.x(al)
... the command in full is SHOW_VALUE
GM.X(AL)=-79930.097
POLY: @@ This is not the same as the chemical potential. It actually
POLY: @@ is equal to the so-called diffusion potential:  $\mu(al) - \mu(cu)$ .
POLY:
POLY: ent fun diffmu= $\mu(al) - \mu(cu)$ ;
... the command in full is ENTER_SYMBOL
POLY: show diffmu
... the command in full is SHOW_VALUE
DIFFMU=-79930.097
POLY: @@ The relation between the chemical potential and the partial derivative is
POLY: @@  $\mu(al) = gm + gm.x(al) - x(al)*gm.x(al)$ 
POLY:
POLY: @@ We can also enter this as a function.
POLY: enter fun dgdx= $gm + gm.x(al) - x(al)*gm.x(al)$ ;
... the command in full is ENTER_SYMBOL
POLY: sh dgdx
... the command in full is SHOW_VALUE
DGDx=-157243.97
POLY: sh mu(al)
... the command in full is SHOW_VALUE
MU(AL)=-157243.97
POLY: @@ Partial entropy is the negative of  $\mu(al).t$ 
POLY: ent fun ps=- $\mu(al).t$ ;
... the command in full is ENTER_SYMBOL
POLY: sh ps
... the command in full is SHOW_VALUE
PS=95.218667
POLY: @@ Partial enthalpy is  $h = g + s*t$ 
POLY: enter fun ph= $\mu(al) + ps*t$ ;
... the command in full is ENTER_SYMBOL
POLY: sh ph
... the command in full is SHOW_VALUE
PH=-23937.838
POLY: @@ Partial enthalpy can also be calculated in a similar way as chemical
POLY: @@ potential
POLY: @@ partial enthalpy =  $hm + hm.x(al) - x(al)*hm.x(al)$ 
POLY: ent fun ph1= $hm + hm.x(al) - x(al)*hm.x(al)$ ;
... the command in full is ENTER_SYMBOL
POLY: sh ph1
... the command in full is SHOW_VALUE
PH1=-23937.838
POLY: @@ As can be seen,  $ph1 = ph$ .
POLY: @@ Another useful quantity is  $\mu(al).x(al)$ . That is related to
POLY: @@ the thermodynamic factor and part of the diffusion coefficient.
POLY: show  $\mu(al).x(al)$ 
... the command in full is SHOW_VALUE
MU(AL).X(AL)=324789.82
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```


tcex03

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex03\tcex03.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating an isothermal section using the Ternary module

SYS:

SYS: set-log ex03,,

SYS:

SYS: go tern

... the command in full is GOTO_MODULE

Quick ternary phase diagram calculation module

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Current database: Iron Demo Database v6.0

VA /- DEFINED

Database: /FEDEMO/: FEDEMO

First element: ?

The following assessed systems

C-Cr-Fe-Mn C-Cr-Fe-Ni C-Cr-Fe C-Cr-Mn C-Cr-Ni C-Cr C-Fe-Mn C-Fe-Ni

C-Fe C-Mn C-Ni Cr-Fe-Mn Cr-Fe-Ni Cr-Fe Cr-Mn-Ni Cr-Mn Cr-Ni

Fe-Mn-Ni Fe-Mn Fe-Ni Mn-Ni

First element: fe

Second element: c

Third element: cr

Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: Phase_Diagram

Temperature (C) /1000/: 1200

Global minimization on: /Y/: Y

VA /- DEFINED

REINITIATING GES

C CR

FE

DEFINED

GAS:G REJECTED

08:37:16,578 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set FCC_A1#2

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set HCP_A3#2

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

... the command in full is ADD_INITIAL_EQUILIBRIUM

... the command in full is ADD_INITIAL_EQUILIBRIUM

... the command in full is ADD_INITIAL_EQUILIBRIUM

... the command in full is ADD_INITIAL_EQUILIBRIUM

Start points provided by database

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Phase region boundary 1 at: 8.888E-01 7.693E-03

BCC_A2

** M23C6_D84

Calculated 14 equilibria

Phase region boundary 2 at: 8.888E-01 7.693E-03

BCC_A2

** M23C6_D84

Calculated 54 equilibria

Phase region boundary 3 at: 3.620E-01 5.294E-01

BCC_A2

** FCC_A1#2

** M23C6_D84

Phase region boundary 4 at: 2.028E-01 7.787E-01

BCC_A2

** FCC_A1#1

Calculated 28 equilibria

Phase region boundary 5 at: 3.450E-01 5.382E-01

```

** FCC_A1#1
M23C6_D84
Calculated.                2 equilibria

Phase region boundary 6 at: 3.367E-01 5.459E-01
** FCC_A1#1
M23C6_D84
** M7C3_D101

Phase region boundary 7 at: 5.141E-01 2.324E-01
M23C6_D84
** M7C3_D101
Calculated                33 equilibria

Phase region boundary 8 at: 3.565E-01 4.793E-01
FCC_A1#1
** M7C3_D101
Calculated.                30 equilibria

Phase region boundary 9 at: 1.646E-01 6.458E-01
** LIQUID
FCC_A1#1
** M7C3_D101

Phase region boundary 10 at: 6.933E-02 8.073E-01
** LIQUID
FCC_A1#1
Calculated                23 equilibria

Phase region boundary 11 at: 1.820E-01 5.842E-01
** LIQUID
M7C3_D101
Calculated.                7 equilibria

Phase region boundary 12 at: 1.414E-01 6.131E-01
** LIQUID
** CEMENTITE_D011
M7C3_D101

Phase region boundary 13 at: 1.610E-01 5.640E-01
** CEMENTITE_D011
M7C3_D101
Calculated.                3 equilibria

Phase region boundary 14 at: 1.457E-01 5.793E-01
** CEMENTITE_D011
** GRAPHITE_A9
M7C3_D101

Phase region boundary 15 at: 9.822E-02 2.518E-01
** GRAPHITE_A9
M7C3_D101
Calculated.                18 equilibria

Phase region boundary 16 at: 2.652E-01 8.482E-02
** GRAPHITE_A9
** M3C2_D510
M7C3_D101

Phase region boundary 17 at: 5.652E-01 8.482E-02
** M3C2_D510
M7C3_D101
Calculated                20 equilibria

Phase region boundary 18 at: 3.000E-01 0.000E+00
GRAPHITE_A9
** M3C2_D510

Phase region boundary 19 at: 4.753E-02 3.275E-01
CEMENTITE_D011
** GRAPHITE_A9
Calculated.                3 equilibria

Phase region boundary 20 at: 3.674E-02 3.383E-01
** LIQUID
CEMENTITE_D011
** GRAPHITE_A9

Phase region boundary 21 at: 6.004E-02 7.169E-01
** LIQUID
CEMENTITE_D011
Calculated.                5 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 2.330E-02 3.787E-01
** LIQUID
GRAPHITE_A9
Calculated                19 equilibria

Phase region boundary 23 at: 3.620E-01 5.294E-01
BCC_A2
** M23C6_D84
Calculated                65 equilibria

Phase region boundary 24 at: 1.167E-01 2.333E-01
** GRAPHITE_A9
M7C3_D101
Calculated.                16 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 1.167E-01 2.333E-01
** GRAPHITE_A9
M7C3_D101
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 26 at: 1.750E-01 1.750E-01
** GRAPHITE_A9
M7C3_D101
Calculated.                11 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 1.750E-01 1.750E-01
** GRAPHITE_A9
M7C3_D101
Calculated.                9 equilibria

```

```

Terminating at known equilibrium

Phase region boundary 28 at: 1.262E-02 8.673E-01
** LIQUID
FCC_A1#1
Calculated 10 equilibria

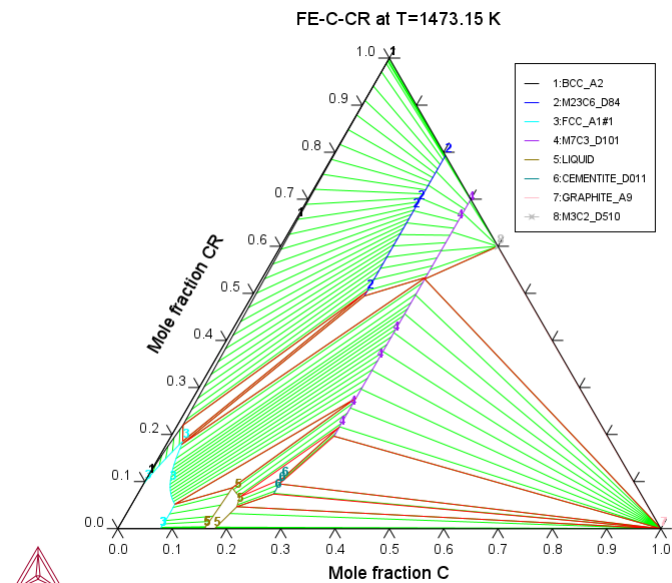
Phase region boundary 29 at: 1.262E-02 8.673E-01
** LIQUID
FCC_A1#1
Calculated. 7 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\ISOTHER_002.POLY3
CPU time for mapping 6 seconds
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

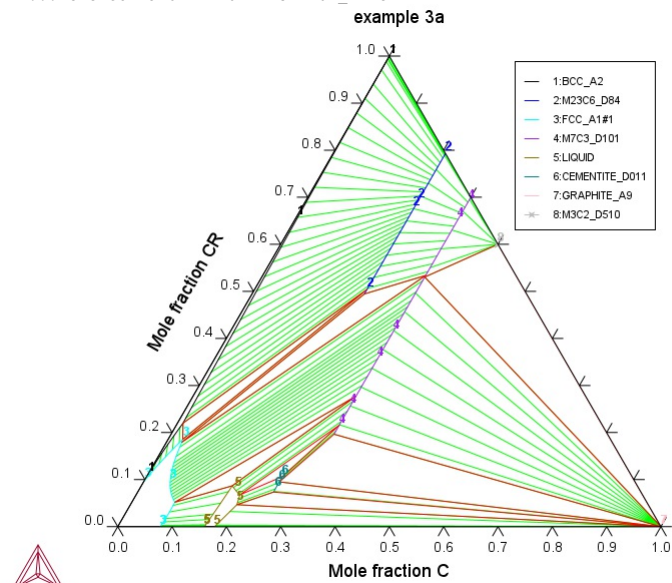
```



```

POST: N
No such command, use HELP
POST:
POST: set-title example 3a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



```

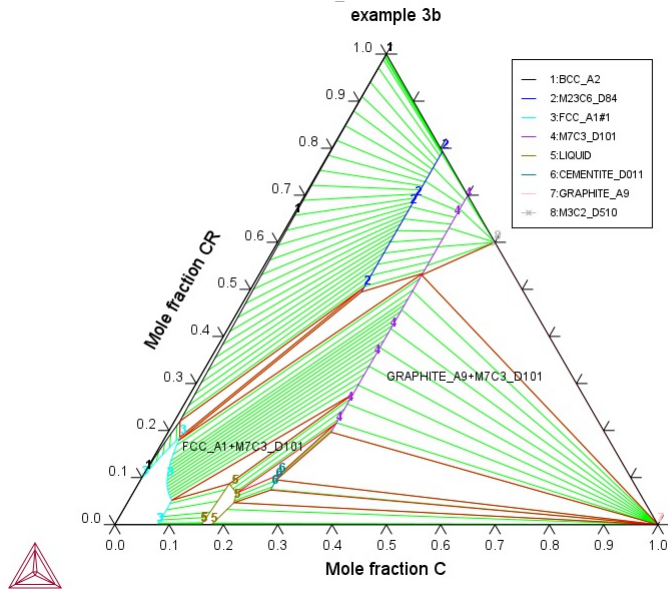
POST:
POST:Hit RETURN to continue
POST: @@ Add some labels
POST: add .35 .3
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in 0.006 s
Calculated POLY solution 0.017 s, total time 0.023 s
Stable phases are: GRAPHITE_A9+M7C3_D101
Text size: /.36/:
POST: add .05 .15

```

```

... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0.009 s
Calculated POLY solution      0.027 s, total time      0.036 s
Stable phases are: FCC_A1+M7C3_D101
Text size: /.36/:
POST: set-title example 3b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

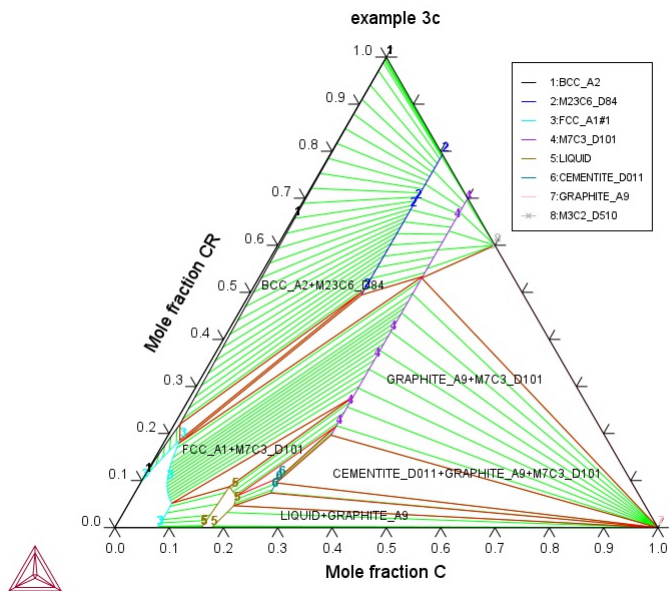
```



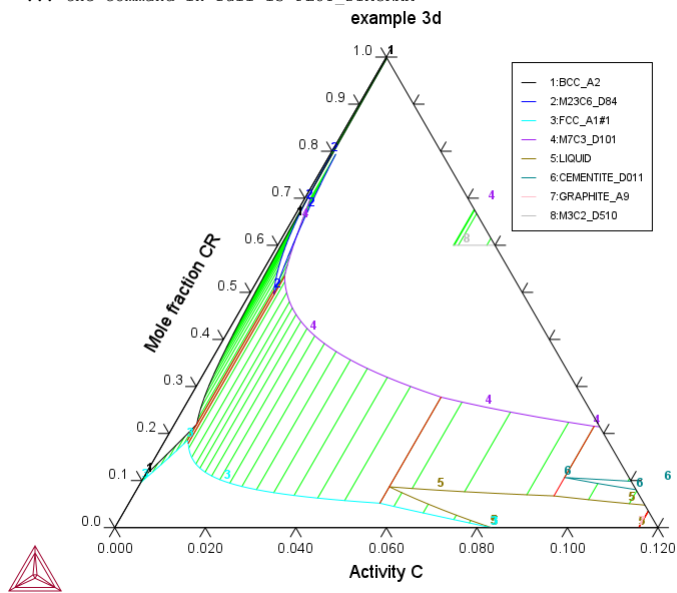
```

POST:
POST:Hit RETURN to continue
POST: add .3 .01
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0.004 s
Calculated POLY solution      0.016 s, total time      0.020 s
Stable phases are: LIQUID+GRAPHITE_A9
Text size: /.36/:
POST: add .35 .1
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0.004 s
Calculated POLY solution      0.025 s, total time      0.029 s
Stable phases are: CEMENTITE_D011+GRAPHITE_A9+M7C3_D101
Text size: /.36/:
POST: add .02 .5
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0.005 s
Calculated POLY solution      0.034 s, total time      0.039 s
Stable phases are: BCC_A2+M23C6_D84
Text size: /.36/:
POST: set-title example 3c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

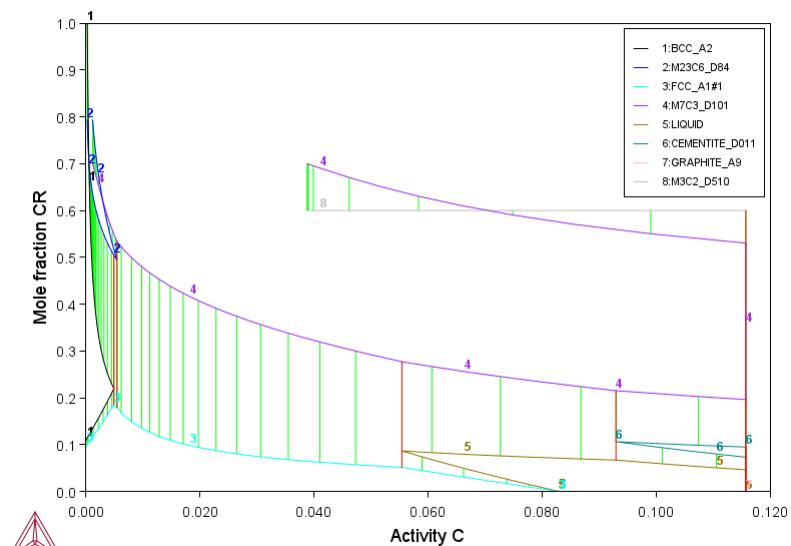


```
POST:
POST:Hit RETURN to continue
POST: @@ We can try the same exercise as in TCEX_01 which uses
POST: @@ carbon activity on one axis
POST: s-d-a x ac c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 3d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ With these axes it is better to have a square diagram.
POST: s-dia-type
... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM (Y OR N) /N/: N
CREATE TETRAHEDRON WRML FILE (Y OR N) /N/:
POST:
POST: set-title example 3e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 3e

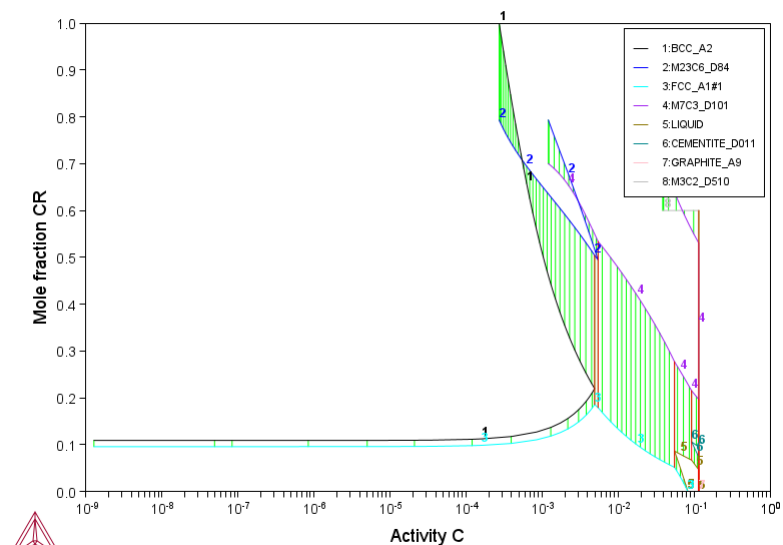


```

POST:
POST:Hit RETURN to continue
POST: @@ The activity axis is probably better as logarithmic
POST: s-a-ty x
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 3f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 3f



```

POST:
POST:Hit RETURN to continue
POST: @@ In order for pure graphite to have activity one, the reference
POST: @@ state of C should be set to graphite. In addition,
POST: @@ the solubility lines now cross. Is the diagram wrong?
POST: @@ No, in this case one should not use the mole fraction of Cr
POST: @@ but the metallic fraction. This can be fixed by setting
POST: @@ the status of C to "special". All species set as special
POST: @@ are excluded from the summation of fractions.
POST: @@ The special status is set in the POLY module
POST: ba
... the command in full is BACK
SYS: go p-3
... the command in full is GOTO_MODULE
POLY:
POLY: s-r-s
... the command in full is SET_REFERENCE_STATE
Component: c
Reference phase: gra
Temperature /*/:
Pressure /1E5/:
POLY: ch-st
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/: c
Name(s): c
Status: /ENTERED/: ?
FILE SYSTEM ERROR IN FILHLP
ERROR 1717 READING HELP FILE
Status: /ENTERED/: special
POLY:
POLY: post

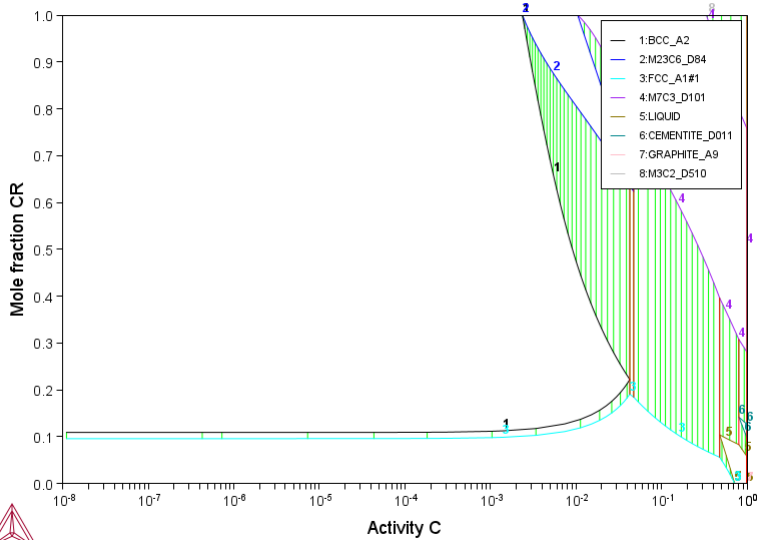
```

```

POST:
POST: set-title example 3g
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 3g

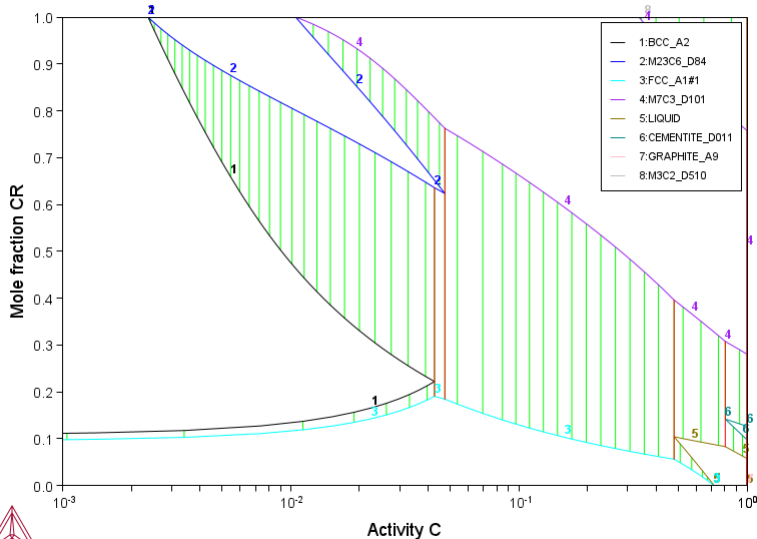


```

POST:
POST:Hit RETURN to continue
POST: @@ Finally scale
POST: s-s x n .001 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 3h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

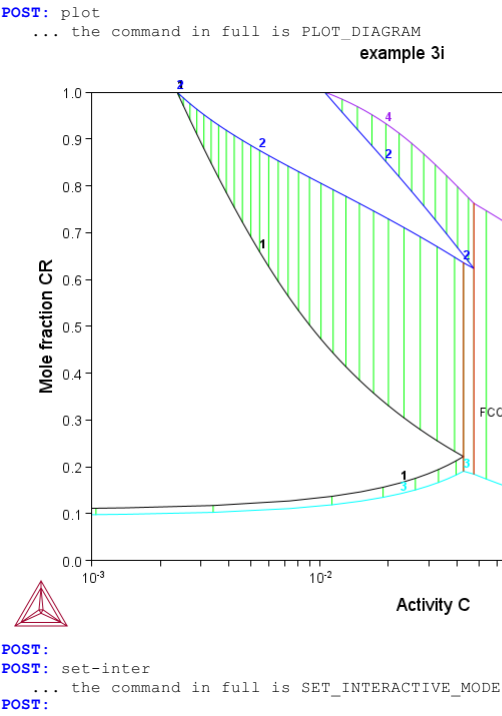
example 3h



```

POST:
POST:Hit RETURN to continue
POST: @@ This kind of diagram is useful to understand diffusion paths.
POST:
POST: @@ The phase labels were lost when we changed axis
POST: @@ To add them back
POST: add .05 .3
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Stable phases are: FCC_A1+M7C3_D101
Text size: /.36/:
POST: set-title example 3i
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:

```



tcex04

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex04\tcex04.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating the miscibility gap in the Fe-Cr system.

SYS:

SYS: set-log ex04,,,

SYS:

SYS: go data

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw FEDEMO

... the command in full is SWITCH_DATABASE

Current database: Iron Demo Database v6.0

VA /- DEFINED

TDB_FEDEMO: def-sys

... the command in full is DEFINE_SYSTEM

ELEMENTS: fe cr

FE CR DEFINED

TDB_FEDEMO: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:

GAS:G :CR CR2 FE FE2:

#Gas # # # #6038cfcf41046d48150aa2e6

LIQUID:L :CR FE:

#Liquid # # # #6038cfcf41046d48150aa2e7

BCC_A2 :CR FE:VA:

#Body-Centered Cubic (W, A2, bcc) #cI2 #Im-3m # #602e7f15105f8553a825b4e4

C14 LAVES :CR FE:CR FE:

#MgZn2 Hexagonal Laves (C14) #hP12 #P6_3/mmc # #602e7f15105f8553a825b52b

CBCC_A12 :CR FE:VA:

#a1pha-Mn (A12) #cI58 #I-43m # #602e7f15105f8553a825b4dc

CHI_A12 :CR FE:CR:CR FE:

#a1pha-Mn (A12) #cI58 #I-43m # #602e7f15105f8553a825b4dc

CUB_A13 :CR FE:VA:

#beta-Mn (A13) #cP20 #P4_132 # #602e7f15105f8553a825b4dd

FCC_A1 :CR FE:VA:

#Face-Centered Cubic (Cu, A1, fcc) #cF4 #Fm-3m # #602e7f15105f8553a825b4d9

HCP_A3 :CR FE:VA:

#Hexagonal Close Packed (Mg, A3, hcp) #hP2 #P6_3/mmc #

#602e7f15105f8553a825b4e6

SIGMA_D8B :CR FE:CR:CR FE:

#sigma-CrFe (D8b) #tP30 #P4_2/mnm # #602e7f15105f8553a825b5b9

TDB_FEDEMO: rej ph /all

... the command in full is REJECT

GAS:G LIQUID:L BCC_A2

C14 LAVES CBCC_A12 CHI_A12

CUB_A13 FCC_A1 HCP_A3

SIGMA_D8B REJECTED

TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 sigma

... the command in full is RESTORE

LIQUID:L FCC_A1 BCC_A2

SIGMA_D8B RESTORED

TDB_FEDEMO: get

... the command in full is GET_DATA

08:38:50,778 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_FEDEMO: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: l-st

... the command in full is LIST_STATUS

Option /CPS/:

*** STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)

VA	ENTERED	SER		

CR	ENTERED	SER		

FE	ENTERED	SER		

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES

SIGMA_D8B	ENTERED	0.000000E+00	0.000000E+00

FCC_A1	ENTERED	0.000000E+00	0.000000E+00

BCC_A2	ENTERED	0.000000E+00	0.000000E+00

LIQUID	ENTERED	0.000000E+00	0.000000E+00

*** STATUS FOR ALL SPECIES

CR	ENTERED	CR2	ENTERED	FE	ENTERED	FE2	ENTERED	VA	ENTERED

POLY:Hit RETURN to continue

POLY: @@ There is a miscibility gap in BCC Fe-Cr.

POLY: @@ Let us first calculate the low temperature region.

```

POLY: s-c x(cr)=.6 t=700 p=101325 n=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      2579 grid points in      0.346 s
Found the set of lowest grid points in      0.001 s
Creating a new composition set BCC_A2#2
Calculated POLY solution      0.099 s, total time      0.446 s
Creating a new composition set BCC_A2#3
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0 , database: FEDEMO

Conditions:
X(CR)=0.6, T=700, P=101325, N=1
DEGREES OF FREEDOM 0

Temperature      700.00 K ( 426.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.35364E+01
Total Gibbs energy -2.30658E+04, Enthalpy 1.31801E+04, Volume 7.26548E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
CR      6.0000E-01  5.8274E-01 2.3703E-02 -2.1780E+04 SER
FE      4.0000E-01  4.1726E-01 1.3643E-02 -2.4995E+04 SER

BCC_A2#3      Status ENTERED      Driving force 0.0000E+00
Moles 6.0116E-01, Mass 3.1437E+01, Volume fraction 6.0322E-01 Mass fractions:
CR 9.17514E-01 FE 8.24857E-02

BCC_A2#1      Status ENTERED      Driving force 0.0000E+00
Moles 3.9884E-01, Mass 2.2100E+01, Volume fraction 3.9678E-01 Mass fractions:
FE 8.93487E-01 CR 1.06513E-01
POLY:Hit RETURN to continue
POLY: @@ Now make a calculation at a higher temperature
POLY: s-c t=900
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      2579 grid points in      0.034 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.023 s, total time      0.057 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0 , database: FEDEMO

Conditions:
X(CR)=0.6, T=900, P=101325, N=1
DEGREES OF FREEDOM 0

Temperature      900.00 K ( 626.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.35364E+01
Total Gibbs energy -3.49346E+04, Enthalpy 2.36851E+04, Volume 7.26372E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
CR      6.0000E-01  5.8274E-01 1.2779E-02 -3.2626E+04 SER
FE      4.0000E-01  4.1726E-01 5.9087E-03 -3.8398E+04 SER

SIGMA_D8B      Status ENTERED      Driving force 0.0000E+00
Moles 6.4237E-01, Mass 3.4605E+01, Volume fraction 6.3941E-01 Mass fractions:
FE 5.04665E-01 CR 4.95335E-01

BCC_A2#3      Status ENTERED      Driving force 0.0000E+00
Moles 3.5763E-01, Mass 1.8932E+01, Volume fraction 3.6059E-01 Mass fractions:
CR 7.42495E-01 FE 2.57505E-01
POLY:Hit RETURN to continue
POLY: @@ The Fe-Cr phase diagram has three non-connected two-phase regions.
POLY:
POLY: s-a-v 1 x(cr)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/:
POLY: s-a-v 2
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: t
Min value /0/: 600
Max value /1/: 2200
Increment /40/:
POLY: @@ Always use a SAVE command before MAP (or STEP) otherwise unless
POLY: @@ you want to overlay this calculation with an earlier one
POLY: save tcex04 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7

```

```

Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Working hard

Phase region boundary 1 at: 1.067E-02 1.169E+03
  BCC_A2#1
  ** FCC_A1
Calculated 12 equilibria

Phase region boundary 2 at: 1.067E-02 1.169E+03
  BCC_A2#1
  ** FCC_A1
Calculated 42 equilibria

Phase region boundary 3 at: 5.119E-01 6.100E+02
  ** BCC_A2#1
  BCC_A2#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 4 at: 5.112E-01 6.000E+02
  BCC_A2#1
  ** BCC_A2#2
Calculated. 10 equilibria

Phase region boundary 5 at: 5.192E-01 7.875E+02
  BCC_A2#1
  ** BCC_A2#2
  ** SIGMA_D8B

Phase region boundary 6 at: 6.762E-01 7.875E+02
  BCC_A2#1
  ** SIGMA_D8B
Calculated.. 54 equilibria
Calculated 54 equilibria

Phase region boundary 7 at: 6.762E-01 7.875E+02
  BCC_A2#1
  ** SIGMA_D8B
Calculated. 58 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 5.119E-01 6.100E+02
  ** BCC_A2#1
  BCC_A2#2
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 9 at: 5.119E-01 6.100E+02
  ** BCC_A2#1
  BCC_A2#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 10 at: 5.119E-01 6.100E+02
  ** BCC_A2#1
  BCC_A2#2
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 4.325E-02 1.137E+03
  BCC_A2#1
  ** FCC_A1
Calculated 49 equilibria

Phase region boundary 12 at: 4.325E-02 1.137E+03
  BCC_A2#1
  ** FCC_A1
Calculated 14 equilibria

Phase region boundary 13 at: 1.006E-01 1.137E+03
  BCC_A2#1
  ** FCC_A1
Calculated 25 equilibria

Phase region boundary 14 at: 1.006E-01 1.137E+03
  BCC_A2#1
  ** FCC_A1
Calculated 34 equilibria

Phase region boundary 15 at: 1.224E-02 1.663E+03
  ** BCC_A2#1
  FCC_A1
Calculated 43 equilibria

Phase region boundary 16 at: 1.224E-02 1.663E+03
  ** BCC_A2#1
  FCC_A1
Calculated 12 equilibria

Phase region boundary 17 at: 9.640E-03 1.809E+03
  LIQUID
  ** BCC_A2#1
Calculated 11 equilibria

Phase region boundary 18 at: 9.640E-03 1.809E+03
  LIQUID
  ** BCC_A2#1
Calculated 93 equilibria

Phase region boundary 19 at: 3.471E-01 1.807E+03
  LIQUID

```

```

** BCC_A2#1
Calculated                      38  equilibria

Phase region boundary  20 at:    3.471E-01  1.807E+03
LIQUID
** BCC_A2#1
Calculated                      64  equilibria

Phase region boundary  21 at:    6.881E-01  2.007E+03
LIQUID
** BCC_A2#1
Calculated                      68  equilibria

Phase region boundary  22 at:    6.881E-01  2.007E+03
LIQUID
** BCC_A2#1
Calculated                      39  equilibria

Phase region boundary  23 at:    9.910E-01  2.176E+03
LIQUID
** BCC_A2#1
Calculated                      90  equilibria

Phase region boundary  24 at:    9.910E-01  2.176E+03
LIQUID
** BCC_A2#1
Calculated                      12  equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex04\tcex04.POLY3
CPU time for mapping                      9  seconds

```

```

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

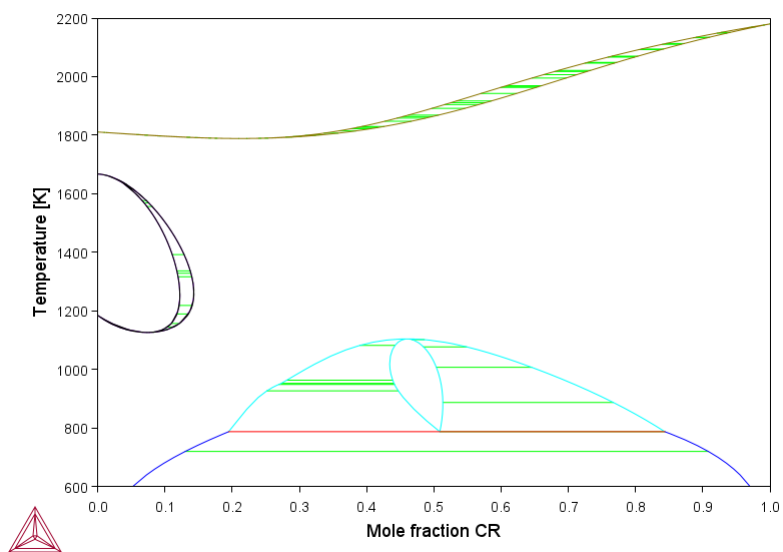
Setting automatic diagram axes

```

POST:
POST: s-t-s 6
... the command in full is SET_TIELINE_STATUS
POST: set_title example 4a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 4a



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex05

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex05\tcex05.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a vertical section in the Al-Cu-Si system

SYS:

SYS: @@ This example calculates a vertical section in the Al-Cu-Si

SYS: @@ system and of a vertical section from Al to 10% Cu2Si.

SYS:

SYS: set-log ex05,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_Al REJECTED

TDB_TCFE11: sw ALDEMO

... the command in full is SWITCH_DATABASE
Current database: Aluminum Demo Database v5.0

VA /- DEFINED

TDB_ALDEMO: def-sys al Cu si

... the command in full is DEFINE_SYSTEM

AL CU SI

DEFINED

TDB_ALDEMO: get

... the command in full is GET_DATA

08:39:55,994 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_ALDEMO: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: s-c t=1000,p=1e5,n=1

... the command in full is SET_CONDITION

POLY: @@ We shall calculate along a line where the Cu content is twice

POLY: @@ that of the Si content. This can be used as a condition.

POLY: @@ Note that the whole equation must be given before the equal sign.

POLY: @@ It is wrong to write s-c x(cu)=2*x(si).

POLY: s-c x(cu)-2*x(si)=0

... the command in full is SET_CONDITION

POLY: l-c

... the command in full is LIST_CONDITIONS

T=1000, P=100000, N=1, X(CU)-2*X(SI)=0

DEGREES OF FREEDOM 1

POLY: s-c w(si)=0.05

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 17676 grid points in 0.304 s

38 ITS, CPU TIME USED 2 SECONDS

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: ALDEMO

Conditions:

T=1000, P=100000, N=1, X(CU)-2*X(SI)=0, W(SI)=5E-2

DEGREES OF FREEDOM 0

Temperature 1000.00 K (726.85 C), Pressure 1.000000E+05

Number of moles of components 1.000000E+00, Mass in grams 3.10908E+01

Total Gibbs energy -5.01533E+04, Enthalpy 2.90243E+04, Volume 1.09580E-05

Component	Moles	W-Fraction	Activity	Potential	Ref.stat

AL	8.3395E-01	7.2374E-01	4.7926E-03	-4.4405E+04	SER

CU	1.1070E-01	2.2626E-01	9.6970E-06	-9.5980E+04	SER

SI	5.5351E-02	5.0000E-02	4.4065E-03	-4.5103E+04	SER

LIQUID Status ENTERED Driving force 0.0000E+00

Moles 1.0000E+00, Mass 3.1091E+01, Volume fraction 1.0000E+00 Mass fractions:

AL 7.23737E-01 CU 2.26263E-01 SI 5.00000E-02

POLY: @?<Hit_return_to_continue>

POLY: ?

... the command in full is HELP

ADD_INITIAL_EQUILIBRIUM GOTO_MODULE REINITIATE_MODULE

ADVANCED_OPTIONS HELP SAVE_WORKSPACES

AMEND_STORED_EQUILIBRIA INFORMATION SELECT_EQUILIBRIUM

BACK LIST_AXIS_VARIABLE SET_ALL_START_VALUES

CHANGE_STATUS LIST_CONDITIONS SET_AXIS_VARIABLE

COMPUTE_EQUILIBRIUM LIST_EQUILIBRIUM SET_CONDITION

COMPUTE_TRANSITION LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS

CREATE_NEW_EQUILIBRIUM LIST_STATUS SET_INTERACTIVE

```

DEFINE_COMPONENTS      LIST_SYMBOLS      SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM         LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
DEFINE_MATERIAL        MACRO_FILE_OPEN    SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB MAKE_COMPONENT_ENTERED SET_START_VALUE
DELETE_SYMBOL          MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL           MAP                STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS     POST              TABULATE
EXIT                  READ_WORKSPACES

POLY: s-a-v 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w (si)
Min value /0/: 0
Max value /1/: .1
Increment /.0025/: .0025
POLY: s-a-v 2
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: t
Min value /0/: 500
Max value /1/: 1300
Increment /20/: 10
POLY: l-a-v
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W (SI)           Min: 0           Max: 0.1           Inc: 2.5E-3
Axis No 2: T               Min: 500          Max: 1300          Inc: 10
POLY:@?<Hit_return_to_continue>
POLY: save tcex05 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Working hard

Phase region boundary 1 at: 2.500E-03 6.461E+02
** AL2CU_C16
   DIAMOND_A4
   FCC_A1
Calculated.. 16 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 3.656E-04 5.000E+02
** AL2CU_C16
   DIAMOND_A4
   FCC_A1
Calculated. 31 equilibria

Phase region boundary 3 at: 1.067E-02 7.948E+02
** LIQUID
** AL2CU_C16
   DIAMOND_A4
   FCC_A1

Phase region boundary 4 at: 5.846E-02 7.948E+02
LIQUID
AL2CU_C16
** DIAMOND_A4
Calculated. 2 equilibria

Phase region boundary 5 at: 6.069E-02 8.026E+02
LIQUID
** AL2CU_C16
** DIAMOND_A4

Phase region boundary 6 at: 6.069E-02 8.026E+02
LIQUID
** DIAMOND_A4
Calculated.. 18 equilibria
Terminating at axis limit.

Phase region boundary 7 at: 6.069E-02 8.026E+02
LIQUID
** AL2CU_C16
Calculated. 3 equilibria

Phase region boundary 8 at: 5.704E-02 7.964E+02
LIQUID
** AL2CU_C16

```

```

** FCC_A1
Phase region boundary 9 at: 5.704E-02 7.964E+02
LIQUID
** AL2CU_C16
FCC_A1
Calculated. 17 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 5.704E-02 7.964E+02
LIQUID
** FCC_A1
Calculated 41 equilibria

Phase region boundary 11 at: 5.704E-02 7.964E+02
LIQUID
AL2CU_C16
** FCC_A1
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 6.069E-02 8.026E+02
LIQUID
** AL2CU_C16
DIAMOND_A4
Calculated. 22 equilibria

Phase region boundary 13 at: 9.890E-02 8.509E+02
LIQUID
** AL2CU_C16
** ALCU_ETA
DIAMOND_A4

Phase region boundary 14 at: 1.058E-01 8.509E+02
** LIQUID
AL2CU_C16
DIAMOND_A4

Phase region boundary 15 at: 9.890E-02 8.509E+02
LIQUID
** ALCU_ETA
DIAMOND_A4
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 16 at: 1.350E-01 8.509E+02
** LIQUID
ALCU_ETA
DIAMOND_A4

Phase region boundary 17 at: 1.058E-01 8.509E+02
AL2CU_C16
** ALCU_ETA
DIAMOND_A4

Phase region boundary 18 at: 1.350E-01 8.509E+02
** AL2CU_C16
ALCU_ETA
DIAMOND_A4

Phase region boundary 19 at: 1.036E-01 7.948E+02
** LIQUID
AL2CU_C16
DIAMOND_A4

Phase region boundary 20 at: 1.669E-02 7.948E+02
LIQUID
** DIAMOND_A4
FCC_A1
Calculated. 4 equilibria

Phase region boundary 21 at: 1.013E-02 7.966E+02
** LIQUID
** DIAMOND_A4
FCC_A1

Phase region boundary 22 at: 1.013E-02 7.966E+02
** DIAMOND_A4
FCC_A1
Calculated.. 31 equilibria
Terminating at axis limit.

Phase region boundary 23 at: 1.013E-02 7.966E+02
** LIQUID
FCC_A1
Calculated 26 equilibria

Phase region boundary 24 at: 1.013E-02 7.966E+02
** LIQUID
DIAMOND_A4
FCC_A1
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 1.036E-01 7.948E+02
AL2CU_C16
DIAMOND_A4
** FCC_A1

Phase region boundary 26 at: 2.500E-03 6.461E+02
** AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated. 16 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.417E-02 7.948E+02
** LIQUID
AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 3.417E-02 7.948E+02
** LIQUID

```

```

AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 29 at: 6.583E-02 7.948E+02
** LIQUID
AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 24 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 6.583E-02 7.948E+02
** LIQUID
AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 31 at: 9.750E-02 7.948E+02
** LIQUID
AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 36 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 9.750E-02 7.948E+02
** LIQUID
AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 33 at: 7.899E-03 7.700E+02
** DIAMOND_A4
FCC_A1
Calculated.. 29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 34 at: 7.899E-03 7.700E+02
** DIAMOND_A4
FCC_A1
Calculated.. 4 equilibria
Terminating at known equilibrium

Phase region boundary 35 at: 8.449E-03 7.700E+02
** AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 36 at: 8.449E-03 7.700E+02
** AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 4 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.500E-03 9.291E+02
LIQUID
** FCC_A1
Calculated 18 equilibria

Phase region boundary 38 at: 2.500E-03 9.291E+02
LIQUID
** FCC_A1
Calculated.. 23 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 3.417E-02 8.648E+02
LIQUID
** FCC_A1
Calculated 26 equilibria

Phase region boundary 40 at: 3.417E-02 8.648E+02
LIQUID
** FCC_A1
Calculated.. 11 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 6.583E-02 8.227E+02
LIQUID
** DIAMOND_A4
Calculated.. 4 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 6.583E-02 8.227E+02
LIQUID
** DIAMOND_A4
Calculated.. 20 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 43 at: 9.750E-02 9.579E+02
LIQUID
** DIAMOND_A4
Calculated.. 20 equilibria
Terminating at known equilibrium

Phase region boundary 44 at: 9.750E-02 9.579E+02
LIQUID
** DIAMOND_A4
Calculated.. 4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

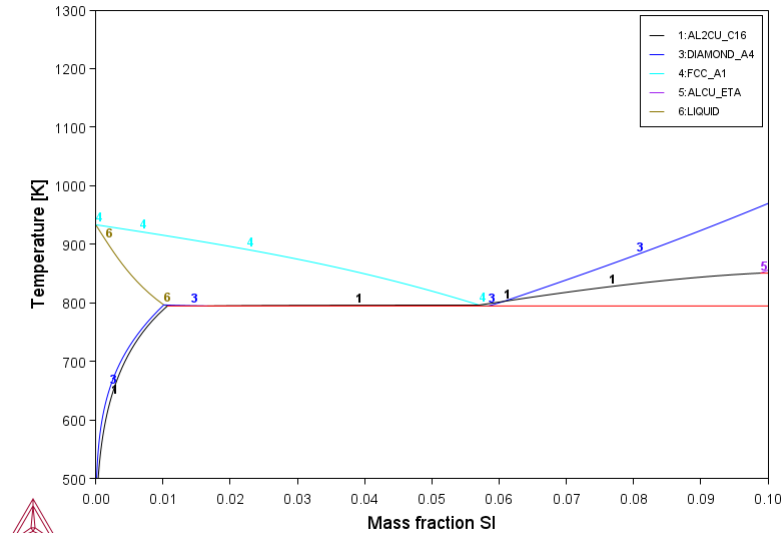
```


*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex05\tcex05.POLY3
CPU time for mapping 18 seconds

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

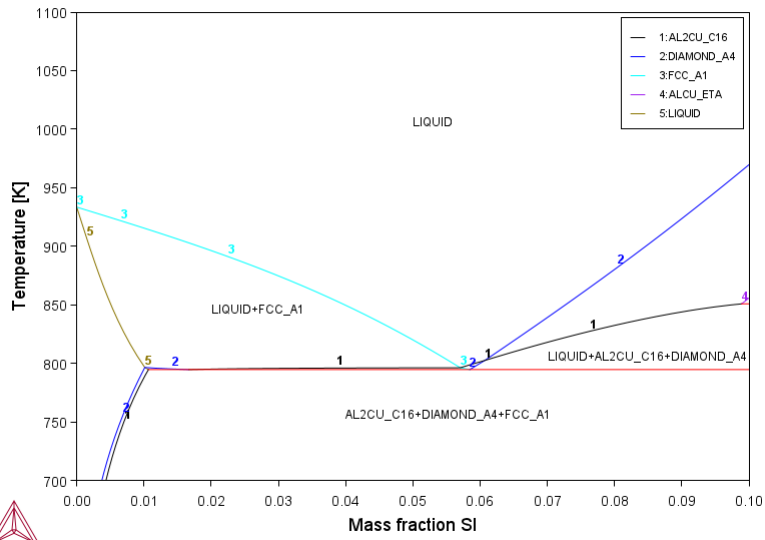
Setting automatic diagram axes

POST: s-lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: b
POST:
POST:
POST: set-title example 5a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 5a



POST:
POST:@?<Hit_return_to_continue>
POST: s-s y n 700 1100
... the command in full is SET_SCALING_STATUS
POST: @@ Note that the three-phase region LIQ-Si-Al2Cu is an area and not
POST: @@ a single line as in a binary system. This is called a pseudo-binary section
POST: add .05 1000
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Stable phases are: LIQUID
Text size: /.36/:
POST: add .02 840
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated 17676 grid points in 0.076 s
Stable phases are: LIQUID+FCC_A1
Text size: /.36/:
POST: add .04 750
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated 17676 grid points in 0.066 s
Stable phases are: AL2CU_C16+DIAMOND_A4+FCC_A1
Text size: /.36/:
POST: add .07 800
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated 17676 grid points in 0.088 s
Stable phases are: LIQUID+AL2CU_C16+DIAMOND_A4
Text size: /.36/:
POST:
POST: set-title example 5b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

example 5b



POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex06\tcex06.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculation of an isopleth in low alloyed

SYS: @@ Fe-Mn-Si-Cr-Ni-C steel.

SYS:

SYS: @@ This example calculates a multicomponent phase diagram using

SYS: @@ the Define Material command in POLY and the TCFE steel

SYS: @@ database. Note that TCFE database license is required to run the

SYS: @@ example.

SYS:Hit RETURN to continue

SYS: set-log ex06,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: @@ The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C

POLY: @@ (by weight). These conditions are set by the command and in

POLY: @@ addition the temperature. Hidden commands set the pressure to 1 bar

POLY: @@ and that iron is "the rest".

POLY: @@ After calculating the first equilibrium we calculate a phase diagram

POLY: @@ with one axis variable as temperature and the other as the

POLY: @@ carbon content

POLY:

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfell

Major element or alloy: ?

FILE SYSTEM ERROR IN FILHLP

ERROR 1717 READING HELP FILE

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: y

1st alloying element: c

Mass (weight) percent /1/: 1

2nd alloying element: si .3

Next alloying element: mn .4

Next alloying element: ni 3.5

Next alloying element: cr 1.5

Next alloying element:

Temperature (C) /1000/: 1000

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

NI DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M5C2	M3C2_D510
KSI_CARBIDE	FE4N_LP1	SIGMA_D8B
HIGH_SIGMA	CHI_A12	C14_LAVES
C15_LAVES	M3SI	MN9SI2
MN11SI19	MN6SI	G_PHASE
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	NB5SI3_D8L	MSI2_C40
M11SI8	M6SI5	AL4C3_D71
FE8SI2C	SIC_B3	MN5SI2C
CRZN17	CUZN_EPSILON	NI2N_B2
NI2N_L10	NI2ZN11_D82	AL5FE4
MNP_B31	M2P_C22	M4SI1_G3
NI3SI12	CO2SI_C37	M2SI_TETA
NISI_B31	NI3SI2	CR5SI3_D8M

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3

CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M5C2	M3C2_D510
KSI_CARBIDE	FE4N_LP1	SIGMA_D8B
HIGH_SIGMA	CHI_A12	C14_LAVES
C15_LAVES	M3SI	MN9SI2
MN11SI19	MN6SI	G_PHASE
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	NB5SI3_D8L	MSI2_C40
M11SI8	M6SI5	AL4C3_D71
FE8SI2C	SIC_B3	MN5SiC
CRZN17	CUZN_EPSILON	NIZN_B2
NIZN_L10	NI2ZN11_D82	AL5FE4
MNP_B31	M2P_C22	M4SI1_G3
NI3SI12	CO2SI_C37	M2SI_TETA
NISI_B31	NI3SI2	CR5SI3_D8M

.....

OK? /Y/: Y

08:41:11,457 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set FCC_A1#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set HCP_A3#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 45065 grid points in 1.186 s
 Found the set of lowest grid points in 0.020 s
 Calculated POLY solution 0.959 s, total time 2.165 s

POLY:

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=1273.15, W(C)=1E-2, W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2,
 P=100000, N=1

DEGREES OF FREEDOM 0

Temperature 1273.15 K (1000.00 C), Pressure 1.000000E+05
 Number of moles of components 1.00000E+00, Mass in grams 5.37536E+01
 Total Gibbs energy -6.46661E+04, Enthalpy 3.76396E+04, Volume 7.13974E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	4.4754E-02	1.0000E-02	8.5166E-02	-2.6074E+04	SER
CR	1.5507E-02	1.5000E-02	1.3307E-04	-9.4473E+04	SER
FE	8.9803E-01	9.3300E-01	2.4799E-03	-6.3509E+04	SER
MN	3.9138E-03	4.0000E-03	3.3252E-06	-1.3353E+05	SER
NI	3.2056E-02	3.5000E-02	5.8057E-05	-1.0325E+05	SER
SI	5.7419E-03	3.0000E-03	4.4487E-09	-2.0357E+05	SER

FCC A1#1 Status ENTERED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 5.3754E+01, Volume fraction 1.0000E+00 Mass fractions:
 FE 9.33000E-01 CR 1.50000E-02 MN 4.00000E-03
 NI 3.50000E-02 C 1.00000E-02 SI 3.00000E-03

POLY:Hit RETURN to continue

POLY: @@ Note that values now must be set in fractions and Kelvin.

POLY: s-a-v 1 w(c)

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 0

Max value /1/: .01

Increment /2.5E-04/: 1E-4

POLY: s-a-v 2 t

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 700

Max value /1/: 1300

Increment /15/:

POLY: save tcex06 y

... the command in full is SAVE_WORKSPACES

POLY: map

Version S mapping is selected

Generating start equilibrium 1
 Generating start equilibrium 2
 Generating start equilibrium 3
 Generating start equilibrium 4
 Generating start equilibrium 5
 Generating start equilibrium 6
 Generating start equilibrium 7
 Generating start equilibrium 8
 Generating start equilibrium 9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1

Generating start point 2

```

Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 1.348E-03 7.100E+02
  BCC_A2
  FCC_A1#1
  ** M3C2_D510
  M7C3_D101
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 1.356E-03 7.000E+02
  BCC_A2
  FCC_A1#1
  ** M3C2_D510
  M7C3_D101
Calculated. 22 equilibria

Phase region boundary 3 at: 2.413E-03 7.877E+02
  BCC_A2
  FCC_A1#1
  ** GRAPHITE_A9
  ** M3C2_D510
  M7C3_D101

Phase region boundary 4 at: 2.413E-03 7.877E+02
  BCC_A2
  FCC_A1#1
  GRAPHITE_A9
  ** M3C2_D510
  M7C3_D101
Calculated.. 78 equilibria
Terminating at axis limit.

Phase region boundary 5 at: 2.413E-03 7.877E+02
  BCC_A2
  FCC_A1#1
  ** GRAPHITE_A9
  M7C3_D101
Calculated. 7 equilibria

Phase region boundary 6 at: 2.693E-03 8.693E+02
  BCC_A2
  ** CEMENTITE_D011
  FCC_A1#1
  ** GRAPHITE_A9
  M7C3_D101

Phase region boundary 7 at: 2.693E-03 8.693E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
  ** GRAPHITE_A9
  M7C3_D101
Calculated. 22 equilibria

Phase region boundary 8 at: 4.767E-03 8.798E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
  ** GRAPHITE_A9
  ** M7C3_D101

Phase region boundary 9 at: 4.767E-03 8.798E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
  ** GRAPHITE_A9
Calculated.. 55 equilibria
Terminating at axis limit.

Phase region boundary 10 at: 4.767E-03 8.798E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
  ** M7C3_D101
Calculated. 27 equilibria

Phase region boundary 11 at: 5.567E-03 9.868E+02
  ** BCC_A2
  CEMENTITE_D011
  FCC_A1#1
  ** M7C3_D101

Phase region boundary 12 at: 5.567E-03 9.868E+02
  CEMENTITE_D011
  FCC_A1#1
  ** M7C3_D101
Calculated. 7 equilibria

```

Phase region boundary 13 at: 5.692E-03 1.066E+03
 ** CEMENTITE_D011
 FCC_A1#1
 ** M7C3_D101

Phase region boundary 14 at: 5.692E-03 1.066E+03
 FCC_A1#1
 ** M7C3_D101
 Calculated. 27 equilibria

Phase region boundary 15 at: 3.176E-03 9.980E+02
 ** BCC_A2
 FCC_A1#1
 ** M7C3_D101

Phase region boundary 16 at: 3.176E-03 9.980E+02
 BCC_A2
 FCC_A1#1
 ** M7C3_D101
 Calculated.. 51 equilibria
 Terminating at axis limit.

Phase region boundary 17 at: 3.176E-03 9.980E+02
 ** BCC_A2
 FCC_A1#1
 Calculated 38 equilibria

Phase region boundary 18 at: 3.176E-03 9.980E+02
 ** BCC_A2
 FCC_A1#1
 M7C3_D101
 Calculated. 19 equilibria

Phase region boundary 19 at: 4.977E-03 9.872E+02
 ** BCC_A2
 ** CEMENTITE_D011
 FCC_A1#1
 M7C3_D101

Phase region boundary 20 at: 4.977E-03 9.872E+02
 ** BCC_A2
 CEMENTITE_D011
 FCC_A1#1
 M7C3_D101
 Calculated. 7 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 4.977E-03 9.872E+02
 ** CEMENTITE_D011
 FCC_A1#1
 M7C3_D101
 Calculated. 12 equilibria
 Terminating at known equilibrium

Phase region boundary 22 at: 4.977E-03 9.872E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1#1
 M7C3_D101
 Calculated. 38 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 5.692E-03 1.066E+03
 ** CEMENTITE_D011
 FCC_A1#1
 Calculated.. 46 equilibria
 Terminating at axis limit.

Phase region boundary 24 at: 5.567E-03 9.868E+02
 ** BCC_A2
 CEMENTITE_D011
 FCC_A1#1
 Calculated.. 47 equilibria
 Terminating at axis limit.

Phase region boundary 25 at: 4.767E-03 8.798E+02
 BCC_A2
 CEMENTITE_D011
 FCC_A1#1
 GRAPHITE_A9
 ** M7C3_D101
 Calculated.. 55 equilibria
 Terminating at axis limit.

Phase region boundary 26 at: 2.693E-03 8.693E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1#1
 GRAPHITE_A9
 M7C3_D101
 Calculated.. 76 equilibria
 Terminating at axis limit.

Phase region boundary 27 at: 2.413E-03 7.877E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 M7C3_D101
 Calculated. 5 equilibria

Phase region boundary 28 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101

Phase region boundary 29 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 Calculated.. 5 equilibria
 Terminating at axis limit.

Phase region boundary 30 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 M3C2_D510
 ** M7C3_D101
 Calculated.. 29 equilibria
 Terminating at axis limit.

Phase region boundary 31 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated.. 82 equilibria
 Terminating at axis limit.

Phase region boundary 32 at: 1.348E-03 7.100E+02
 BCC_A2
 FCC_A1#1
 ** M3C2_D510
 M7C3_D101
 Calculated. 23 equilibria
 Terminating at known equilibrium

Phase region boundary 33 at: 1.000E-04 9.392E+02
 BCC_A2
 FCC_A1#1
 ** M7C3_D101
 Calculated.. 18 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 34 at: 1.000E-04 9.392E+02
 BCC_A2
 FCC_A1#1
 ** M7C3_D101
 Calculated. 32 equilibria
 Terminating at known equilibrium

Phase region boundary 35 at: 3.367E-03 7.586E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated. 14 equilibria
 Terminating at known equilibrium

Phase region boundary 36 at: 3.367E-03 7.586E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated.. 69 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 37 at: 6.633E-03 7.586E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated. 47 equilibria
 Terminating at known equilibrium

Phase region boundary 38 at: 6.633E-03 7.586E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated.. 36 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 39 at: 2.166E-03 7.100E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 40 at: 2.166E-03 7.100E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 Calculated. 5 equilibria
 Terminating at known equilibrium

Phase region boundary 41 at: 9.900E-03 7.586E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated. 80 equilibria
 Terminating at known equilibrium

Phase region boundary 42 at: 9.900E-03 7.586E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated.. 4 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 43 at: 2.556E-03 9.033E+02
 BCC_A2

```

** CEMENTITE_D011
  FCC_A1#1
  M7C3_D101
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 44 at:  2.556E-03  9.033E+02
  BCC_A2
** CEMENTITE_D011
  FCC_A1#1
  M7C3_D101
Calculated.          31 equilibria
Terminating at known equilibrium

Phase region boundary 45 at:  5.545E-03  9.033E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
** GRAPHITE_A9
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 46 at:  5.545E-03  9.033E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
** GRAPHITE_A9
Calculated..         47 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 47 at:  6.691E-03  1.097E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 48 at:  6.691E-03  1.097E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated..         36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 49 at:  6.691E-03  1.097E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 50 at:  6.691E-03  1.097E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated..         36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 51 at:  1.000E-04  1.050E+03
** BCC_A2
  FCC_A1#1
Calculated           5 equilibria

Phase region boundary 52 at:  1.000E-04  1.050E+03
** BCC_A2
  FCC_A1#1
Calculated.          32 equilibria
Terminating at known equilibrium

Phase region boundary 53 at:  3.367E-03  1.004E+03
  FCC_A1#1
** M7C3_D101
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 54 at:  3.367E-03  1.004E+03
  FCC_A1#1
** M7C3_D101
Calculated.          25 equilibria
Terminating at known equilibrium

Phase region boundary 55 at:  6.633E-03  1.095E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 56 at:  6.633E-03  1.095E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated..         36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 57 at:  9.900E-03  1.189E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated.          44 equilibria
Terminating at known equilibrium

Phase region boundary 58 at:  9.900E-03  1.189E+03
** CEMENTITE_D011
  FCC_A1#1
Calculated..         4 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex06\tcex06.POLY3
CPU time for mapping          69 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 6a
POST:

```

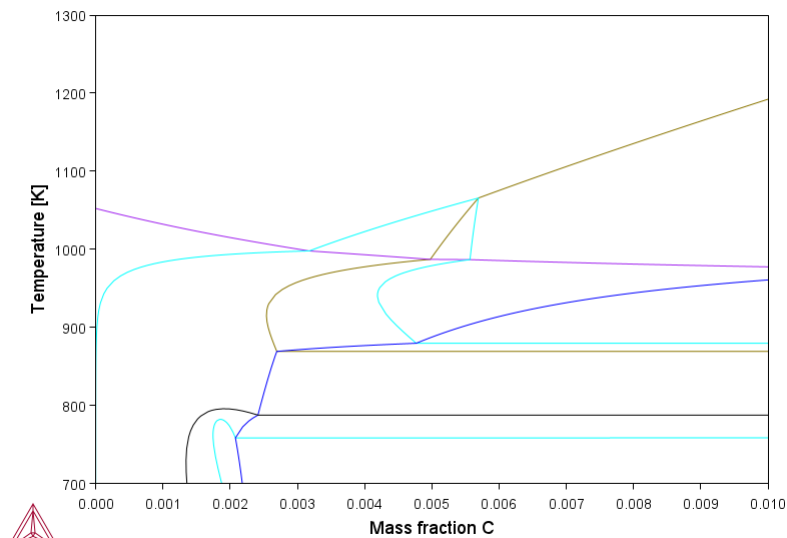


```

POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 6a

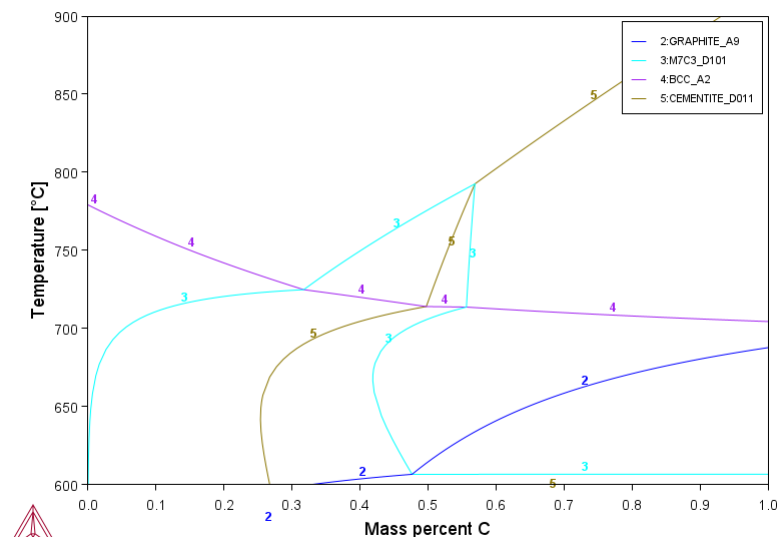


```

POST:
POST:Hit RETURN to continue
POST: @@ Use more practical quantities in the plot and
POST: @@ label the curves
POST: s-d-a x w-p c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST:
POST: s-s y n 600 900
... the command in full is SET_SCALING_STATUS
POST:
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 6b



```

POST:
POST:Hit RETURN to continue
POST: @@ Determine the phase region at the iron rich side
POST: add .2 850
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 45065 grid points in 0.215 s
Found the set of lowest grid points in 0.011 s
Calculated POLY solution 0.256 s, total time 0.482 s
Stable phases are: FCC_A1
Text size: /.36/:
POST: @@ Knowing that only FCC (or austenite) is stable in that region and
POST: @@ which phase is stable along each line, one can determine the phases

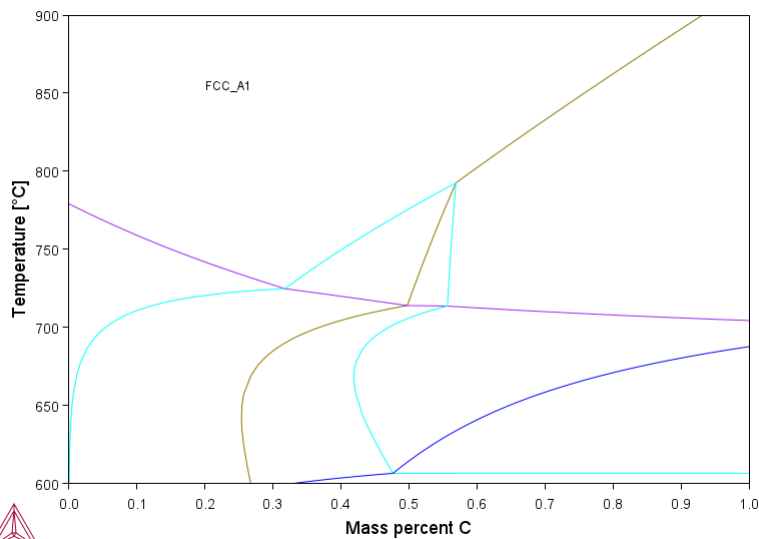
```

```

POST: @@ in each region. For example at 0.3 % C and 630 degree C one should
POST: @@ have FCC+BCC+M7C3+CEMENTITE.
POST: @@ Check by adding a label
POST:
POST: add .3 630
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      45065 grid points in      0.214 s
Found the set of lowest grid points in      0.013 s
Calculated POLY solution      0.258 s, total time      0.485 s
Stable phases are: BCC_A2+CEMENTITE_D011+FCC_A1+M7C3_D101
Text size: /.36/: @@ We remove the labels again.
*** ERROR 1034 IN GETREL: NO DIGIT
POST:
POST: s-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 6c



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex07

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex07\tcex07.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating single equilibria in low alloyed

SYS: @@ Fe-Mn-Si-Cr-Ni-C steel

SYS:

SYS: @@ There are 2 common ways to perform a single equilibrium

SYS: @@ calculation.

SYS:

SYS: @@ 1) Get data from database, then in POLY use SET_CONDITION

SYS: @@ and COMPUTE_EQUILIBRIUM.

SYS: @@ 2) Go directly to POLY and use DEFINE_MATERIAL.

SYS:

SYS: @@ The COMPUTE_TRANSITION command is also used to determine the

SYS: @@ temperature or composition where one phase forms or

SYS: @@ disappears. It is the same as the CHANGE_STATUS -->

SYS: @@ SET_CONDITION --> COMPUTE_EQUILIBRIUM sequence of commands.

SYS: @@ Note that a TCFE database license is required to run the

SYS: @@ example.

SYS:Hit RETURN to continue

SYS:

SYS: set-log ex07,,

SYS: @@ The alloy composition is 1 wt% Cr, 0.3 wt% Si, 0.3wt% Mn,

SYS: @@ 2.8 wt% Ni and 0.55 wt% C

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfell

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/:

1st alloying element: c .55

2nd alloying element: cr 1

Next alloying element: mn .3 ni 2.8 si .3

Next alloying element:

Temperature (C) /1000/: 600

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

NI DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M5C2	M3C2_D510
KSI_CARBIDE	FE4N_LP1	SIGMA_D8B
HIGH_SIGMA	CHI_A12	C14_LAVES
C15_LAVES	M3SI	MN9SI2
MN11SI19	MN6SI	G_PHASE
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	NB5SI3_D8L	MSI2_C40
M11SI8	M6SI5	AL4C3_D71
FE8SI2C	SIC_B3	MN5SIC
CRZN17	CUZN_EPSILON	NIZN_B2
NIZN_L10	NI2ZN11_D82	AL5FE4
MNP_B31	M2P_C22	M4SI1_G3
NI3SI12	CO2SI_C37	M2SI_TETA
NISI_B31	NI3SI2	CR5SI3_D8M

Reject phase(s) /NONE/:

Restore phase(s): /NONE/:

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M5C2	M3C2_D510

KSI_CARBIDE	FE4N_LP1	SIGMA_D8B
HIGH_SIGMA	CHI_A12	C14_LAVES
C15_LAVES	M3SI	MN9SI2
MN11SI19	MN6SI	G_PHASE
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	NB5SI3_D8L	MSI2_C40
M11SI8	M6SI5	AL4C3_D71
FE8SI2C	SIC_B3	MN5SIC
CRZN17	CUZN_EPSILON	NIZN_B2
NIZN_L10	NI2ZN11_D82	AL5FE4
MNP_B31	M2P_C22	M4SI1_G3
NI3SI12	CO2SI_C37	M2SI_TETA
NISI_B31	NI3SI2	CR5SI3_D8M

.....

OK? /Y/: Y

08:43:21,673 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set FCC_A1#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set HCP_A3#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 45065 grid points in 1.281 s

Found the set of lowest grid points in 0.268 s

Calculated POLY solution 0.943 s, total time 2.492 s

POLY:

POLY: @@ The first equilibrium is calculated automatically

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0, database: TCFE11

Conditions:

T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,

P=100000, N=1

DEGREES OF FREEDOM 0

Temperature 873.15 K (600.00 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.46196E+01

Total Gibbs energy -3.56755E+04, Enthalpy 1.80441E+04, Volume 7.19873E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	2.5011E-02	5.5000E-03	2.6153E-01	-9.7369E+03	SER
CR	1.0505E-02	1.0000E-02	3.0144E-04	-5.8855E+04	SER
FE	9.2961E-01	9.5050E-01	8.6912E-03	-3.4451E+04	SER
MN	2.9826E-03	3.0000E-03	2.7817E-05	-7.6155E+04	SER
NI	2.6058E-02	2.8000E-02	3.2474E-04	-5.8314E+04	SER
SI	5.8344E-03	3.0000E-03	2.1186E-11	-1.7843E+05	SER

BCC_A2 Status ENTERED Driving force 0.0000E+00

Moles 9.4807E-01, Mass 5.2841E+01, Volume fraction 9.5831E-01 Mass fractions:

FE 9.63018E-01 SI 3.10097E-03 MN 2.01890E-03

NI 2.88252E-02 CR 3.01634E-03 C 2.00700E-05

CEMENTITE_D011 Status ENTERED Driving force 0.0000E+00

Moles 2.4898E-02, Mass 1.1032E+00, Volume fraction 2.0766E-02 Mass fractions:

FE 7.19940E-01 C 6.77718E-02 NI 4.39878E-03

CR 1.71965E-01 MN 3.59240E-02 SI 4.75407E-13

M7C3_D101 Status ENTERED Driving force 0.0000E+00

Moles 1.1910E-02, Mass 4.9370E-01, Volume fraction 9.6222E-03 Mass fractions:

FE 4.75579E-01 C 8.69279E-02 NI 2.71291E-03

CR 3.99236E-01 MN 3.55437E-02 SI 2.83764E-12

GRAPHITE_A9 Status ENTERED Driving force 0.0000E+00

Moles 1.5125E-02, Mass 1.8167E-01, Volume fraction 1.1300E-02 Mass fractions:

C 1.00000E+00 NI 0.00000E+00 FE 0.00000E+00

SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00

POLY: ?

... the command in full is HELP

ADD_INITIAL_EQUILIBRIUM GOTO_MODULE REINITIATE_MODULE

ADVANCED_OPTIONS HELP SAVE_WORKSPACES

AMEND_STORED_EQUILIBRIA INFORMATION SELECT_EQUILIBRIUM

BACK LIST_AXIS_VARIABLE SET_ALL_START_VALUES

CHANGE_STATUS LIST_CONDITIONS SET_AXIS_VARIABLE

COMPUTE_EQUILIBRIUM LIST_EQUILIBRIUM SET_CONDITION

COMPUTE_TRANSITION LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS

CREATE_NEW_EQUILIBRIUM LIST_STATUS SET_INTERACTIVE

DEFINE_COMPONENTS LIST_SYMBOLS SET_NUMERICAL_LIMITS

DEFINE_DIAGRAM LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE

DEFINE_MATERIAL MACRO_FILE_OPEN SET_START_CONSTITUITION

DELETE_INITIAL_EQUILIB MAKE_COMPONENT_ENTERED SET_START_VALUE

DELETE_SYMBOL MAKE_COMPONENT_SUSPENDED SHOW_VALUE

ENTER_SYMBOL MAP STEP_WITH_OPTIONS

EVALUATE_FUNCTIONS POST TABULATE

EXIT READ_WORKSPACES

POLY:Hit RETURN to continue

POLY: @@ Increase Cr until all Graphite disappears. Calculate this

POLY: @@ directly using the COMPUTE-TRANSITION command. You

POLY: @@ must release the Cr content

POLY: c-t

```

... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: grap
You must release one of these conditions
T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: w(cr)
Testing POLY result by global minimization procedure
Using already calculated grid
To form GRAP the condition is set to W(CR)=.0287719523467
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=873.15, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 873.15 K ( 600.00 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45454E+01
Total Gibbs energy -3.61530E+04, Enthalpy 1.78811E+04, Volume 7.15509E-06

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
C      2.4977E-02  5.5000E-03  2.6153E-01 -9.7369E+03 SER
CR     3.0183E-02  2.8772E-02  3.0842E-04 -5.8689E+04 SER
FE     9.1001E-01  9.3173E-01  8.6876E-03 -3.4454E+04 SER
MN     2.9786E-03  3.0000E-03  2.0228E-05 -7.8467E+04 SER
NI     2.6023E-02  2.8000E-02  3.3357E-04 -5.8119E+04 SER
SI     5.8265E-03  3.0000E-03  2.1648E-11 -1.7827E+05 SER

BCC_A2      Status ENTERED      Driving force 0.0000E+00
Moles 9.1702E-01, Mass 5.1108E+01, Volume fraction 9.3254E-01 Mass fractions:
FE 9.62515E-01 SI 3.20176E-03 MN 1.47289E-03
NI 2.96997E-02 CR 3.09060E-03 C 1.98381E-05

M7C3_D101    Status ENTERED      Driving force 0.0000E+00
Moles 8.2976E-02, Mass 3.4372E+00, Volume fraction 6.7456E-02 Mass fractions:
FE 4.73949E-01 C 8.69853E-02 NI 2.72688E-03
CR 4.10632E-01 MN 2.57069E-02 SI 2.90090E-12

GRAPHITE_A9   Status ENTERED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
C 1.00000E+00 NI 0.00000E+00 FE 0.00000E+00
SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Graphite disappears when we have this chromium content 2.89 w/o
POLY: @@ The amount of Cr can be obtained directly with a Show command
POLY: show w(cr)
... the command in full is SHOW_VALUE
W(CR)=2.8771952E-2
POLY: @@ This is automatically set as a new condition by the C-T command
POLY: @@ and the amount of graphite is zero.
POLY: l-st ph
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
M7C3_D101  ENTERED      0.000000E+00      8.297554E-02
GRAPHITE_A9 ENTERED      0.000000E+00      0.000000E+00
BCC_A2     ENTERED      0.000000E+00      9.170245E-01
BCC_B2     ENTERED      -1.377319E-04      0.000000E+00
CEMENTITE_D011 ENTERED      -4.665913E-03      0.000000E+00
FCC_A1#1   ENTERED      -1.129409E-02      0.000000E+00
FCC_A1#2   ENTERED      -1.129409E-02      0.000000E+00
FCC_L12    ENTERED      -1.143122E-02      0.000000E+00
M23C6_D84  ENTERED      -8.127100E-02      0.000000E+00
M3C2_D510  ENTERED      -1.346313E-01      0.000000E+00
HCP_A3#2   ENTERED      -2.666922E-01      0.000000E+00
HCP_A3#1   ENTERED      -2.666922E-01      0.000000E+00
M5C2       ENTERED      -2.780639E-01      0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -5.489230E-01
CUB_A13 M4SI1_G3 FE4N_LP1 LIQUID NBN13_D0A CHI_A12 SIGMA_D8B DIAMOND_A4
CBCC_A12 C14 LAVES C15 LAVES AL5FE4 KSI_CARBIDE NI3TI_D024 CRZN17 FE8SI2C
NI3SI12 G_PHASE M3SI CO2SI_C37 M2SI_TETA M2P_C22 CR3SI_A15 NI2ZN11_D82
NI3SI2 M5SI3_D88 NIZN_L10 NIZN_B2 MN5SIC HIGH_SIGMA CR5SI3_D8M MN6SI MSI_B20
CUZN_EPSILON MN9SI2 NISI_B31 MNP_B31 SIC_B3 M6SI5 FESI2_L AL4C3_D71 MN11SI19
MSI2_C40 FESI2_H M11SI8 NB5SI3_D8L GAS
POLY: @@ Now determine the maximum temperature with no Austenite (FCC_A1),
POLY: @@ i.e. Al temperature.
POLY: @@ Use the command COMPUTE-TRANSITION again
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: fcc_al
You must release one of these conditions
T=873.15, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 45065 grid points in 0.263 s
To form FCC_A1 the condition is set to T=910.926169574
POLY: l-c
... the command in full is LIST_CONDITIONS
T=910.9261696, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0
POLY: @@ This command does the same as Change-Status/Set-Cond/Compute-Equil sequence.
POLY: @@ Notice that the temperature is set back as condition with the new value.
POLY: @@ If we want temperatures in Celsius enter a function.
POLY: ent fun tc=t-273;
... the command in full is ENTER_SYMBOL
POLY: sh tc
... the command in full is SHOW_VALUE
TC=637.92617
POLY:Hit RETURN to continue
POLY:
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS

```

```

Output from POLY-3, equilibrium =      1, label A0  , database: TCFE11

Conditions:
T=910.9261696, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature      910.93 K (   637.78 C), Pressure  1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.45454E+01
Total Gibbs energy -3.85270E+04, Enthalpy  1.95997E+04, Volume  7.16809E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C               2.4977E-02  5.5000E-03 2.1677E-01 -1.1580E+04 SER
CR              3.0183E-02  2.8772E-02 3.1863E-04 -6.0981E+04 SER
FE              9.1001E-01  9.3173E-01 7.7657E-03 -3.6794E+04 SER
MN              2.9786E-03  3.0000E-03 1.7785E-05 -8.2837E+04 SER
NI              2.6023E-02  2.8000E-02 2.7915E-04 -6.1983E+04 SER
SI              5.8265E-03  3.0000E-03 4.2177E-11 -1.8093E+05 SER

BCC_A2          Status ENTERED      Driving force  0.0000E+00
Moles 9.1675E-01, Mass 5.1087E+01, Volume fraction 9.3232E-01 Mass fractions:
FE 9.61370E-01 CR 3.99660E-03 MN 1.69140E-03
NI 2.97053E-02 SI 3.20309E-03 C 3.31203E-05

M7C3_D101       Status ENTERED      Driving force  0.0000E+00
Moles 8.0497E-02, Mass 3.3366E+00, Volume fraction 6.5375E-02 Mass fractions:
FE 4.85354E-01 C 8.69306E-02 NI 2.74957E-03
CR 4.02641E-01 MN 2.23247E-02 SI 6.70624E-12

CEMENTITE_D011  Status ENTERED      Driving force  0.0000E+00
Moles 2.7483E-03, Mass 1.2174E-01, Volume fraction 2.3072E-03 Mass fractions:
FE 7.26713E-01 C 6.77895E-02 NI 4.43780E-03
CR 1.78567E-01 MN 2.24927E-02 SI 4.75531E-13

FCC_A1#1        Status ENTERED      Driving force  0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 8.44258E-01 MN 1.10217E-02 CR 5.80937E-03
NI 1.27409E-01 SI 9.74493E-03 C 1.75747E-03

POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: cps
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)          P(Pa)
VA              ENTERED      SER
C               ENTERED      SER
CR              ENTERED      SER
FE              ENTERED      SER
MN              ENTERED      SER
NI              ENTERED      SER
SI              ENTERED      SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
M7C3_D101      ENTERED      0.000000E+00      8.049708E-02
FCC_A1#2       ENTERED      0.000000E+00      0.000000E+00
FCC_A1#1       ENTERED      0.000000E+00      0.000000E+00
CEMENTITE_D011 ENTERED      0.000000E+00      2.748313E-03
BCC_A2         ENTERED      0.000000E+00      9.167546E-01
FCC_L12        ENTERED      -1.309646E-04      0.000000E+00
BCC_B2         ENTERED      -1.320120E-04      0.000000E+00
M23C6_D84      ENTERED      -6.812021E-02      0.000000E+00
GRAPHITE_A9     ENTERED      -1.334968E-01      0.000000E+00
M3C2_D510      ENTERED      -1.866450E-01      0.000000E+00
HCP_A3#2       ENTERED      -2.563175E-01      0.000000E+00
HCP_A3#1       ENTERED      -2.563175E-01      0.000000E+00
M5C2           ENTERED      -2.766353E-01      0.000000E+00
CUB_A13        ENTERED      -5.142755E-01      0.000000E+00
FE4N_LP1       ENTERED      -5.394909E-01      0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -5.870182E-01
M4S11_G3 LIQUID CHI_A12 NBN13_D0A SIGMA_D8B CBCC_A12 C14_LAVES C15_LAVES
DIAMOND_A4 AL5FE4_KSI_CARBIDE_CRZN17_NI3TI_D024 FE8SI2C_NI31SI12_G_PHASE M3SI
CO2SI_C37 M2SI_TETA_M2P_C22 CR3SI_A15 NI2ZN11_D82 M5SI3_D88 NI3SI2_NIZN_L10
NIZN_B2 MN5SIC_HIGH_SIGMA_CR5SI3_D8M MSI_B20 MN6SI_CUZN_EPSILON_MN9SI2
NIS1_B31 MNP_B31 SIC_B3 M6SI5_FESI2_L_AL4C3_D71 MN11SI19 MSI2_C40 FESI2_H
M11SI8 NB5SI3_D8L GAS
*** STATUS FOR ALL SPECIES
C      ENTERED      C60 ENTERED      FE+2 ENTERED      MN+3 ENTERED      SI      ENTERED
C2     ENTERED      CR      ENTERED      FE+3 ENTERED      MN+4 ENTERED      SI+4 ENTERED
C3     ENTERED      CR+2 ENTERED      FE+4 ENTERED      NI      ENTERED      VA      ENTERED
C4     ENTERED      CR+3 ENTERED      MN      ENTERED      NI+2 ENTERED
C5     ENTERED      FE      ENTERED      MN+2 ENTERED      NI+3 ENTERED
POLY: @@ Now determine maximum temperature where no Ferrite (BCC_A2) exists
POLY: @@ Use
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
You want to find when the current major phase is formed, please give
New major phase: fcc_a1
You must release one of these conditions
T=910.9261696, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated      45065 grid points in      0.274 s
To form BCC_A2 the condition is set to T=1008.10465885
POLY:
POLY: show tc
... the command in full is SHOW_VALUE
TC=735.10466
POLY:Hit RETURN to continue
POLY: @@ Check how this varies with the carbon content
POLY: ch-st phase fcc_a1
... the command in full is CHANGE_STATUS
Status: /ENTERED/: ent
Start value, number of mole formula units /0/: 1
POLY: ch-st phase bcc_a2
... the command in full is CHANGE_STATUS
Status: /ENTERED/: fix
Number of mole formula units /0/: 0
POLY:
POLY: s-c t=none
... the command in full is SET_CONDITION
POLY:
POLY: c-e

```

```

... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
  7 ITS, CPU TIME USED  0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
P=100000, N=1
FIXED PHASES
BCC_A2=0
DEGREES OF FREEDOM 0

Temperature 1008.10 K ( 734.95 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.45454E+01
Total Gibbs energy -4.50693E+04, Enthalpy 2.77195E+04, Volume 7.08502E-06

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
C                2.4977E-02  5.5000E-03  8.7621E-02 -2.0408E+04 SER
CR               3.0183E-02  2.8772E-02  5.0980E-04 -6.3547E+04 SER
FE               9.1001E-01  9.3173E-01  5.8696E-03 -4.3066E+04 SER
MN               2.9786E-03  3.0000E-03  5.0117E-06 -1.0229E+05 SER
NI               2.6023E-02  2.8000E-02  7.6292E-05 -7.9468E+04 SER
SI               5.8265E-03  3.0000E-03  2.5738E-10 -1.8508E+05 SER

FCC_A1#1        Status ENTERED      Driving force  0.0000E+00
Moles 9.6475E-01, Mass 5.3092E+01, Volume fraction 9.7087E-01  Mass fractions:
FE 9.45651E-01 CR 1.63193E-02 SI 3.08210E-03
NI 2.87421E-02 C 3.25815E-03 MN 2.94707E-03

M7C3_D101       Status ENTERED      Driving force  0.0000E+00
Moles 3.5250E-02, Mass 1.4529E+00, Volume fraction 2.9128E-02  Mass fractions:
CR 4.83816E-01 C 8.74213E-02 NI 8.82838E-04
FE 4.22946E-01 MN 4.93402E-03 SI 4.97830E-11

BCC_A2          Status FIXED        Driving force  0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
FE 9.71935E-01 CR 1.08640E-02 MN 9.22867E-04
NI 1.29484E-02 SI 3.24854E-03 C 8.13589E-05
POLY: show tc
... the command in full is SHOW_VALUE
TC=735.10466
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 1 w(c) 0 .08 0.001,,,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex07 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.550000E-02
...OK

Phase Region from 0.550000E-02 for:
  BCC_A2
  FCC_A1#1
  M7C3_D101
Global check of adding phase at 7.92117E-03
Calculated 5 equilibria

Phase Region from 0.792117E-02 for:
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
  M7C3_D101
Global check of removing phase at 1.03956E-02
Calculated 5 equilibria

Phase Region from 0.103956E-01 for:
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
Global test at 1.75000E-02 .... OK
Global check of adding phase at 2.24931E-02
Calculated 15 equilibria

Phase Region from 0.224931E-01 for:
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
  GRAPHITE_A9
Global test at 3.05000E-02 .... OK
Global test at 4.05000E-02 .... OK
Global test at 5.05000E-02 .... OK
Global test at 6.05000E-02 .... OK
Global test at 7.05000E-02 .... OK
Global test at 8.00000E-02 .... OK
Terminating at 0.800000E-01
Calculated 61 equilibria

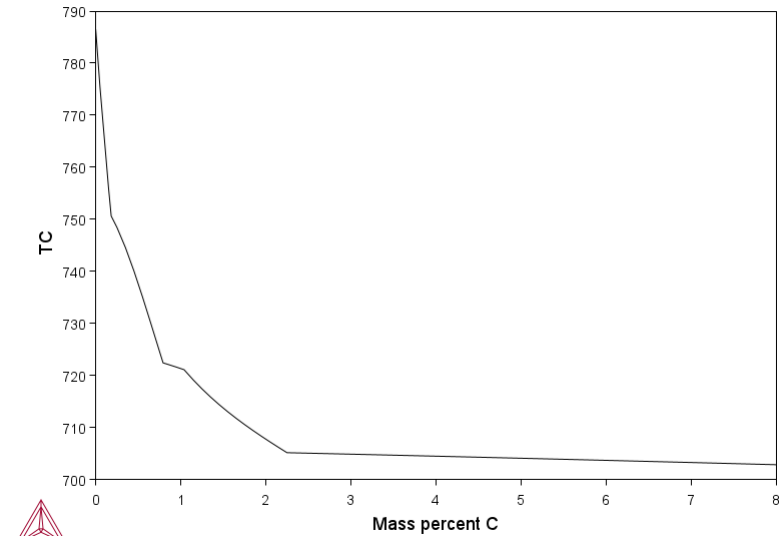
Phase Region from 0.550000E-02 for:
  BCC_A2
  FCC_A1#1
  M7C3_D101
Global check of removing phase at 1.81940E-03
Calculated 6 equilibria

Phase Region from 0.181940E-02 for:
  BCC_A2
  FCC_A1#1
Global test at 9.99526E-16 .... OK
Terminating at 0.215885E-12
Calculated 6 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex07\tcex07.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w-p c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y tc
... the command in full is SET_DIAGRAM_AXIS
POST:

```

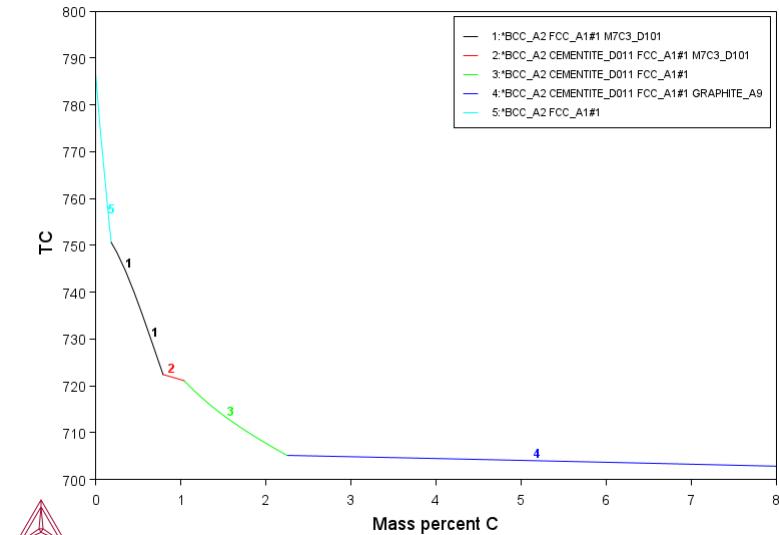
```
POST: set-title example 7a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 7a



```
POST:
POST:Hit RETURN to continue
POST: s-s y n 700 800
... the command in full is SET_SCALING_STATUS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 7b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 7b



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```


tcex08

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex08\tcex08.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculation of a property diagram for a high speed steel

SYS:

SYS: @@ This example shows how to calculate property diagrams

SYS: @@ for a high speed steel i.e. phase fraction plots,

SYS: @@ activity vs temperature, and so forth.

SYS: @@ Note that a TCFE database license is required to run

SYS: @@ the example.

SYS:

SYS: set-log ex08,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-dia

... the command in full is DEFINE_DIAGRAM

For binary or ternary diagrams you may prefer the special modules

You must specify a value for all compositions and the temperature even if you want to use it as axis.

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfell

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/:

1st alloying element: c .9 cr 4 mn .3 si .3 w 8 mo 5 v 2

Next alloying element:

Temperature (C) /1000/: 1300

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

W DEFINED

... the command in full is DEFINE_ELEMENTS

MO DEFINED

... the command in full is DEFINE_ELEMENTS

V DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	MC_ETA	MC_SHP
KSI_CARBIDE	Z_PHASE	FE4N_LP1
SIGMA_D8B	HIGH_SIGMA	MU_D85
P_PHASE	R_PHASE	CHI_A12
CL4_LAVES	CL5_LAVES	M3SI
MN9SI2	MN11SI19	MN6SI
G_PHASE	CR3SI_A15	FESI2_H
FESI2_L	MSI_B20	M5SI3_D88
NBNI3_D0A	CO3V	MOSI2_C11B
MO5SI3_D8M	NB5SI3_D8L	MSI2_C40
M11SI8	M6SI5	AL4C3_D71
FE8SI2C	SIC_B3	MN5SiC
CRZN17	CUZN_EPSILON	AL5FE4
MNP_B31	M2P_C22	NI31SI12
CO2SI_C37	M2SI_TETA	NISI_B31
NI3SI2	CR5SI3_D8M	DELTA_TIH2
DIS_BETA	BETA_PHASE	

Reject phase(s) /NONE/: NONE

Restore phase(s) /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	MC_ETA	MC_SHP
KSI_CARBIDE	Z_PHASE	FE4N_LP1
SIGMA_D8B	HIGH_SIGMA	MU_D85

P_PHASE	R_PHASE	CHI_A12
C14_LAVES	C15_LAVES	M3SI
MN9SI2	MN11SI19	MN6SI
G_PHASE	CR3SI_A15	FESI2_H
FESI2_L	MSI_B20	M5SI3_D88
NBNI3_D0A	CO3V	MOSI2_C11B
MO5SI3_D8M	NB5SI3_D8L	MSI2_C40
M11SI8	M6SI5	AL4C3_D71
FE8SI2C	SIC_B3	MN5SIC
CRZN17	CUZN_EPSILON	AL5FE4
MNP_B31	M2P_C22	NI3SI12
CO2SI_C37	M2SI_TETA	NISI_B31
NI3SI2	CR5SI3_D8M	DELTA_TIH2
DIS_BETA	BETA_PHASE	

.....

OK? /Y/: Y

08:44:40,193 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set FCC_A1#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set HCP_A3#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 48087 grid points in 1.126 s

Found the set of lowest grid points in 0.046 s

Calculated POLY solution 1.209 s, total time 2.381 s

You must now set an independent axis for your diagram

as one of the following conditions:

Condition 1 is temperature (Celsius)

Condition 2 is mass percent of C

Condition 3 is mass percent of CR

Condition 4 is mass percent of MN

Condition 5 is mass percent of SI

Condition 6 is mass percent of W

Condition 7 is mass percent of MO

Condition 8 is mass percent of V

Give the number of the condition to vary /1/: 1

Minimum value (C) /800/: 600

Maximum value (C) /1800/: 1600

The second axis can be another of the conditions above and you will then calculate a phase diagram.

Or you may want to plot how some other quantities depend on the selected condition and you will then calculate a "property" diagram.

In addition to the conditions above you may use these selected dependent quantities on the vertical axis:

Dependent 9 is mass fraction of all phases

Dependent 10 is composition of a phase

Dependent 11 is the fraction of a component in all phases

(In the post processor you may select many other quantities)

Give the number of the quantity on second axis /9/: 9 tcex08 y

No initial equilibrium, using default

Step will start from axis value 1573.15

...OK

Phase Region from 1573.15 for:

LIQUID

BCC_A2

FCC_A1#1

M6C_E93

Global Check of removing phase at 1.57870E+03

Calculated 3 equilibria

Phase Region from 1578.70 for:

LIQUID

BCC_A2

FCC_A1#1

Global Check of removing phase at 1.59784E+03

Calculated 5 equilibria

Phase Region from 1597.84 for:

LIQUID

BCC_A2

Global test at 1.67315E+03 OK

Global check of removing phase at 1.69235E+03

Calculated 12 equilibria

Phase Region from 1692.35 for:

LIQUID

BCC_A2

Global test at 1.76315E+03 OK

Global test at 1.86315E+03 OK

Terminating at 1873.15

Calculated 22 equilibria

Phase Region from 1573.15 for:

LIQUID

BCC_A2

FCC_A1#1

M6C_E93

Global check of removing phase at 1.57109E+03

Calculated 3 equilibria

```

Phase Region from 1571.09 for:
LIQUID
FCC_A1#1
M6C_E93
Global Check of adding phase at 1.52095E+03
Calculated 8 equilibria

Phase Region from 1520.95 for:
LIQUID
FCC_A1#1
FCC_A1#2
M6C_E93
Global Check of removing phase at 1.52080E+03
Calculated 3 equilibria

Phase Region from 1520.80 for:
FCC_A1#1
FCC_A1#2
M6C_E93
Global test at 1.44315E+03 .... OK
Global test at 1.34315E+03 .... OK
Global test at 1.24315E+03 .... OK
Global test at 1.14315E+03 .... OK
Global check of adding phase at 1.12062E+03
Calculated 43 equilibria

Phase Region from 1120.62 for:
FCC_A1#1
FCC_A1#2
M23C6_D84
M6C_E93
Global check of adding phase at 1.11212E+03
Calculated 4 equilibria

Phase Region from 1112.12 for:
BCC_A2
FCC_A1#1
FCC_A1#2
M23C6_D84
M6C_E93
Global check of removing phase at 1.09550E+03
Calculated 4 equilibria

Phase Region from 1095.50 for:
BCC_A2
FCC_A1#2
M23C6_D84
M6C_E93
Global test at 1.02315E+03 .... OK
Global test at 9.23150E+02 .... OK
Terminating at 873.150
Calculated 26 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex08\tcex08.POLY3
POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

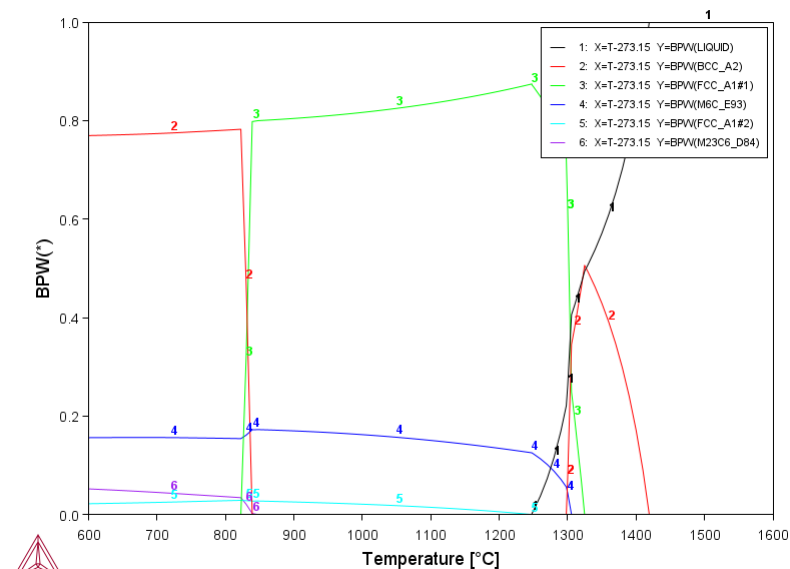
... the command in full is REINITIATE_PLOT_SETTINGS
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is SET_AUTOMATIC_DIAGRAM_A

Setting automatic diagram axes

... the command in full is PLOT_DIAGRAM

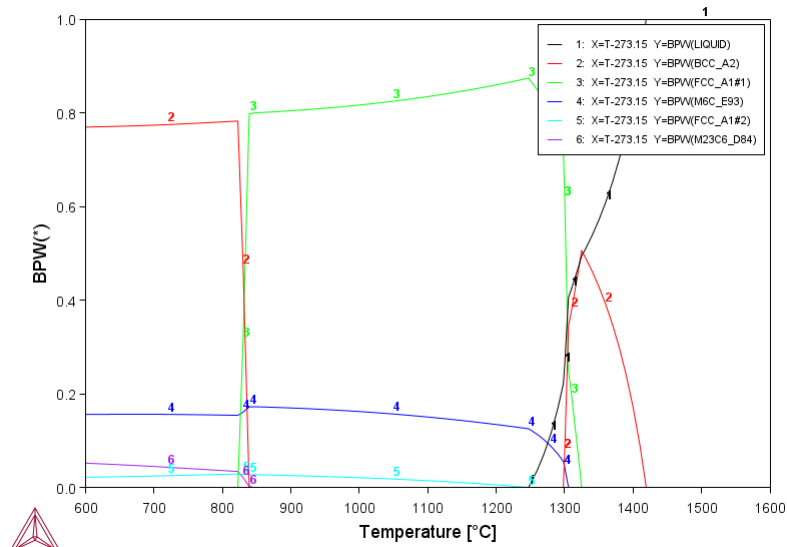


```

POST:
POST:Hit RETURN to continue
POST: set-title example 8a
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 8a

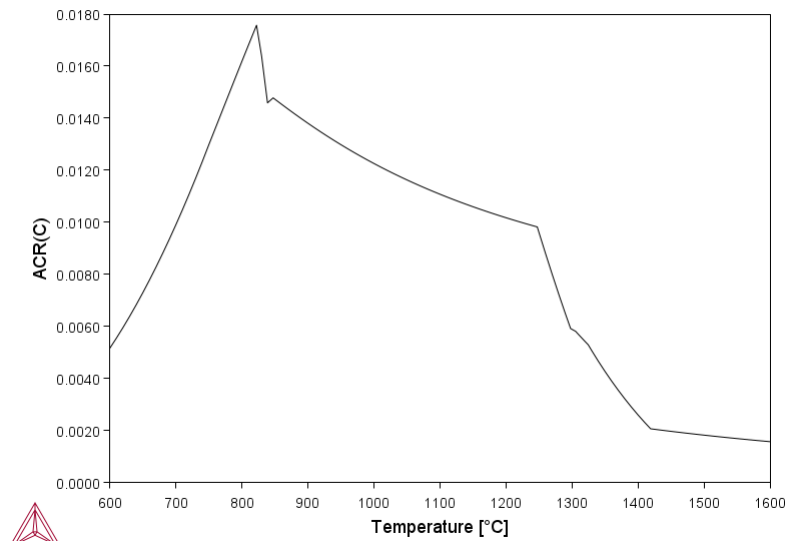


```

POST:
POST:Hit RETURN to continue
POST: s-d-a y acr(c)
... the command in full is SET_DIAGRAM_AXIS
POST: set_lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: n
POST: set-title example 8b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 8b

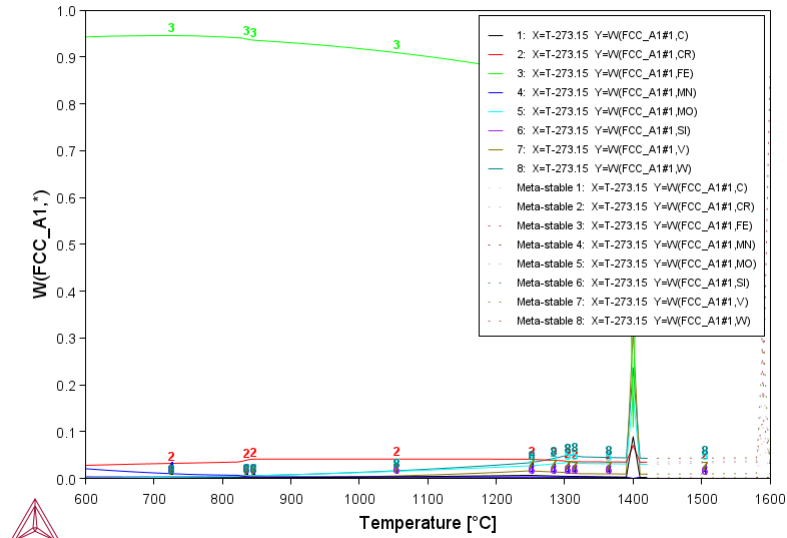


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot how the composition of the austenite (called fcc) varies
POST: @@ Note this is plotted also where the austenite is not stable.
POST: s-d-a y w(fcc_a1,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set_lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 8c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 8c

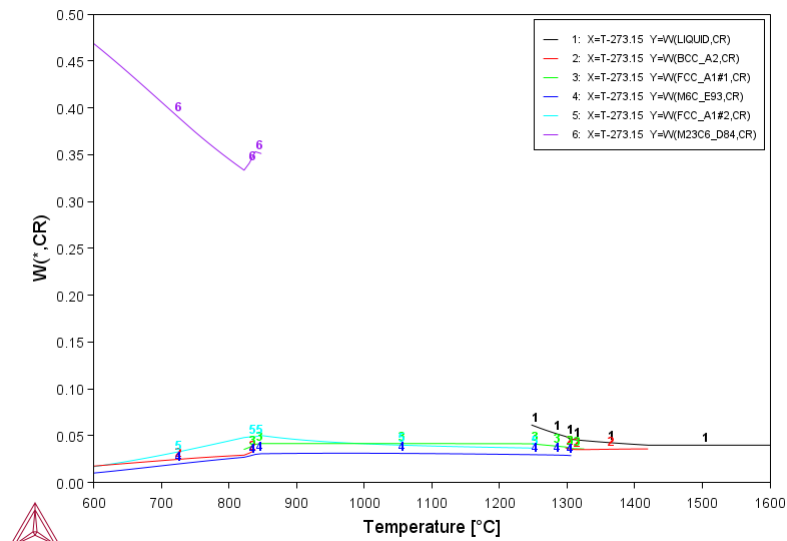


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot the fraction of Cr in all phases
POST: s-d-a y w(*,cr)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 8d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 8d



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex09

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex09\tcex09.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a dew point with the POLY3 module

SYS:

SYS: go data

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw subdemo

Current database: Substance Demo Database v1.0

VA /- DEFINED

TDB_SUBDEMO: def-sp h2 h2o1

H2 H2O1 DEFINED

TDB_SUBDEMO: get

08:46:25,334 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_SUBDEMO: go p-3

POLY version 3.32

POLY: s-c n=1 p=1e5 t=233

POLY: ch-st ph h2o_l=f 0

POLY: c-e

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 210 grid points in 0.020 s

22 ITS, CPU TIME USED 1 SECONDS

POLY: l-e,,,

Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:

N=1, P=100000, T=233

FIXED PHASES

H2O1_L=0

DEGREES OF FREEDOM 0

Temperature 233.00 K (-40.15 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 1.00931E+00

Total Gibbs energy -1.53589E+04, Enthalpy -9.53654E+02, Volume 9.68549E-03

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
H	9.9991E-01	9.9851E-01	3.6499E-04	-1.5335E+04	SER
O	9.3929E-05	1.4889E-03	1.0377E-61	-2.7203E+05	SER

GAS Status ENTERED Driving force 0.0000E+00

Moles 1.0000E+00, Mass 1.0093E+00, Volume fraction 1.0000E+00 Mass fractions:

H 9.9851E-01 O 1.4889E-03

Constitution:

H2 9.99812E-01 H2O1 1.87875E-04

H2O1_L Status FIXED Driving force 0.0000E+00

Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:

O 8.88103E-01 H 1.11897E-01

POLY: ent fun ph2_h2o=acr(h2,gas)/acr(h2o,gas);

POLY: s-a-v l t 173.15 373.15 ,

POLY: save dew y

POLY: step normal

No initial equilibrium, using default

Step will start from axis value 233.000

...OK

Phase Region from 233.000 for:

GAS

H2O1_L

Global test at 2.73000E+02 OK

Global test at 3.23000E+02 OK

Global test at 3.73000E+02 OK

Terminating at 373.150

Calculated 32 equilibria

Phase Region from 233.000 for:

GAS

H2O1_L

Global test at 1.93000E+02 OK

Terminating at 173.150

Calculated 15 equilibria

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex09\dew.POLY3

POLY: post

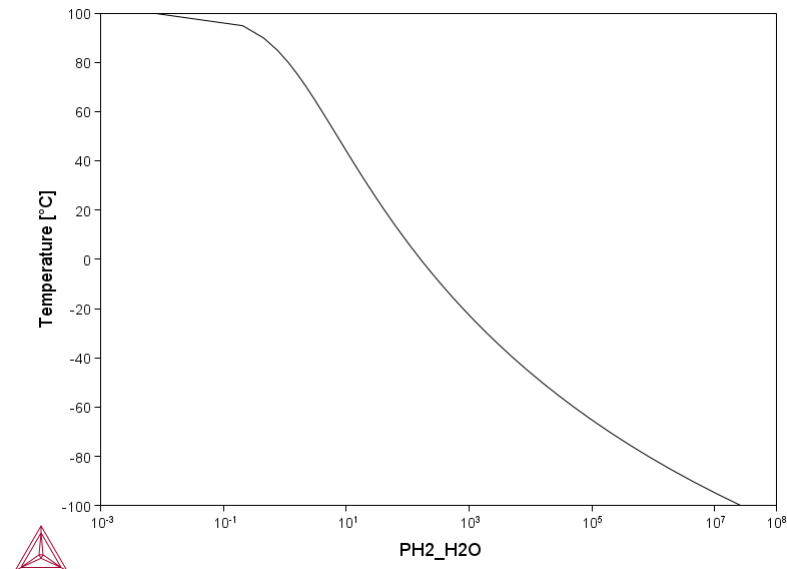
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x ph2_h2o

POST: s-a-ty x log

```
POST: s-d-a y t-c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```



```
POST:
POST:
POST: set-inter
POST:
```

tcex10

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex10\tcex10.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Preventing Cr304 clogging in a continuous casting process

SYS:

SYS: @@ This example calculates an equilibrium with suspended or

SYS: @@ dormant phases and shows how to avoid Cr-oxide clogging in

SYS: @@ a continuous casting process.

SYS: @@ Note that a license for the TCOX13 database is required to

SYS: @@ run the example.

SYS:

SYS: @@ The background to this example is that a manufacturer

SYS: @@ wanted to increase the Cr content of a material from 18

SYS: @@ to 25 weight percent. He then had trouble in the continous

SYS: @@ casting of this material because solid Cr304 was formed.

SYS: @@ By calculating the equilibria in the steel/slag system a

SYS: @@ simple correction could be found: modify the Mn or Si

SYS: @@ content, thus decrease the oxygen potential.

SYS:

SYS: @@ In Thermo-Calc, you can FIX a phase with zero amount to

SYS: @@ simulate how to avoid forming this phase. You can then

SYS: @@ release one of the conditions, usually one of the

SYS: @@ compositions, and this composition is determined by the

SYS: @@ equilibrium calculation.

SYS:

SYS: set-log ex10,,,,

SYS: @@ Go to the database module to obtain data

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: @@ Switch to the database with slag data

TDB_TCFE11: sw TCOX13

... the command in full is SWITCH_DATABASE

Current database: Metal Oxide Solutions v13.0

VA /- DEFINED

PEROVSKITE:I REJECTED

TDB_TCOX13: @@ Some information about the database is given by this command

TDB_TCOX13: d-i

... the command in full is DATABASE_INFORMATION

Current database: Metal Oxide Solutions v13.0

TCOX: TCS Metal Oxide Solutions Database

(Version 13.0, November 2023)

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The TCOX, Metal Oxide Solutions Database - Version 13.0, contains critically assessed data for many multicomponent oxides, fluorides and sulfides, as well as all alloy phases needed to calculate the Me-O, Me-F and Me-S binary phase diagrams. The intended application is for solid and liquid ionized materials, such as development of ceramics, metallurgical processing, materials corrosion, solid oxide fuel cell materials, ESR slags, sulfide formation, dephosphorization, desulfurization and Thermal Barrier Coatings (TBC) but the database is of course not limited to this. TCOX has been developed in a CALPHAD spirit with all of the oxygen (and sulfur and fluor) containing binary systems assessed for their full range of composition including all phases, plus the majority of the ternary oxide/fluoride/sulfide systems, and many quaternary oxide/fluoride/sulfide systems, including also oxy-fluoride and oxy-sulfide systems as well, in order to give an accurate thermodynamic description of the multicomponent systems of interest.

Since version 11, carbides and nitrides are included in TCOX. However, other intermetallic compounds (Me1-Me2) and order-disorder transformations are not included in the database. For those phases, the TCOX database is compatible with TCFE Steels/Fe-Alloys Database, TCNI Ni-based Superalloys Database and SSOL Solutions Database. Thus, if needed, more solid metallic phases can be obtained by appending from TCFE, TCNI, SSOL and/or other appropriate databases. However, one must keep in mind that the LIQUID phase from other databases and the IONIC_LIQ phase from TCOX should never be simultaneously considered in the same defined system/calculation, as they both represent the liquid phase using two different models. Viscosity, surface tension and electrical conductivity of the ionic liquid phase are incorporated in TCOX.

Now it is able to calculate the viscosity, surface tension and electrical conductivities of the molten slags for various industrial applications. The calculated viscosity, surface tension and electrical conductivity of the ionic liquid phase are connected to the distribution and connectivity of species in the oxide melts in the whole composition and a broad range of temperatures.

Molar volumes are described, both for liquid and solid oxides.

The primary thermodynamic models applied for various solution phases are:
- Compound Energy Formalism with several sublattices and neutral or ionic constituents (Hillert, 2001) for various solid solution phases.

- Ionic Two-Sublattice Liquid Model (Hillert et al., 1985) for the ionic liquid solution phase (IONIC_LIQ). The same model is used both for metallic and ionized melts. At low levels of ionization, the model becomes equivalent to a substitutional solution model between metallic atoms.

Different composition sets of IONIC_LIQ designated by #1, #2 etc. (e.g. IONIC_LIQ#1) may be observed which often represent the metallic and ionized liquid phases. Different composition sets also describe miscibility gaps frequently found in e.g. Silicate systems. The #n suffix

(where n is an integer) is generated dynamically by Thermo-Calc when using global minimization and therefore the identification of the phases should be determined from their compositions.

- Ideal Gas Model (GAS). Since version 12, the TCOX database contains an extensive GAS mixture phase.

ALLOY ELEMENTS (32): Al Ar B C Ca Co Cr Cu F Fe
Gd H Hf K La Mg Mn Mo N Na Nb
Ni O P S Si Ti V W Y Yb Zr

Ar and H is only included in the gas phase. There are 606 different phases included in the database. Many of the solid oxide and sulfide phases are modelled as solution phases.

The assessed systems in TCOX are given in the extended information, found on the Thermo-Calc website.

The TCOX database was called ION prior to version 4.0.

Release History of the TCOX database:

Version 1.0: Aug. 1992 (initial release)
Version 1.1: Nov. 1994 (with some modifications)
Version 1.2: Nov. 2001 (with some modifications)
Version 2.0: Aug. 2002 (with major updates and improvements)
Version 2.1: Apr. 2004 (with major improvements)
Version 2.2: Jun. 2005 (with minor improvements)
Version 2.3: Mar. 2006 (with minor improvements)
Version 3.0: May 2009 (with major updates and improvements)
Version 4.0: Mar. 2011 (with major updates and improvements)
Version 4.1: Aug. 2012 (with minor improvements)
Version 5.0: Oct. 2012 (with major improvements)
Version 5.1: Jan. 2013 (with major improvements)
Version 5.2: Sep. 2014 (with major improvements)
Version 6.0: Jan. 2015 (with major improvements)
Version 7.0: Mar. 2017 (with major improvements)
Version 8.0: May 2018 (with major improvements)
Version 9.0: May 2019 (with major improvements)
Version 9.0.1: Aug. 2019 (with minor modifications)
Version 9.0.2: Dec. 2019 (with minor modifications)
Version 10.0: Apr. 2020 (with major improvements)
Version 10.1: Dec. 2020 (with minor improvements)
Version 10.2: Dec. 2021 (bugfix)
Version 11.0: May 2021 (with major improvements)
Version 11.1: Dec. 2021 (bugfix)
Version 12.0: Nov. 2022 (with major improvements)
Version 13.0: Nov. 2023 (with major improvements)

Edited by: Lina Kjellqvist, Thermo-Calc Software AB, Stockholm, Sweden.

Revision info: \$Rev: 15284 \$

Revision date: \$Date: 2023-11-10 12:45:37 +0000 (Fri, 10 Nov 2023) \$

TDB_TCOX13: Hit RETURN to continue

TDB_TCOX13: @@ Define the system by giving the elements.

TDB_TCOX13:

TDB_TCOX13: d-sys Fe o mn si cr al

... the command in full is DEFINE_SYSTEM

FE	O	MN
SI	CR	AL

DEFINED

TDB_TCOX13: @@ 'GET' reads thermodynamic data from the database files to the

TDB_TCOX13: @@ program

TDB_TCOX13: get

... the command in full is GET_DATA

08:47:27,739 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set IONIC_LIQ#2

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set IONIC_LIQ#3

... the command in full is AMEND_PHASE_DESCRIPTION

AL+3 IN ALPO4_S1:I SUBLATTICE 1 REJECTED

FE+3 IN ALPO4_S1:I SUBLATTICE 1 REJECTED

MN+3 IN ALPO4_S1:I SUBLATTICE 1 REJECTED

AL+3 IN ALPO4_S2:I SUBLATTICE 1 REJECTED

AL+3 IN ALPO4_S3:I SUBLATTICE 1 REJECTED

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

FE+2 IN CORUNDUM:I SUBLATTICE 1 REJECTED

MN+2 IN CORUNDUM:I SUBLATTICE 1 REJECTED

VA IN CORUNDUM:I SUBLATTICE 1 REJECTED

... the command in full is AMEND_PHASE_DESCRIPTION

AL+3 IN CRISTOBALITE:I SUBLATTICE 1 REJECTED

... the command in full is AMEND_PHASE_DESCRIPTION

AL+3 IN GARNET:I SUBLATTICE 3 REJECTED

CR+3 IN GARNET:I SUBLATTICE 3 REJECTED

FE+3 IN GARNET:I SUBLATTICE 3 REJECTED

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

MN+4 IN NIMNO3:I SUBLATTICE 1 REJECTED

AL+3 IN QUARTZ:I SUBLATTICE 1 REJECTED

... the command in full is AMEND_PHASE_DESCRIPTION

AL+3 IN TRIDYMITE:I SUBLATTICE 1 REJECTED

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_TCOX13: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ There are many commands in the POLY-3 module

POLY: ?

... the command in full is HELP

ADD_INITIAL_EQUILIBRIUM	GOTO_MODULE	REINITIATE_MODULE

ADVANCED_OPTIONS	HELP	SAVE_WORKSPACES

AMEND_STORED_EQUILIBRIA	INFORMATION	SELECT_EQUILIBRIUM

BACK	LIST_AXIS_VARIABLE	SET_ALL_START_VALUES

CHANGE_STATUS	LIST_CONDITIONS	SET_AXIS_VARIABLE

COMPUTE_EQUILIBRIUM	LIST_EQUILIBRIUM	SET_CONDITION

COMPUTE_TRANSITION	LIST_INITIAL_EQUILIBRIA	SET_INPUT_AMOUNTS

CREATE_NEW_EQUILIBRIUM	LIST_STATUS	SET_INTERACTIVE

DEFINE_COMPONENTS	LIST_SYMBOLS	SET_NUMERICAL_LIMITS

DEFINE_DIAGRAM	LOAD_INITIAL_EQUILIBRIUM	SET_REFERENCE_STATE

DEFINE_MATERIAL	MACRO_FILE_OPEN	SET_START_CONSTITUITION

DELETE_INITIAL_EQUILIB	MAKE_COMPONENT_ENTERED	SET_START_VALUE

DELETE_SYMBOL	MAKE_COMPONENT_SUSPENDED	SHOW_VALUE

ENTER_SYMBOL	MAP	STEP_WITH_OPTIONS

```

EVALUATE_FUNCTIONS      POST                TABULATE
EXIT                    READ_WORKSPACES
POLY:Hit RETURN to continue
POLY: @@ Some basic information is given by the INFORMATION command
POLY: @@ Look at TCEX-01 for more details.
POLY: info
... the command in full is INFORMATION
FILE SYSTEM ERROR      37
*** ERROR 1717 IN MOPEN: FILE DOES NOT EXIST: c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\help\poly3.hlp
POLY: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM GOTO_MODULE          REINITIATE_MODULE
ADVANCED_OPTIONS        HELP                 SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA INFORMATION          SELECT_EQUILIBRIUM
BACK                   LIST_AXIS_VARIABLE    SET_ALL_START_VALUES
CHANGE_STATUS          LIST_CONDITIONS       SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM    LIST_EQUILIBRIUM    SET_CONDITION
COMPUTE_TRANSITION     LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_STATUS         SET_INTERACTIVE
DEFINE_COMPONENTS      LIST_SYMBOLS        SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM         LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
DEFINE_MATERIAL        MACRO_FILE_OPEN       SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB MAKE_COMPONENT_ENTERED SET_START_VALUE
DELETE_SYMBOL          MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL          MAP                 STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS    POST                TABULATE
EXIT                  READ_WORKSPACES
POLY:
POLY:Hit RETURN to continue
POLY: @@ Now set the conditions i.e. the temperature, pressure and
POLY: @@ composition. We are interested in the situation at the
POLY: @@ outflow of steel
POLY:
POLY: s-c t=1800,p=101325,n=1
... the command in full is SET_CONDITION
POLY: @@ As conditions you can specify that the steel should have
POLY: @@ 18 weight percent of Cr, 0.1 w/o Mn and 0.4 w/o Si
POLY: @@ (Note that the overall amount of Cr and Mn is not specified).
POLY:
POLY: s-c w(mn)=.001,w(cr)=.18,w(si)=.004
... the command in full is SET_CONDITION
POLY: @@ The amount of Al is very small, assume 4 ppm
POLY: s-c w(al)=4e-6
... the command in full is SET_CONDITION
POLY: @@ We will later assume that the oxygen potential is determined
POLY: @@ by the equilibrium with liquid slag but initially we assume
POLY: @@ there is 50 ppm O
POLY:
POLY: s-c w(o)=5e-5
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=4E-6,
W(O)=5E-5
DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ Check what phases there are
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE	STATUS	DRIVING FORCE	MOLES
ZRTIO4_BETA	ENTERED	0.000000E+00	0.000000E+00
ZRO2_TETR	ENTERED	0.000000E+00	0.000000E+00
ZRO2_MONO	ENTERED	0.000000E+00	0.000000E+00
WOLLASTONITE	ENTERED	0.000000E+00	0.000000E+00
V3O5_HT	ENTERED	0.000000E+00	0.000000E+00
TRIDYMIT	ENTERED	0.000000E+00	0.000000E+00
SPINEL	ENTERED	0.000000E+00	0.000000E+00
SILLIMANITE	ENTERED	0.000000E+00	0.000000E+00
RUTILE	ENTERED	0.000000E+00	0.000000E+00
RHODONITE	ENTERED	0.000000E+00	0.000000E+00
QUARTZ	ENTERED	0.000000E+00	0.000000E+00
PSEUDO_BROOKITE	ENTERED	0.000000E+00	0.000000E+00
PROTO_PYROXENE	ENTERED	0.000000E+00	0.000000E+00
ORTHO_PYROXENE	ENTERED	0.000000E+00	0.000000E+00
OLIVINE	ENTERED	0.000000E+00	0.000000E+00
NIMNO3	ENTERED	0.000000E+00	0.000000E+00
NAFEO2_G	ENTERED	0.000000E+00	0.000000E+00
NAFEO2_B	ENTERED	0.000000E+00	0.000000E+00
NAALO2_D	ENTERED	0.000000E+00	0.000000E+00
MULLITE	ENTERED	0.000000E+00	0.000000E+00
MALINKOITE	ENTERED	0.000000E+00	0.000000E+00
M4O7	ENTERED	0.000000E+00	0.000000E+00
M2O3H	ENTERED	0.000000E+00	0.000000E+00
M2O3C	ENTERED	0.000000E+00	0.000000E+00
M2O3B	ENTERED	0.000000E+00	0.000000E+00
KYANITE	ENTERED	0.000000E+00	0.000000E+00
KAPPA_E21	ENTERED	0.000000E+00	0.000000E+00
K2MGSI04_LT	ENTERED	0.000000E+00	0.000000E+00
K2MGSI04_HT	ENTERED	0.000000E+00	0.000000E+00
HCP_A3	ENTERED	0.000000E+00	0.000000E+00
HALITE	ENTERED	0.000000E+00	0.000000E+00
GARNET	ENTERED	0.000000E+00	0.000000E+00
FLUORITE	ENTERED	0.000000E+00	0.000000E+00
FE4N_LP1	ENTERED	0.000000E+00	0.000000E+00
FCC_A1	ENTERED	0.000000E+00	0.000000E+00
DIAMOND_FCC_A4	ENTERED	0.000000E+00	0.000000E+00
DHCP	ENTERED	0.000000E+00	0.000000E+00
CUB_A13	ENTERED	0.000000E+00	0.000000E+00
CRNBO4	ENTERED	0.000000E+00	0.000000E+00
CRISTOBALITE	ENTERED	0.000000E+00	0.000000E+00
CORUNDUM	ENTERED	0.000000E+00	0.000000E+00
CORDIERITE	ENTERED	0.000000E+00	0.000000E+00
COLUMBITE	ENTERED	0.000000E+00	0.000000E+00
CLINO_PYROXENE	ENTERED	0.000000E+00	0.000000E+00
CBCC_A12	ENTERED	0.000000E+00	0.000000E+00
CARNEGIEITE_B	ENTERED	0.000000E+00	0.000000E+00
CARNEGIEITE_A	ENTERED	0.000000E+00	0.000000E+00
CAF2_S2	ENTERED	0.000000E+00	0.000000E+00
CAF2_S1	ENTERED	0.000000E+00	0.000000E+00
BCC_A2	ENTERED	0.000000E+00	0.000000E+00
ANDALUSITE	ENTERED	0.000000E+00	0.000000E+00
ALPO4_S3	ENTERED	0.000000E+00	0.000000E+00
ALPO4_S2	ENTERED	0.000000E+00	0.000000E+00

```

ALPO4_S1          ENTERED      0.000000E+00   0.000000E+00
ALPHA_SPINEL      ENTERED      0.000000E+00   0.000000E+00
AF                ENTERED      0.000000E+00   0.000000E+00
IONIC_LIQ#3       ENTERED      0.000000E+00   0.000000E+00
IONIC_LIQ#2       ENTERED      0.000000E+00   0.000000E+00
IONIC_LIQ#1       ENTERED      0.000000E+00   0.000000E+00
GAS               ENTERED      0.000000E+00   0.000000E+00
POLY: @@ Start by assuming all other phases except Metallic liquid are suspended
POLY: @@ In TCOX13 the liquid metal and Liquid slag(s) are modelled as the same phase
POLY: @@ IONIC LIQ, were miscibility gap(s) are separating the Liquid Metal
POLY: @@ and Liquid slag(s). By default IONIC_LIQ#1 is Liquid metals and
POLY: @@ IONIC_LIQ#2... are liquid slag(s).
POLY: @@ In order to secure that only Liquid metal is stable in the calculation
POLY: @@ we first need to turn Global minimization off.
POLY: advance glob n n
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY:
POLY: ch-st p *=sus
... the command in full is CHANGE_STATUS
POLY: ch-st p Ionic_Liq#1=ent 0
... the command in full is CHANGE_STATUS
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=4E-6,
W(O)=5E-5
DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ The degree of freedom is zero and we can make a calculation.
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
*** ERROR 1611 IN QTHISS: TOO MANY ITERATIONS
Give the command INFO TROUBLE for help
POLY:
POLY: @@ The calculation failed and
POLY: @@ we need to change the start values for the phase in order
POLY: @@ to find equilibrium.
POLY: @@ The metallic elements can be set as the alloy composition and the
POLY: @@ Oxide constituents should be low (Log amount of slag formers).
POLY: s-a-s n
... the command in full is SET_ALL_START_VALUES
Should IONIC_LIQ#1 be stable? /N/: y
Major constituent(s) /*/: Fe
No such constituent
Y(IONIC_LIQ#1,AL+3) /1/: 8e-6
Y(IONIC_LIQ#1,CR+2) /1/: .18
Y(IONIC_LIQ#1,FE+2) /1/: .8
Y(IONIC_LIQ#1,MN+2) /1/: 4e-3
Y(IONIC_LIQ#1,SI+4) /1/: 4e-3
Y(IONIC_LIQ#1,ALO2-1#2) /1/: 1e-8
Y(IONIC_LIQ#1,O-2#2) /1/: 5e-5
Y(IONIC_LIQ#1,SIO4-4#2) /1/: 1e-8
Y(IONIC_LIQ#1,VA#2) /1/: .99
Y(IONIC_LIQ#1,CRO3/2#2) /1/: 1e-8
Y(IONIC_LIQ#1,FE03/2#2) /1/: 1e-8
Y(IONIC_LIQ#1,MNO3/2#2) /1/: 1e-8
Y(IONIC_LIQ#1,SIO2#2) /1/: 1e-8
POLY:
POLY: @@ Now we can calculate equilibrium again
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
16 ITS, CPU TIME USED 0 SECONDS
POLY:
POLY: @@ Now set the suspended phases as dormant and keep Metalic liquid entered.
POLY:
POLY: c-st p *s=d
... the command in full is CHANGE_STATUS
POLY:
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
18 ITS, CPU TIME USED 2 SECONDS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE	STATUS	DRIVING FORCE	MOLES
IONIC_LIQ#1	ENTERED	0.000000E+00	1.000000E+00
PSEUDO_BROOKITE	DORMANT	3.415359E+00	
MULLITE	DORMANT	2.482896E+00	
SPINEL	DORMANT	9.316834E-02	
M2O3C	DORMANT	-1.836644E-01	
CORUNDUM	DORMANT	-1.898450E-01	
SILLIMANITE	DORMANT	-3.123170E-01	
ANDALUSITE	DORMANT	-3.305096E-01	
KYANITE	DORMANT	-4.137814E-01	
M2O3B	DORMANT	-4.219409E-01	
FE4N_LP1	DORMANT	-4.256096E-01	
CUB_A13	DORMANT	-4.655151E-01	
IONIC_LIQ#3	DORMANT	-4.736338E-01	
IONIC_LIQ#2	DORMANT	-4.736338E-01	
DORMANT PHASES WITH DRIVING FORCE LESS THAN		-5.348030E-01	
CORIERITE CBCC A12 HALITE CRISTOBALITE TRIDYMITTE GARNET QUARTZ ALPHA SPINEL			
CARNEGIEITE_B CARNEGIEITE_A K2MGSIO4 LT K2MGSIO4_HT MALINKOITE CRNB04			
PROTO_PYROXENE OLIVINE NAALO2_D RHODONITE WOLLASTONITE NAFEO2_G NAFEO2_B			
ZRTIO4 BETA HCP A3 ALPO4_S3 ALPO4_S2 FCC_A1 ALPO4_S1 FLUORITE ORTHO_PYROXENE			
CLINO_PYROXENE V3O5_HT ZRO2 TETR ZRO2 MONO AF RUTILE M4O7 KAPPA_E21 BCC_A2			
COLUMBITE CAF2_S2 CAF2_S1 NIMNO3 M2O3H GAS DIAMOND_FCC_A4 DHCP			

```

POLY:Hit RETURN to continue
POLY: @@ If the stable phases do not change in 12 iterations the program
POLY: @@ terminates even if the program has not calculated the correct
POLY: @@ driving forces for the metastable phases.
POLY: @@ You can change this with the command SET-NUMERICAL-LIMITS
POLY: @@ Use this command to change the lowest value of a fraction variable.
POLY:
POLY: s-n-l 500 1E-6 1E-12 n
... the command in full is SET_NUMERICAL_LIMITS
LIMITATIONS of the present version of Thermo-Calc
Max number of elements      : 80
Max number of species       : 5000
Max number of sublattices in a phase : 10

```

```

Max number of constituents in a phase:      : 200
Max number of constituents in an ideal phase :5000
POLY:Hit RETURN to continue
POLY: @@ Calculate again
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
65 ITS, CPU TIME USED 0 SECONDS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS    DRIVING FORCE    MOLES
IONIC_LIQ#1     ENTERED    0.000000E+00    1.000000E+00
BCC_A2          DORMANT    -6.736046E-03
CORUNDUM        DORMANT    -1.202849E-02
FCC_A1          DORMANT    -3.396264E-02
SPINEL          DORMANT    -1.086331E-01
MULLITE         DORMANT    -1.351453E-01
IONIC_LIQ#3     DORMANT    -1.974908E-01
IONIC_LIQ#2     DORMANT    -1.974908E-01
HCP_A3          DORMANT    -3.040706E-01
SILLIMANITE     DORMANT    -3.123170E-01
ANDALUSITE      DORMANT    -3.305096E-01
DORMANT PHASES WITH DRIVING FORCE LESS THAN -3.633275E-01
CUB_A13 PSEUDO BROOKITE KYANITE CBCC_A12 M2O3C FE4N_LP1 M2O3B CORDIERITE
ALPHA_SPINEL HALITE CRISTOBALITE TRIDYMIT GARNET QUARTZ CARNEGIEITE B
CARNEGIEITE A K2MGSIO4 LT K2MGSIO4 HT MALINKOITE CRNBO4 PROTO PYROXENE
OLIVINE NAAIO2_D RHODONITE WOLLASTONITE NAFEO2_G NAFEO2_B ZRTIO4 BETA
FLUORITE ZRO2_TETR ALPO4_S3 ALPO4_S2 ALPO4_S1 ORTHO PYROXENE CLINO PYROXENE
V3O5_HT RUTILE ZRO2_MONO_AF M4O7 KAPPA_E21 COLUMBITE CAF2_S2 CAF2_S1 NIMNO3
M2O3H GAS DIAMOND FCC_A4 DHCP O
POLY:Hit RETURN to continue
POLY: @@ The driving forces are quite stable.
POLY: @@ Now set the slag phase to stable and let the program
POLY: @@ adjust the amount of oxygen to make it stable
POLY:
POLY: c-st p Ionic_Liq#2=fix 0
... the command in full is CHANGE_STATUS
POLY: s-c w(o)
... the command in full is SET_CONDITION
Value /5.000000273E-05/: none
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=4E-6
FIXED PHASES
IONIC_LIQ#2=0
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
12 ITS, CPU TIME USED 1 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCOX13

Conditions:
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=4E-6
FIXED PHASES
IONIC_LIQ#2=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.48875E+01
Total Gibbs energy -1.12448E+05, Enthalpy 6.88237E+04, Volume 8.01468E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
AL              8.1369E-06  4.0000E-06  3.0008E-10 -3.2816E+05 SER
CR              1.9001E-01  1.8000E-01  4.9679E-04 -1.1385E+05 SER
FE              8.0092E-01  8.1493E-01  6.2391E-04 -1.1044E+05 SER
MN              9.9908E-04  1.0000E-03  3.3922E-07 -2.2294E+05 SER
O               2.4114E-04  7.0288E-05  3.5414E-13 -4.2907E+05 SER
SI              7.8173E-03  4.0000E-03  2.9075E-08 -2.5971E+05 SER

IONIC_LIQ#1     Status ENTERED    Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4887E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 8.14926E-01 SI 4.00000E-03 O 7.02882E-05
CR 1.80000E-01 MN 1.00000E-03 AL 4.00000E-06

IONIC_LIQ#2     Status FIXED    Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.30413E-01 CR 1.16242E-01 MN 3.20913E-02
AL 3.14573E-01 SI 8.52728E-02 FE 2.14072E-02

CORUNDUM        Status DORMANT    Driving force 1.7609E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
AL 4.90617E-01 CR 4.99519E-02 MN 9.56016E-07
O 4.59425E-01 FE 4.88863E-06 SI 0.00000E+00

MULLITE         Status DORMANT    Driving force 5.8222E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.82648E-01 SI 1.12314E-01 FE 1.07093E-07
AL 3.92032E-01 CR 1.30057E-02 MN 0.00000E+00

SPINEL          Status DORMANT    Driving force 7.9096E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
AL 4.83690E-01 CR 4.50640E-02 MN 6.67611E-03
O 4.55474E-01 FE 9.09583E-03 SI 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ List the status of the phases.
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS    DRIVING FORCE    MOLES
IONIC_LIQ#2     FIXED      0.000000E+00    0.000000E+00
IONIC_LIQ#1     ENTERED    0.000000E+00    1.000000E+00
CORUNDUM        DORMANT    1.760860E-01
SPINEL          DORMANT    7.909554E-02
MULLITE         DORMANT    5.822201E-02
IONIC_LIQ#3     DORMANT    -7.293661E-15
BCC_A2          DORMANT    -6.798103E-03
FCC_A1          DORMANT    -3.401624E-02
SILLIMANITE     DORMANT    -1.161407E-01
ANDALUSITE      DORMANT    -1.343334E-01
PSEUDO_BROOKITE DORMANT    -2.127232E-01
KYANITE          DORMANT    -2.176052E-01

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M2O3C          DORMANT      -2.304962E-01
M2O3B          DORMANT      -3.009092E-01
HCP_A3         DORMANT      -3.041529E-01
DORMANT PHASES WITH DRIVING FORCE LESS THAN -3.398449E-01
CORDIERITE CUB_A13 CBCC_A12 FE4N_LP1 HALITE ALPHA_SPINEL CRISTOBALITE
TRIDYMITITE QUARTZ GARNET CARNEGIEITE_B CARNEGIEITE_A K2MGSIO4_LT K2MGSIO4_HT
MALINKOITE CRNB04 PROTO_PYROXENE OLIVINE_NAALO2_D RHODONITE WOLLASTONITE
NAFEO2_G NAFEO2_B ZRTIO4_BETA FLUORITE ZRO2_TETR ALPO4_S3 ALPO4_S2 ALPO4_S1
ORTHO_PYROXENE CLINO_PYROXENE V3O5_HT RUTILE ZRO2_MONO_AF M4O7_KAPPA_E21
COLUMBITE CAF2_S2 CAF2_S1 NIMNO3 M2O3H GAS DIAMOND_FCC_A4 DHCP_K
POLY:Hit RETURN to continue
POLY: @@ Note that mullite, corundum and spinel are stable.
POLY: @@ All Al-rich oxides.
POLY: @@ The amount of Al is probably too high, set it
POLY: @@ to 1/4 of the initial value
POLY:
POLY: s-c w(al)=1e-6
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
42 ITS, CPU TIME USED 1 SECONDS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
IONIC_LIQ#2     FIXED        0.000000E+00      0.000000E+00
IONIC_LIQ#1     ENTERED       0.000000E+00      1.000000E+00
IONIC_LIQ#3     DORMANT        1.683761E-14
BCC_A2          DORMANT        -6.924146E-03
FCC_A1          DORMANT        -3.412641E-02
CORUNDUM        DORMANT        -3.485769E-02
SPINEL          DORMANT        -5.836783E-02
MULLITE         DORMANT        -6.498640E-02
SILLIMANITE     DORMANT        -1.986305E-01
ANDALUSITE      DORMANT        -2.168231E-01
CRISTOBALITE    DORMANT        -2.555783E-01
TRIDYMITITE     DORMANT        -2.559763E-01
CORDIERITE      DORMANT        -2.684734E-01
DORMANT PHASES WITH DRIVING FORCE LESS THAN -2.787991E-01
QUARTZ_PSEUDO Brookite Kyanite HCP_A3 CARNEGIEITE_B CARNEGIEITE_A CUB_A13
K2MGSIO4_LT M2O3C HALITE K2MGSIO4_HT MALINKOITE CBCC_A12 FE4N_LP1 GARNET
ALPHA_SPINEL CRNB04 PROTO_PYROXENE_NAALO2_D OLIVINE M2O3B RHODONITE
WOLLASTONITE NAFEO2_G NAFEO2_B ALPO4_S3 ALPO4_S2 ALPO4_S1 ORTHO_PYROXENE
CLINO_PYROXENE FLUORITE V3O5_HT ZRO2_TETR ZRTIO4_BETA ZRO2_MONO_AF RUTILE
M4O7_KAPPA_E21 COLUMBITE CAF2_S2 CAF2_S1 NIMNO3 M2O3H GAS DIAMOND_FCC_A4 DHCP_K
POLY: @@ Now the Al-oxide phases are not stable.
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0, database: TCOX13

Conditions:
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=1E-6
FIXED PHASES
IONIC_LIQ#2=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.48821E+01
Total Gibbs energy -1.12492E+05, Enthalpy 6.87930E+04, Volume 8.01449E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              2.0340E-06  1.0000E-06  7.4801E-11 -3.4895E+05 SER
CR              1.8999E-01  1.8000E-01  4.9646E-04 -1.1386E+05 SER
FE              8.0081E-01  8.1489E-01  6.2391E-04 -1.1044E+05 SER
MN              9.9898E-04  1.0000E-03  3.3903E-07 -2.2295E+05 SER
O               3.8382E-04  1.1189E-04  5.4091E-13 -4.2273E+05 SER
SI              7.8166E-03  4.0000E-03  2.9092E-08 -2.5970E+05 SER

IONIC_LIQ#1     Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4882E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 8.14887E-01 SI 4.00000E-03 O 1.11891E-04
CR 1.80000E-01 MN 1.00000E-03 AL 1.00000E-06

IONIC_LIQ#2     Status FIXED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.11908E-01 SI 1.75856E-01 MN 4.99086E-02
CR 2.01791E-01 AL 1.43088E-01 FE 1.74489E-02

IONIC_LIQ#3     Status DORMANT      Driving force 1.6838E-14
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.11908E-01 SI 1.75856E-01 MN 4.99086E-02
CR 2.01791E-01 AL 1.43088E-01 FE 1.74489E-02
POLY:Hit RETURN to continue
POLY: @@ We assume that this describes the situation at 18 w/o Cr. Some
POLY: @@ liquid slag that later will form mainly SiO2-Al2O3-MnO is present.
POLY: @@ Now increase the Cr-content to 25 w/o
POLY:
POLY: s-c w(cr)=.25
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
13 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0, database: TCOX13

Conditions:
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=1E-6
FIXED PHASES
IONIC_LIQ#2=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45982E+01
Total Gibbs energy -1.12536E+05, Enthalpy 6.82543E+04, Volume 8.03374E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              2.0235E-06  1.0000E-06  7.7144E-11 -3.4849E+05 SER
CR              2.6251E-01  2.5000E-01  6.9327E-04 -1.0886E+05 SER
FE              7.2819E-01  7.4484E-01  5.6596E-04 -1.1190E+05 SER
MN              9.9381E-04  1.0000E-03  3.6764E-07 -2.2174E+05 SER
O               5.2773E-04  1.5464E-04  5.1194E-13 -4.2355E+05 SER
SI              7.7761E-03  4.0000E-03  2.7195E-08 -2.6071E+05 SER

IONIC_LIQ#1     Status ENTERED      Driving force 0.0000E+00

```

```

Moles 1.0000E+00, Mass 5.4598E+01, Volume fraction 1.0000E+00  Mass fractions:
FE 7.44844E-01  SI 4.00000E-03  O 1.54642E-04
CR 2.50000E-01  MN 1.00000E-03  AL 1.00000E-06

IONIC_LIQ#2                      Status FIXED          Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
O 3.82867E-01  SI 1.45007E-01  MN 4.34163E-02
CR 2.93640E-01  AL 1.17878E-01  FE 1.71911E-02

CORUNDUM                      Status DORMANT          Driving force 1.8256E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
CR 5.32252E-01  AL 1.17487E-01  MN 3.45291E-06
O 3.50186E-01  FE 7.11812E-05  SI 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Now Cr2O3 (CORUNDUM) would like to be stable. The simplest correction is to modify
POLY: @@ the composition of the steel in order to decrease the oxygen potential.
POLY: @@ For example the Mn or Si content could be changed.
POLY: @@ In order to determine which of these has the largest influence
POLY: @@ on the oxygen potential, calculate this by the partial derivative
POLY: @@ of the oxygen activity w.r.t. the Mn and Si content.
POLY:
POLY: s-ref-s o gas
... the command in full is SET_REFERENCE_STATE
Temperature */:
Pressure /1E5/:
POLY: show acr(o)
... the command in full is SHOW_VALUE
ACR(O)=7.4486595E-7
POLY: show acr(o).w(mn)
... the command in full is SHOW_VALUE
ACR(O).W(MN)=-2.3897642E-5
POLY: show acr(o).w(si)
... the command in full is SHOW_VALUE
ACR(O).W(SI)=-4.635574E-5
POLY:
POLY: @@ The value is largest for Si and thus the smallest change is necessary
POLY: @@ for that. Instead of modifying this content in steps one may
POLY: @@ specify that the Cr2O3 phase should be on its limit of stability, i.e.
POLY: @@ use the command FIX with zero amount and calculate the change
POLY: @@ in composition.
POLY:Hit RETURN to continue
POLY:
POLY: c-s p CORUNDUM=fix 0
... the command in full is CHANGE_STATUS
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=1E-6
FIXED PHASES
IONIC_LIQ#2=0 CORUNDUM=0
DEGREES OF FREEDOM -1
POLY: s-c w(si)=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
9 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCOX13

Conditions:
T=1800, P=101325, N=1, W(MN)=1E-3, W(CR)=0.25, W(AL)=1E-6
FIXED PHASES
IONIC_LIQ#2=0 CORUNDUM=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45711E+01
Total Gibbs energy -1.12681E+05, Enthalpy 6.81427E+04, Volume 8.03708E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
AL              2.0225E-06  1.0000E-06  7.7895E-11 -3.4835E+05 SER
CR              2.6238E-01  2.5000E-01  6.9253E-04 -1.0888E+05 SER
FE              7.2732E-01  7.4432E-01  5.6530E-04 -1.1192E+05 SER
MN              9.9332E-04  1.0000E-03  3.6500E-07 -2.2185E+05 SER
O              5.0666E-04  1.4854E-04  7.2150E-07 -2.1165E+05 GAS
SI              8.8002E-03  4.5290E-03  3.1239E-08 -2.5864E+05 SER

IONIC_LIQ#1                      Status ENTERED          Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4571E+01, Volume fraction 1.0000E+00  Mass fractions:
FE 7.44321E-01  SI 4.52903E-03  O 1.48541E-04
CR 2.50000E-01  MN 1.00000E-03  AL 1.00000E-06

IONIC_LIQ#2                      Status FIXED          Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
O 3.87656E-01  SI 1.53760E-01  MN 4.27058E-02
CR 2.82387E-01  AL 1.17141E-01  FE 1.63509E-02

IONIC_LIQ#3                      Status DORMANT          Driving force 7.3342E-15
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
O 3.87656E-01  SI 1.53760E-01  MN 4.27058E-02
CR 2.82387E-01  AL 1.17141E-01  FE 1.63509E-02

CORUNDUM                      Status FIXED          Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
CR 5.29411E-01  AL 1.19685E-01  MN 3.43000E-06
O 3.50830E-01  FE 7.09236E-05  SI 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ We can read the new Si content from this list but also
POLY: @@ directly show the value of a variable
POLY: sh w(si)
... the command in full is SHOW_VALUE
W(SI)=4.5290293E-3
POLY: @@ Increase the Si content to 0.46 w/o to avoid forming Cr2O3.
POLY: @@ Calculate also how much the Mn content must be changed
POLY: s-c w(si)=.0046
... the command in full is SET_CONDITION
POLY: s-c w(mn)=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
9 ITS, CPU TIME USED 0 SECONDS
POLY: sh w(mn)

```

```

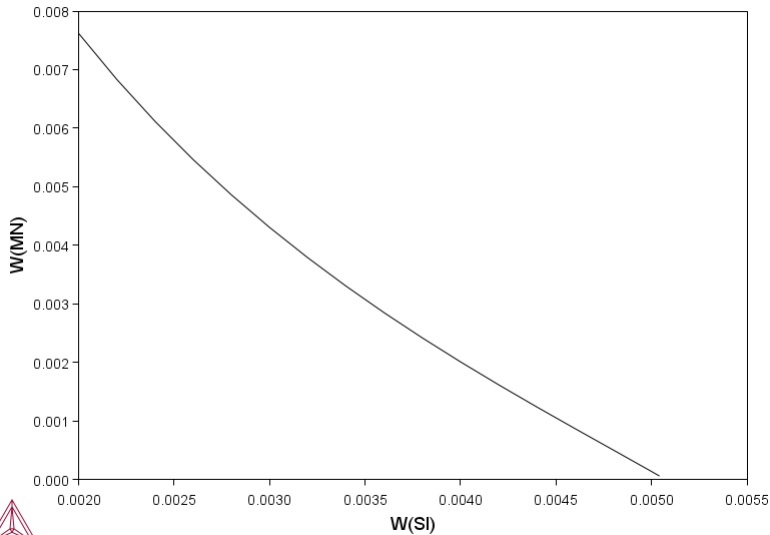
... the command in full is SHOW_VALUE
W(MN)=8.6971545E-4
POLY: @@ Check with Si content equal to .3. It should be consistent with
POLY: @@ the plot below, i.e. Mn content increase with decreasing Si content.
POLY: s-c w(si)=.003
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
16 ITS, CPU TIME USED 1 SECONDS
POLY: sh w(mn)
... the command in full is SHOW_VALUE
W(MN)=4.3046217E-3
POLY:Hit RETURN to continue
POLY: @@ Plot how the Mn content varies when the Si content
POLY: @@ varies between 0.2 and 1 w/o.
POLY: s-a-v 1 w(si) 0.002 .01 0.0002
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex10 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.300000E-02
POLY has calculated initial equilibrium

Phase Region from 0.300000E-02 for:
IONIC_LIQ#1
IONIC_LIQ#2
CORUNDUM
QBSMER trying to find equilibrium at 5.0800000E-03
QBSMER trying to find equilibrium at 5.0800000E-03
QBSMER: Second global calculation
Calculated 14 equilibria
Sorry cannot continue 1717 55 1 5.0400000E-03

Phase Region from 0.300000E-02 for:
IONIC_LIQ#1
IONIC_LIQ#2
CORUNDUM
Terminating at 0.200000E-02
Calculated 8 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex10\tcex10.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w(si)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(mn)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 10a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 10a

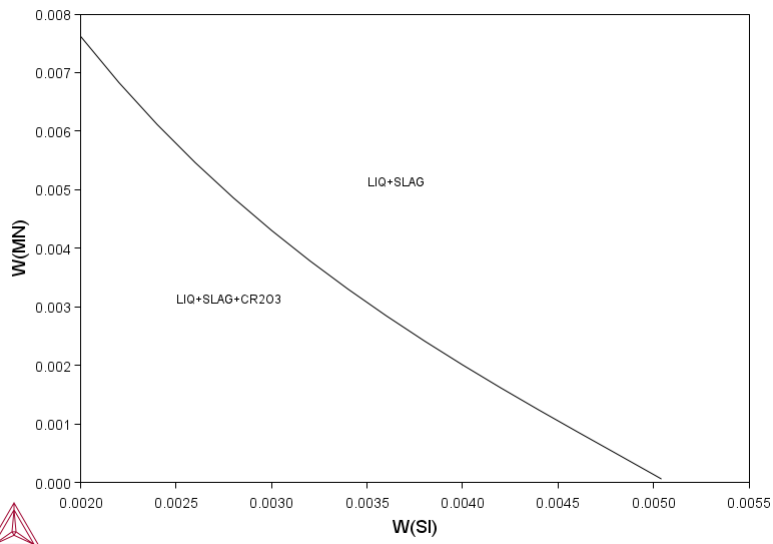


```

POST:Hit RETURN to continue
POST: add .0025 .003 n
... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG+CR2O3
Text size: /.36/:
POST: add .0035 .005 n
... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG
Text size: /.36/:
POST: set-title example 10b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 10b



```
POST:
POST:
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```


tcex11

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex11\tcex11.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Oxidation of Cu2S with an H2O/O2 gas mixture

SYS:

SYS: @@ This example demonstrates the oxidation of Cu2S

SYS: @@ with an H2O/O2 gas mixture. Thermo-Calc is used to find

SYS: @@ the optimum O/H ratio (i.e. oxygen potential) as certain

SYS: @@ oxygen potential values can desulphurize Cu2S without

SYS: @@ forming copper oxides.

SYS:

SYS: @@ In Thermo-Calc, the problem reduces to perform equilibria

SYS: @@ calculations in a Cu-S-H-O system. The amounts of the

SYS: @@ components should be kept to correct ratio corresponding

SYS: @@ to Cu2S and H2O using a command SET_INPUT_AMOUNTS in POLY3.

SYS:

SYS: @@ Initially, O/H = 0.5 is given. Optimum O/H ratio is

SYS: @@ calculated with the desired calculation conditions. For

SYS: @@ example, to simulate one phase disappearing, you can FIX

SYS: @@ the phase with zero amount.

SYS:

SYS: set-log ex11,,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw

... the command in full is SWITCH_DATABASE
Use one of these databases

TCFE11 = Steels/Fe-Alloys v11.0
TCFE9 = Steels/Fe-Alloys v9.3
SSOL7 = SGTE Alloy Solutions v7.0
SSOL6 = SGTE Alloy Solutions v6.0
SSUB6 = SGTE Substances v6.0
TCOX13 = Metal Oxide Solutions v13.0
TCOX12 = Metal Oxide Solutions v12.0
TCOX11 = Metal Oxide Solutions v11.1
FEDEMO = Iron Demo Database v6.0
ALDEMO = Aluminum Demo Database v5.0
OXDEMO = Oxide Demo Database v6.0
SUBDEMO = Substance Demo Database v1.0
PAQ2 = Public Aqueous Solution (SIT) v2.5
PG35 = PG35 Binary Semi-Conductors v1.3
MALDEMO = Al-Alloys Mobility demo database v3.0
USER = User defined Database

DATABASE NAME /TCFE11/: user tcex11.tdb

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

08:48:42,338 [Thread-0] INFO TDBFileParser: USER_386616156_21, number of lines read: 547

08:48:42,759 [Thread-0] INFO DatabaseUtils: Parsing of USER_386616156_21 completed in 493 ms

TDB_USER: def-sys cu s o h

... the command in full is DEFINE_SYSTEM

CU S O

H DEFINED

TDB_USER: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:

GAS:G :CU CU1H1 CU1H1O1 CU1O1 CU1S1 CU2 CU2S1 H H1O1 H1O1S1_HSO
H1O1S1_SOH H1O2 H1S1 H2 H2O1 H2O1S1_H2SO H2O1S1_HSOH H2O2 H2O4S1 H2S1 H2S2
O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8:
CU_S :CU:
CU2O_S :CU2O1:
CU2O_L :CU2O1:
CU2S_S1 :CU2S1:
CU2S04 :CU2O4S1:
CU2S05 :CU2O5S1:
CU2S_L :CU2S1:
CU2S_S2 :CU2S1:
CU2S_S3 :CU2S1:
CUO :CU1O1:
CUS_S :CU1S1:
CUS04 :CU1O4S1:
CU_L :CU:
H2O2_L :H2O2:
H2O_L :H2O1:
H2S04_L :H2O4S1:
SS :S:
S_L :S:
S_S2 :S:

TDB_USER:Hit RETURN to continue

TDB_USER: get

... the command in full is GET_DATA

08:48:43,052 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_USER: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: ?

... the command in full is HELP

ADD_INITIAL_EQUILIBRIUM	GOTO_MODULE	REINITIATE_MODULE
ADVANCED_OPTIONS	HELP	SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA	INFORMATION	SELECT_EQUILIBRIUM
BACK	LIST_AXIS_VARIABLE	SET_ALL_START_VALUES
CHANGE_STATUS	LIST_CONDITIONS	SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM	LIST_EQUILIBRIUM	SET_CONDITION
COMPUTE_TRANSITION	LIST_INITIAL_EQUILIBRIA	SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM	LIST_STATUS	SET_INTERACTIVE
DEFINE_COMPONENTS	LIST_SYMBOLS	SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM	LOAD_INITIAL_EQUILIBRIUM	SET_REFERENCE_STATE
DEFINE_MATERIAL	MACRO_FILE_OPEN	SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB	MAKE_COMPONENT_ENTERED	SET_START_VALUE
DELETE_SYMBOL	MAKE_COMPONENT_SUSPENDED	SHOW_VALUE
ENTER_SYMBOL	MAP	STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS	POST	TABULATE
EXIT	READ_WORKSPACES	

POLY: li-st

... the command in full is LIST_STATUS

Option /CPS/:

COMPONENT	STATUS	REF. STATE	T (K)	P (Pa)
VA	ENTERED	SER		
CU	ENTERED	SER		
H	ENTERED	SER		
O	ENTERED	SER		
S	ENTERED	SER		

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
S_S2	ENTERED	0.000000E+00	0.000000E+00
S_L	ENTERED	0.000000E+00	0.000000E+00
SS	ENTERED	0.000000E+00	0.000000E+00
H2SO4_L	ENTERED	0.000000E+00	0.000000E+00
H2O_L	ENTERED	0.000000E+00	0.000000E+00
H2O2_L	ENTERED	0.000000E+00	0.000000E+00
CU_S	ENTERED	0.000000E+00	0.000000E+00
CU_L	ENTERED	0.000000E+00	0.000000E+00
CUS_S	ENTERED	0.000000E+00	0.000000E+00
CUSO4	ENTERED	0.000000E+00	0.000000E+00
CUO	ENTERED	0.000000E+00	0.000000E+00
CU2S_S3	ENTERED	0.000000E+00	0.000000E+00
CU2S_S2	ENTERED	0.000000E+00	0.000000E+00
CU2S_S1	ENTERED	0.000000E+00	0.000000E+00
CU2S_L	ENTERED	0.000000E+00	0.000000E+00
CU2SO5	ENTERED	0.000000E+00	0.000000E+00
CU2SO4	ENTERED	0.000000E+00	0.000000E+00
CU2O_S	ENTERED	0.000000E+00	0.000000E+00
CU2O_L	ENTERED	0.000000E+00	0.000000E+00
GAS	ENTERED	0.000000E+00	0.000000E+00

*** STATUS FOR ALL SPECIES

CU	ENTERED	H15O10.5S1	ENTERED	O	ENTERED
CU1H1	ENTERED	H1O1	ENTERED	O1S1	ENTERED
CU1H10O9S1	ENTERED	H1O1S1_HSO	ENTERED	O1S2	ENTERED
CU1H1O1	ENTERED	H1O1S1_SOH	ENTERED	O2	ENTERED
CU1H2O2	ENTERED	H1O2	ENTERED	O2S1	ENTERED
CU1H2O5S1	ENTERED	H1S1	ENTERED	O3	ENTERED
CU1H6O7S1	ENTERED	H2	ENTERED	O3S1	ENTERED
CU1O1	ENTERED	H2O1	ENTERED	S	ENTERED
CU1O4S1	ENTERED	H2O1S1_H2SO	ENTERED	S2	ENTERED
CU1S1	ENTERED	H2O1S1_HSOH	ENTERED	S3	ENTERED
CU2	ENTERED	H2O2	ENTERED	S4	ENTERED
CU2O1	ENTERED	H2O4S1	ENTERED	S5	ENTERED
CU2O4S1	ENTERED	H2S1	ENTERED	S6	ENTERED
CU2O5S1	ENTERED	H2S2	ENTERED	S7	ENTERED
CU2S1	ENTERED	H4O5S1	ENTERED	S8	ENTERED
H	ENTERED	H6O6S1	ENTERED	VA	ENTERED
H10O8S1	ENTERED	H8O7S1	ENTERED		

POLY:

POLY:Hit RETURN to continue

POLY: @@ Assume initially that we have one mole of Cu2S and 50 moles water vapor

POLY: s-i-a n(cu2s1)=1,n(h2o1)=50

... the command in full is SET_INPUT_AMOUNTS

POLY: set-cond t=1400,p=101325

... the command in full is SET_CONDITION

POLY: l-c

... the command in full is LIST_CONDITIONS

N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=101325
DEGREES OF FREEDOM 0

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

08:48:43,811 [Thread-0] INFO Database: Preparing system for use: USER_386616156_21

08:48:45,151 [Thread-0] INFO Phase: Preparing phase for use: GAS

Using global minimization procedure

08:48:45,703 [Thread-0] INFO Phase: Preparing phase for use: CU2O_L

08:48:46,016 [Thread-0] INFO Phase: Preparing phase for use: CU2O_S

08:48:46,331 [Thread-0] INFO Phase: Preparing phase for use: CU2SO4

08:48:46,656 [Thread-0] INFO Phase: Preparing phase for use: CU2SO5

08:48:46,944 [Thread-0] INFO Phase: Preparing phase for use: CU2S_L

08:48:47,231 [Thread-0] INFO Phase: Preparing phase for use: CU2S_S1

08:48:47,534 [Thread-0] INFO Phase: Preparing phase for use: CU2S_S2

08:48:47,836 [Thread-0] INFO Phase: Preparing phase for use: CU2S_S3

08:48:48,186 [Thread-0] INFO Phase: Preparing phase for use: CUO

08:48:48,441 [Thread-0] INFO Phase: Preparing phase for use: CUSO4

08:48:48,702 [Thread-0] INFO Phase: Preparing phase for use: CUS_S

08:48:48,954 [Thread-0] INFO Phase: Preparing phase for use: CU_L

08:48:49,331 [Thread-0] INFO Phase: Preparing phase for use: CU_S

08:48:49,759 [Thread-0] INFO Phase: Preparing phase for use: H2O2_L

08:48:50,015 [Thread-0] INFO Phase: Preparing phase for use: H2O_L

08:48:50,252 [Thread-0] INFO Phase: Preparing phase for use: H2SO4_L

08:48:50,515 [Thread-0] INFO Phase: Preparing phase for use: SS

08:48:50,766 [Thread-0] INFO Phase: Preparing phase for use: S_L

08:48:51,015 [Thread-0] INFO Phase: Preparing phase for use: S_S2

Calculated 685 grid points in 5.597 s

Found the set of lowest grid points in 0.001 s

Calculated POLY solution 0.029 s, total time 5.627 s

POLY: l-e

```

... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0  , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=101325
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.53000E+02, Mass in grams 1.05989E+03
Total Gibbs energy -2.75931E+07, Enthalpy -9.82382E+06, Volume 5.76972E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CU              2.0000E+00  1.1991E-01 1.6098E-03 -7.4867E+04 SER
H              1.0000E+02  9.5095E-02 9.5714E-06 -1.3452E+05 SER
O              5.0000E+01  7.5475E-01 5.1729E-11 -2.7570E+05 SER
S              1.0000E+00  3.0248E-02 2.0746E-08 -2.0593E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.5022E+02, Mass 9.0794E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.81060E-01 H 1.11009E-01 S 7.92556E-03 CU 5.01241E-06
Constitution:
H2O1 9.86660E-01 CU1H1O1 1.96753E-08 CU1O1 8.58177E-12
H2 8.86811E-03 O3S1 1.43507E-08 H2O2 5.46461E-12
O2S1 4.44169E-03 H2O1S1_HSOH 7.52014E-09 H2O1S1_H2SO 3.12748E-12
H2S1 2.10471E-05 S 4.30477E-09 H2O4S1 3.10120E-12
O1S1 5.63051E-06 O2 2.46248E-09 S3 1.29650E-12
CU 1.32327E-06 H1O1S1_SOH 1.77241E-09 H1O2 4.13438E-13
H1O1 1.00104E-06 CU1S1 1.23642E-09 S4 3.25596E-18
H 4.55656E-07 CU2 4.47851E-10 S5 1.21560E-21
H1S1 3.40802E-07 CU2S1 2.11636E-10 O3 1.70006E-22
S2 1.38936E-07 H2S2 1.77731E-10 S6 5.54892E-27
CU1H1 8.04525E-08 O 4.66615E-11 S8 1.00000E-30
O1S2 2.49875E-08 H1O1S1_HSO 3.35706E-11 S7 1.00000E-30

CU2S_S3          Status ENTERED      Driving force 0.0000E+00
Moles 2.3266E+00, Mass 1.2343E+02, Volume fraction 0.0000E+00 Mass fractions:
CU 7.98557E-01 S 2.01443E-01 O 0.00000E+00 H 0.00000E+00

CU_L              Status ENTERED      Driving force 0.0000E+00
Moles 4.4883E-01, Mass 2.8522E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Now set the status of the diginite (CU2S_S3) to be fixed with
POLY: @@ zero amount. This means that this is reduced completely
POLY: c-s
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): cu2s_s3
Status: /ENTERED/: fix
Number of mole formula units /O/: 0
POLY: @@ There are now too many conditions. The gas must be allowed to vary
POLY: @@ in composition to find the correct oxygen potential
POLY: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=101325
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM -1
POLY:Hit RETURN to continue
POLY: set-c n(o)=none
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=101325
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
10 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0  , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=101325
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.54785E+02, Mass in grams 1.08845E+03
Total Gibbs energy -2.80759E+07, Enthalpy -1.00131E+07, Volume 5.85888E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CU              2.0000E+00  1.1676E-01 1.6098E-03 -7.4867E+04 SER
H              1.0000E+02  9.2600E-02 6.5700E-06 -1.3890E+05 SER
O              5.1785E+01  7.6118E-01 1.0863E-10 -2.6707E+05 SER
S              1.0000E+00  2.9455E-02 2.0746E-08 -2.0593E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.5278E+02, Mass 9.6136E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.61805E-01 H 1.04841E-01 S 3.33486E-02 CU 4.75131E-06
Constitution:
H2O1 9.76211E-01 O1S2 5.24705E-08 H2O4S1 2.84109E-11
O2S1 1.95855E-02 CU1H1O1 2.83599E-08 CU1O1 1.80206E-11
H2 4.17844E-03 O2 1.08582E-08 H2O2 1.13535E-11
O1S1 1.18234E-05 H2O1S1_HSOH 7.44050E-09 H2O1S1_H2SO 3.09435E-12
H2S1 9.91688E-06 S 4.30477E-09 S3 1.29650E-12
H1O1 1.44290E-06 H1O1S1_SOH 2.55475E-09 H1O2 1.25138E-12
CU 1.32327E-06 CU1S1 1.23642E-09 S4 3.25596E-18
H 3.12773E-07 CU2 4.47851E-10 O3 1.57414E-21
H1S1 2.33934E-07 CU2S1 2.11636E-10 S5 1.21560E-21
S2 1.38936E-07 O 9.79832E-11 S6 5.54892E-27
O3S1 1.32878E-07 H2S2 8.37427E-11 S8 1.00000E-30
CU1H1 5.52244E-08 H1O1S1_HSO 4.83886E-11 S7 1.00000E-30

CU_L              Status ENTERED      Driving force 0.0000E+00
Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00 Mass fractions:

```

```

CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00

CU2S_S3 Status FIXED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CU 7.98557E-01 S 2.01443E-01 O 0.00000E+00 H 0.00000E+00
POLY: sh n(*)
... the command in full is SHOW_VALUE
N(CU)=2, N(H)=100., N(O)=51.784749, N(S)=1.
POLY:Hit RETURN to continue
POLY: @@ If we have too much oxygen we may get some copper oxides,
POLY: @@ check which one is the closest to be stable
POLY: 1-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE	STATUS	DRIVING FORCE	MOLES
CU2S_S3	FIXED	0.000000E+00	0.000000E+00
CU_L	ENTERED	0.000000E+00	1.999928E+00
GAS	ENTERED	0.000000E+00	1.527848E+02
CU2S_L	ENTERED	-3.931114E-04	0.000000E+00
CU2S_S2	ENTERED	-3.309936E-02	0.000000E+00
CU_S	ENTERED	-3.549960E-02	0.000000E+00
CU2S_S1	ENTERED	-3.332974E-01	0.000000E+00
CU2O_S	ENTERED	-1.086153E+00	0.000000E+00
CU2O_L	ENTERED	-1.231036E+00	0.000000E+00
H2O_L	ENTERED	-1.738865E+00	0.000000E+00
CUS_S	ENTERED	-3.173417E+00	0.000000E+00
CUO	ENTERED	-3.229722E+00	0.000000E+00
CU2SO4	ENTERED	-3.322206E+00	0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN		-3.797595E+00	
CU2SO5 CUSO4 H2SO4_L H2O2_L S_L S_S2 SS			

```

POLY: @@ Set Cu2O to fix with zero amount and remove the fix status of CU2S_S3
POLY: c-s p cu2o_s=fix 0
... the command in full is CHANGE_STATUS
POLY: c-s p cu2s_s3
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
39 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=101325
FIXED PHASES
CU2O_S=0
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.54993E+02, Mass in grams 1.09178E+03
Total Gibbs energy -2.81294E+07, Enthalpy -1.00609E+07, Volume 5.85900E+00


```

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
CU	2.0000E+00	1.1641E-01	1.6098E-03	-7.4867E+04	SER
H	1.0000E+02	9.2317E-02	1.2909E-06	-1.5784E+05	SER
O	5.1993E+01	7.6191E-01	2.8253E-09	-2.2914E+05	SER
S	1.0000E+00	2.9365E-02	3.0696E-11	-2.8178E+05	SER

```

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.5299E+02, Mass 9.6469E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.62282E-01 H 1.04479E-01 S 3.32335E-02 CU 4.97350E-06
Constitution:

```

H2O1	9.80215E-01	H2O4S1	7.42671E-10	H1O1S1_HSO	3.65881E-13
O2S1	1.96037E-02	H2S1	5.66454E-10	CU2S1	3.13135E-13
H2	1.61310E-04	CU1O1	4.68706E-10	S2	3.04157E-13
H1O1	7.37378E-06	CU2	4.47851E-10	H2O1S1_H2SO	4.59716E-15
O2	7.34547E-06	H2O2	2.96508E-10	O3	2.76971E-17
O3S1	3.45929E-06	H1O2	1.66331E-10	H2S2	7.07748E-18
CU	1.32327E-06	H1S1	6.80080E-11	S3	4.19951E-21
O1S1	4.55002E-07	H1O1S1_SOH	1.93172E-11	S4	1.56044E-29
CU1H1O1	1.44930E-07	H2O1S1_HSOH	1.10541E-11	S7	1.00000E-30
H	6.14543E-08	S	6.36932E-12	S5	1.00000E-30
CU1H1	1.08506E-08	O1S2	2.98765E-12	S6	1.00000E-30
O	2.54848E-09	CU1S1	1.82939E-12	S8	1.00000E-30

```

CU_L Status ENTERED Driving force 0.0000E+00
Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00 Mass fractions:
CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00

CU2O_S Status FIXED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CU 8.88190E-01 O 1.11810E-01 S 0.00000E+00 H 0.00000E+00
POLY: show n(*)
... the command in full is SHOW_VALUE
N(CU)=2, N(H)=100., N(O)=51.992866, N(S)=1.
POLY:Hit RETURN to continue
POLY: @@ The ratio N(O) to N(H) should thus be between 0.5178 and 0.52
POLY: @@ in order to reduce all Cu2S and not forming any Cu2O
POLY: @@ Make a diagram showing this amount of phases
POLY: c-st p cu2o_s
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: s-a-v 1 n(o)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 45
Max value /1/: 55
Increment /.25/:
POLY: s-c n(o)
... the command in full is SET_CONDITION
Value /51.99286556/:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Found the set of lowest grid points in 0.001 s
Calculated POLY solution 0.013 s, total time 0.014 s
POLY: save tcex11 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS

```

```

No initial equilibrium, using default
Step will start from axis value    51.9929
...OK

Phase Region from    51.9929    for:
  GAS
  CU_L
Global check of adding phase at    5.19929E+01
Calculated    2 equilibria

Phase Region from    51.9929    for:
  GAS
  CU2O_S
  CU_L
Global check of removing phase at    5.29928E+01
Calculated    6 equilibria

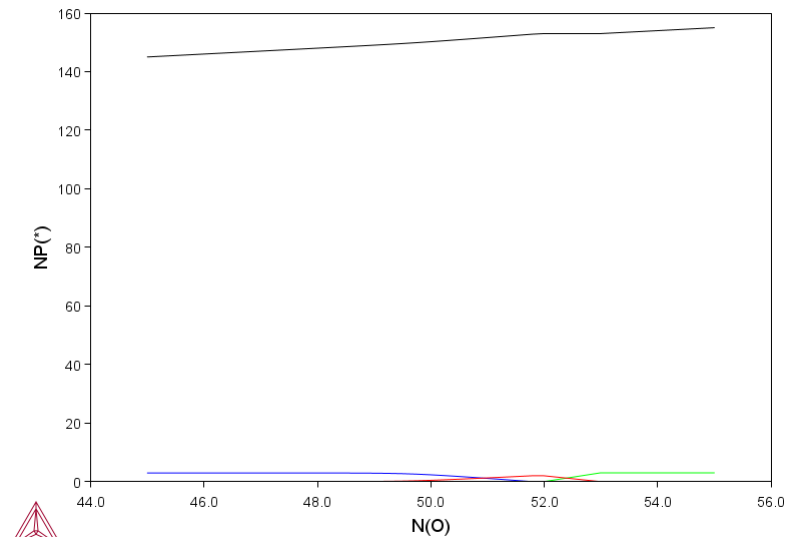
Phase Region from    52.9928    for:
  GAS
  CU2O_S
Global test at    5.49929E+01 .... OK
Terminating at    55.0000
Calculated    12 equilibria

Phase Region from    51.9929    for:
  GAS
  CU_L
Global check of adding phase at    5.17847E+01
Calculated    3 equilibria

Phase Region from    51.7847    for:
  GAS
  CU2S_S3
  CU_L
Global test at    4.99929E+01 .... OK
Global test at    4.74929E+01 .... OK
Global test at    4.50000E+01 .... OK
Terminating at    45.0000
Calculated    31 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex11\tcex11.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 11a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 11a

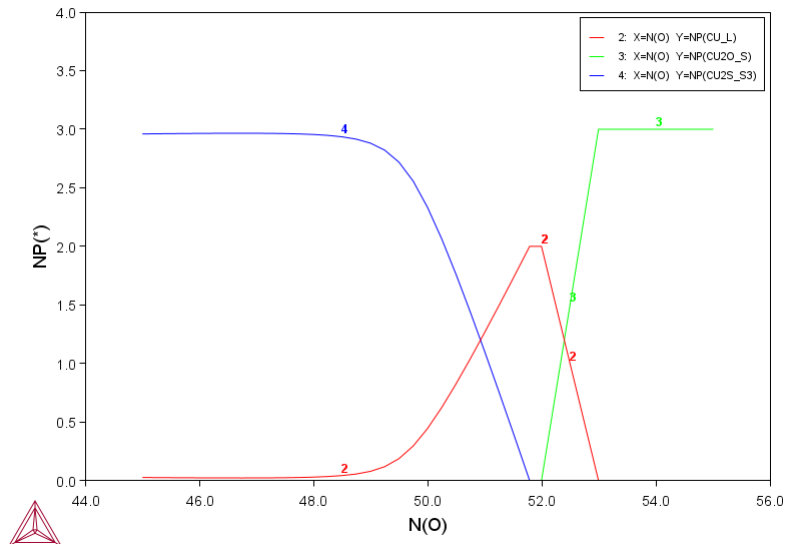


```

POST:
POST:Hit RETURN to continue
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s y n 0 4
... the command in full is SET_SCALING_STATUS
POST: set-title example 11b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 11b



POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tcex12

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex12\tcex12.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Tabulation of thermodynamic data for reactions

SYS:

SYS: @@ This example shows a number of independent cases using

SYS: @@ the TABULATE_REACTION (TAB) module to tabulate thermodynamic

SYS: @@ data for reactions.

SYS:

SYS: @@ Note that a SSUB database license is required to run

SYS: @@ the example.

SYS:

SYS: @@ Each case is separated by a line such as this

SYS: @@ =====

SYS: set-log ex12,,

SYS: go tab

... the command in full is GOTO_MODULE

TAB: ?

... the command in full is HELP

BACK	LIST_SUBSTANCES	SWITCH_DATABASE
ENTER_FUNCTION	MACRO_FILE_OPEN	TABULATE_DERIVATIVES
ENTER_REACTION	PATCH	TABULATE_REACTION
EXIT	SET_ENERGY_UNIT	TABULATE_SUBSTANCE
GOTO_MODULE	SET_INTERACTIVE	
HELP	SET_PLOT_FORMAT	

TAB: @@ Tabulate data for a reaction

TAB: tab-rea 3H2+N2=2NH3;

... the command in full is TABULATE_REACTION

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: SGTE Substances v6.0

VA DEFINED

... the command in full is REJECT

VA DEFINED

REINITIATING GES

... the command in full is DEFINE_SPECIES

H2 N2 H3N1

DEFINED

... the command in full is GET_DATA

08:49:52,097 [Thread=0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Pressure /100000/: SSUB6

Grapical output? /Y/: 100000

*** ERROR 1034 IN TBMOUT: FILE SYSTEM ERROR

Reaction: 3H2<G>+N2<G>=2H3N1<G>

*** ERROR 1114 IN GSSPB: NO SPECIES WITH THIS INDEX

ERROR 1114 RESET

TAB: 298.15

NO SUCH COMMAND, USE HELP *

TAB: 2000

NO SUCH COMMAND, USE HELP *

TAB: 100

NO SUCH COMMAND, USE HELP *

TAB:

TAB:Hit RETURN to continue

TAB: @@ Add a final column with a function. In this function

TAB: @@ you may use G, S, H, V, CP, T and R with the obvious

TAB: @@ meaning. You may also use H298 and ALPHA (thermal expansivity)

TAB: @@ and KAPPA (isothermal compressibility). In most databases

TAB: @@ there are no pressure dependence and thus V, ALPHA and KAPPA

TAB: @@ will not be correct.

TAB:

TAB: e-fun

... the command in full is ENTER_FUNCTION

Name: fef

Function: (g-h298)/t

&

TAB: t-r

... the command in full is TABULATE_REACTION

Same reaction? /Y/: y

Pressure /100000/: 100000

Low temperature limit /1.525346758-311/: 298.15

High temperature limit /4.7430302-322/: 2000

Step in temperature / NaN/: 100

Output file /SCREEN/:

O U T P U T F R O M T H E R M O - C A L C
2025. 5.12 8.49.53

Column 6: fef (G-H298)/T

Reaction: 3H2<G>+N2<G>=2H3N1<G>

H2<GAS>

N2<GAS>

H3N1<GAS>

T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)	fef
298.15	-4.44006E+01	-9.18800E+04	-1.98115E+02	-3.28120E+04	1.98115E+02
300.00	-4.43267E+01	-9.19621E+04	-1.98389E+02	-3.24452E+04	1.98116E+02
400.00	-3.92294E+01	-9.61533E+04	-2.10482E+02	-1.19604E+04	1.99799E+02
500.00	-3.34122E+01	-9.97861E+04	-2.18613E+02	9.52022E+03	2.02800E+02
600.00	-2.77768E+01	-1.02842E+05	-2.24200E+02	3.16779E+04	2.05930E+02
700.00	-2.26324E+01	-1.05358E+05	-2.28088E+02	5.43040E+04	2.08834E+02
800.00	-1.81080E+01	-1.07390E+05	-2.30808E+02	7.72568E+04	2.11421E+02
900.00	-1.41889E+01	-1.09000E+05	-2.32710E+02	1.00438E+05	2.13687E+02
1000.00	-1.08095E+01	-1.10245E+05	-2.34025E+02	1.23779E+05	2.15659E+02
1100.00	-7.77802E+00	-1.11169E+05	-2.34908E+02	1.47229E+05	2.17372E+02
1200.00	-5.07556E+00	-1.11807E+05	-2.35464E+02	1.70750E+05	2.18858E+02
1300.00	-2.93467E+00	-1.12203E+05	-2.35782E+02	1.94314E+05	2.20149E+02
1400.00	-1.19414E+00	-1.12407E+05	-2.35934E+02	2.17901E+05	2.21272E+02
1500.00	2.55400E-01	-1.12452E+05	-2.35966E+02	2.41497E+05	2.22251E+02
1600.00	1.49022E+00	-1.12363E+05	-2.35909E+02	2.65091E+05	2.23107E+02
1700.00	2.56484E+00	-1.12159E+05	-2.35785E+02	2.88676E+05	2.23857E+02
1800.00	3.51909E+00	-1.11854E+05	-2.35611E+02	3.12246E+05	2.24515E+02
1900.00	4.38259E+00	-1.11458E+05	-2.35397E+02	3.35797E+05	2.25093E+02
2000.00	5.17775E+00	-1.10980E+05	-2.35152E+02	3.59325E+05	2.25602E+02

TAB:Hit RETURN to continue

TAB: t-r

... the command in full is TABULATE_REACTION

Same reaction? /Y/: y

Pressure /100000/: 100000

Low temperature limit /298.15/: 298.15

High temperature limit /2000/: 2000

Step in temperature /100/: 100

Output file /SCREEN/: tcex12a

Grapical output? /Y/: y

Plot column? /2/: 6

O U T P U T F R O M T H E R M O - C A L C
2025. 5.12 8.49.54

Column 6: fef (G-H298)/T

Reaction: 3H2<G>+N2<G>=2H3N1<G>

H2<GAS>

N2<GAS>

H3N1<GAS>

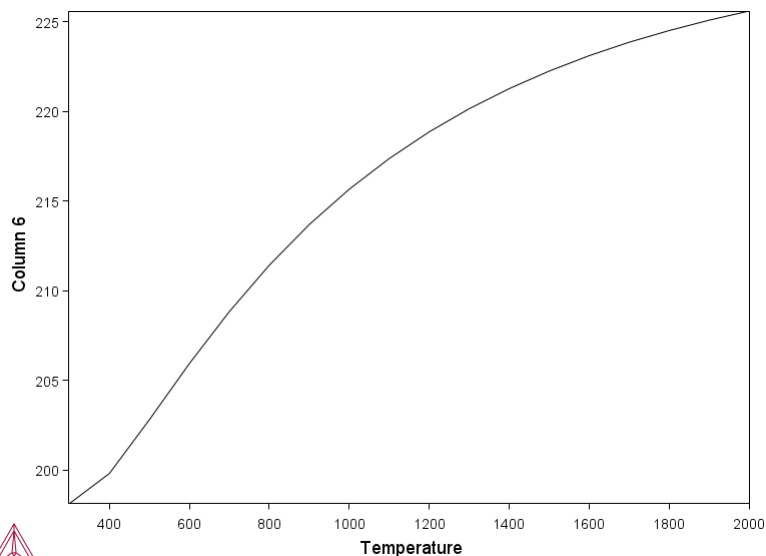
T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)	fef
298.15	-4.44006E+01	-9.18800E+04	-1.98115E+02	-3.28120E+04	1.98115E+02
300.00	-4.43267E+01	-9.19621E+04	-1.98389E+02	-3.24452E+04	1.98116E+02
400.00	-3.92294E+01	-9.61533E+04	-2.10482E+02	-1.19604E+04	1.99799E+02
500.00	-3.34122E+01	-9.97861E+04	-2.18613E+02	9.52022E+03	2.02800E+02
600.00	-2.77768E+01	-1.02842E+05	-2.24200E+02	3.16779E+04	2.05930E+02
700.00	-2.26324E+01	-1.05358E+05	-2.28088E+02	5.43040E+04	2.08834E+02
800.00	-1.81080E+01	-1.07390E+05	-2.30808E+02	7.72568E+04	2.11421E+02
900.00	-1.41889E+01	-1.09000E+05	-2.32710E+02	1.00438E+05	2.13687E+02
1000.00	-1.08095E+01	-1.10245E+05	-2.34025E+02	1.23779E+05	2.15659E+02
1100.00	-7.77802E+00	-1.11169E+05	-2.34908E+02	1.47229E+05	2.17372E+02
1200.00	-5.07556E+00	-1.11807E+05	-2.35464E+02	1.70750E+05	2.18858E+02
1300.00	-2.93467E+00	-1.12203E+05	-2.35782E+02	1.94314E+05	2.20149E+02
1400.00	-1.19414E+00	-1.12407E+05	-2.35934E+02	2.17901E+05	2.21272E+02
1500.00	2.55400E-01	-1.12452E+05	-2.35966E+02	2.41497E+05	2.22251E+02
1600.00	1.49022E+00	-1.12363E+05	-2.35909E+02	2.65091E+05	2.23107E+02
1700.00	2.56484E+00	-1.12159E+05	-2.35785E+02	2.88676E+05	2.23857E+02
1800.00	3.51909E+00	-1.11854E+05	-2.35611E+02	3.12246E+05	2.24515E+02
1900.00	4.38259E+00	-1.11458E+05	-2.35397E+02	3.35797E+05	2.25093E+02
2000.00	5.17775E+00	-1.10980E+05	-2.35152E+02	3.59325E+05	2.25602E+02

POSTPROCESSOR VERSION 3.2

... the command in full is QUICK_EXPERIMENTAL_PLOT

... the command in full is SET_SCALING_STATUS

... the command in full is PLOT_DIAGRAM



POST:
POST: set-title example 12a

POST:
POST: SET_EXP_FILE_FORMAT 5

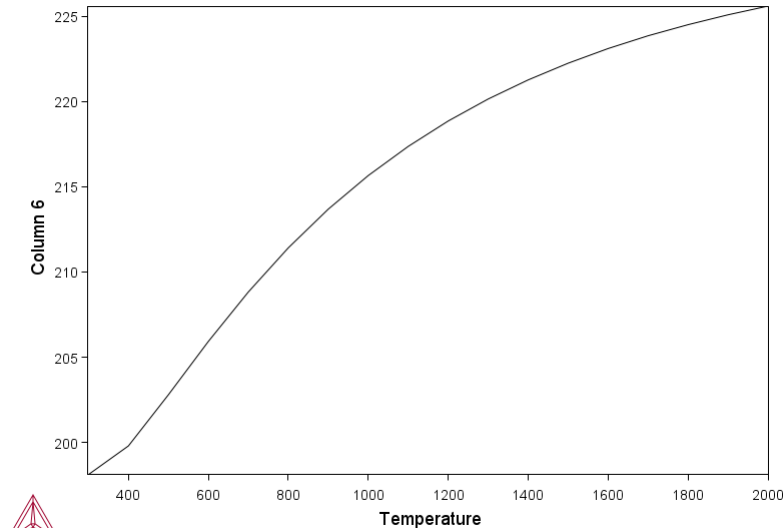
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI


```

*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 12a



```

POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ In the Gibbs-Energy-System list the data using
TAB: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES6: l-d
... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?: ?
FILE SYSTEM ERROR IN FILHLP
ERROR 1717 READING HELP FILE
OPTIONS?: rs

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT      DATE 2025- 5-12
FROM DATABASE: SSUB6

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT STABLE ELEMENT REFERENCE  MASS      H298-H0      S298
0 VA  VACUUM                      0.0000E+00  0.0000E+00  0.0000E+00
1 H    1/2_MOLE_H2(GAS)            1.0079E+00  4.2340E+03  6.5285E+01
2 N    1/2_MOLE_N2(GAS)            1.4007E+01  4.3350E+03  9.5751E+01

SPECIES                                STOICHIOMETRY
1 H                                    H
2 H2                                   H2
3 H3N1                                H3N1
4 N                                    N
5 N2                                   N2
6 VA                                   VA

Property type /ALL/: ALL
GAS:G (H2,H3N1,N2)1.0
- This phase is a gas

==== [H] ====
G(GAS,H2;0)                298.15 F11937T+R*T*LN(1.0E-5*P);      6000 N

==== [N] ====
G(GAS,N2;0)                298.15 F14172T+R*T*LN(1.0E-5*P);      6000 N

==== [H, N] ====
G(GAS,H3N1;0)              298.15 F12196T+R*T*LN(1.0E-5*P);      6000 N

GES6:Hit RETURN to continue
GES6: back
TAB:
TAB: @@ Tabulate another reaction
TAB: @@ =====
TAB: t-r
... the command in full is TABULATE_REACTION
Same reaction? /Y/: n
Reaction: INP+GA=GAP+IN;
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
GA              IN1P1              IN
GA1P1 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

```

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /tcex12a/: tcex12b
Grapical output? /Y/: Y
Plot column? /2/: 2

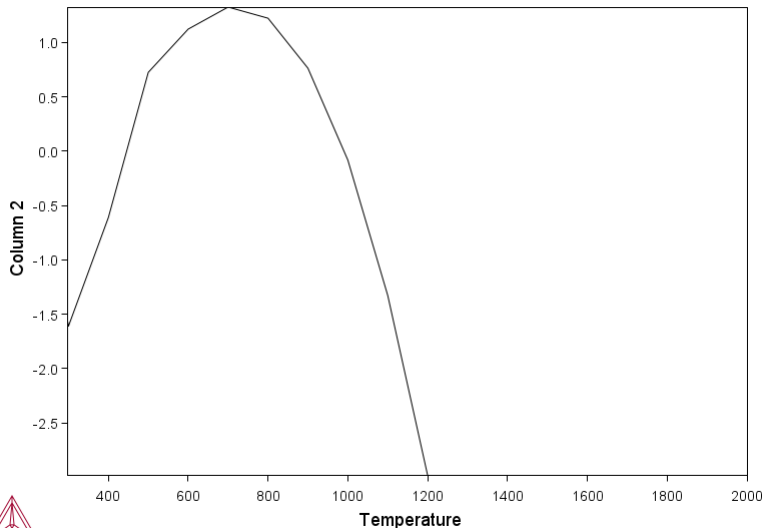
O U T P U T F R O M T H E R M O - C A L C
2025. 5.12 8.50.41

Column 6: fef (G-H298)/T
Reaction: GA+IN1P1=IN+GA1P1
GA stable as GA_S
IN1P1 stable as IN1P1_S
IN stable as IN_S
GA1P1 stable as GA1P1_S

T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)	fef
298.15	-1.56785E+00	-4.01610E+04	4.46600E+00	-4.14925E+04	-4.46600E+00
300.00	-1.60915E+00	-4.01639E+04	4.45617E+00	-4.15008E+04	-4.46597E+00
302.	---- GA becomes GA_L ,delta-H = 5589.80				
400.00	-6.09329E-01	-4.59820E+04	-1.46756E+01	-4.01118E+04	1.23002E-01
430.	---- IN becomes IN_L ,delta-H = 3283.00				
500.00	7.26020E-01	-4.26605E+04	-6.95385E+00	-3.91835E+04	1.95492E+00
600.00	1.12393E+00	-4.25671E+04	-6.78469E+00	-3.84963E+04	2.77457E+00
700.00	1.32655E+00	-4.24423E+04	-6.59282E+00	-3.78274E+04	3.33376E+00
800.00	1.22407E+00	-4.23120E+04	-6.41862E+00	-3.71771E+04	3.72988E+00
900.00	7.64029E-01	-4.22095E+04	-6.29733E+00	-3.65419E+04	4.02125E+00
1000.00	-8.12013E-02	-4.21720E+04	-6.25712E+00	-3.59149E+04	4.24608E+00
1100.00	-1.32730E+00	-4.22391E+04	-6.32007E+00	-3.52870E+04	4.43091E+00
1200.00	-2.98369E+00	-4.24512E+04	-6.50358E+00	-3.46469E+04	4.59509E+00

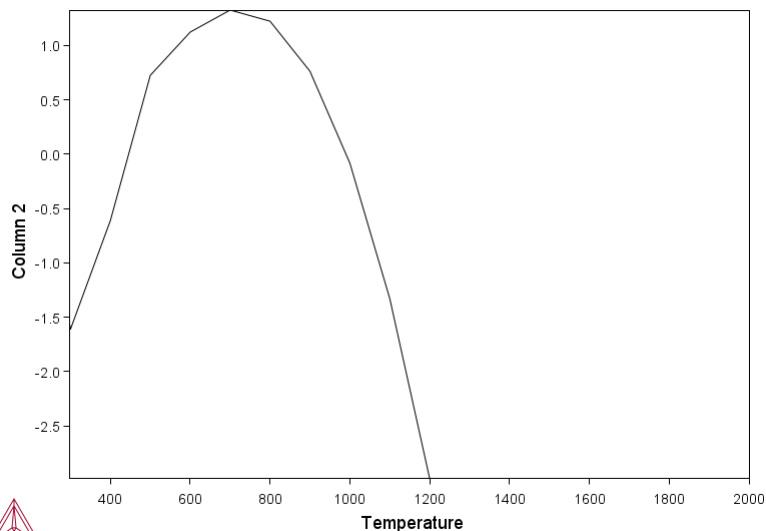
... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is SET_SCALING_STATUS
... the command in full is PLOT_DIAGRAM

example 12a



POST:
POST: set-title example 12b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

example 12b



```

POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ By default a species in a gas is not included in
TAB: @@ a tabulation, you must specify <GAS> if you want that
TAB: t-r n
... the command in full is TABULATE_REACTION
Reaction: INP<gas>+GA=GAP+IN;
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
GA          IN1P1          IN
GA1P1 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 1000
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /tcex12b/:
Graphical output? /Y/: N

      O U T P U T   F R O M   T H E R M O - C A L C
      2025. 5.12                8.51.27

Column 6: fef          (G-H298 )/T
Reaction:  GA+IN1P1<G>=IN+GA1P1
GA stable as GA_L
IN1P1<GAS>
IN1P1<GAS>
IN stable as IN_L
GA1P1 stable as GA1P1_S

*****
      T      Delta-Cp      Delta-H      Delta-S      Delta-G      fef
      (K)      (Joule/K)      (Joule)      (Joule/K)      (Joule)
*****
1000.00  1.57503E+01  -4.65760E+05  -1.78780E+02  -2.86980E+05  1.86368E+02
1100.00  1.60263E+01  -4.64172E+05  -1.77266E+02  -2.69179E+05  1.85608E+02
1200.00  1.63030E+01  -4.62555E+05  -1.75860E+02  -2.51523E+05  1.84854E+02
1300.00  1.65828E+01  -4.60911E+05  -1.74544E+02  -2.34004E+05  1.84111E+02
1400.00  1.68674E+01  -4.59238E+05  -1.73305E+02  -2.16612E+05  1.83383E+02
1500.00  1.71578E+01  -4.57537E+05  -1.72131E+02  -1.99341E+05  1.82672E+02
1600.00  1.74548E+01  -4.55807E+05  -1.71014E+02  -1.82184E+05  1.81978E+02
1700.00  1.77582E+01  -4.54046E+05  -1.69947E+02  -1.65136E+05  1.81301E+02
Temperature range exceeded for GA1P1
TAB:Hit RETURN to continue
TAB: @@ =====
TAB: @@ You can list substances in the database
TAB: li-sub
... the command in full is LIST SUBSTANCES
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
AG DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
With elements /*/: IN P
Exclusively with those elements? /Y/:

```

```

IN                P                IN1P1
IN2              P2                P3
P4
TAB: @@ or all substances with Fe
TAB: li-sub
... the command in full is LIST_SUBSTANCES
With elements /*/: FE
Exclusivly with those elements? /Y/: N
FE                AL1CL6FE1        AL2FE1O4
AS1FE1O4          AS2FE3O8        B1FE1
B1FE2            BA1FE1ND1O4      BA1FE2ND2O7
BR1FE1           BR2FE1          BR3FE1
BR4FE2           BR6FE2          C1FE1O3
C1FE3            C5FE1O5          CA1FE1O6SI2
CA1FE2O4         CA2FE2O5          CD1FE2O4
CL1FE1           CL1FE1O1         CL2FE1
CL3FE1           CL4FE2          CL6FE2
CO1FE2O4         CR2FE1O4          CU1FE1O2
CU1FE1S2         CU1FE2O4          CU2FE2O4
CU5FE1S4         F1FE1            F2FE1
F3FE1            F4FE2            F6FE2
FE0.875S1        FE0.947O1        FE1.04SE1
FE1/+1           FE1/-1           FE1H1
FE1H1O1          FE1H1O2          FE1H2O2
FE1H3O3          FE1H4O6P1        FE1I1
FE1I2            FE1I3            FE1K1O2
FE1K2O2          FE1K4O3          FE1LI1O2
FE1LI5O4         FE1MO1O4         FE1NA1O2
FE1O1            FE1O2            FE1O3SI1
FE1O3TI1         FE1O4P1          FE1O4S1
FE1O4V2          FE1O4W1          FE1O6V2
FE1P1            FE1P2            FE1S1
FE1S2            FE1SE0.96        FE1SE1
FE1SE2           FE1SI1           FE1SI2.33
FE1SI2           FE1TE0.9         FE1TE1
FE1TE2           FE1TI1           FE2
FE2H2O4          FE2I4            FE2I6
FE2LI2O4         FE2MG1O4         FE2MN1O4
FE2N1            FE2NB1           FE2NI1O4
FE2O12S3         FE2O3            FE2O4SI1
FE2O4TI1         FE2O4ZN1         FE2P1
FE2TA1           FE2TI1           FE2U1
FE3LI2O5         FE3MO2           FE3O4
FE3P1            FE3W2            FE4N1
FE5LI1O8
TAB:
TAB:Hit RETURN to continue
TAB: @@ =====
TAB: @@ You can also tabulate data for a substance or phase. This is equivalent
TAB: @@ to those you can find in NIST-JANAF thermochemical tables for example
TAB: t-sub IN1P1
... the command in full is TABULATE_SUBSTANCE
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
IN1P1 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Pressure /100000/: 100000
Low temperature limit /1000/: 300
High temperature limit /2000/: 1300
Step in temperature /100/: 100
Output file /tcex12b/: tcex12c
Grapical output? /Y/: Y
Plot column? /2/: 2

      O U T P U T   F R O M   T H E R M O - C A L C
      2025. 5.12                8.51.28

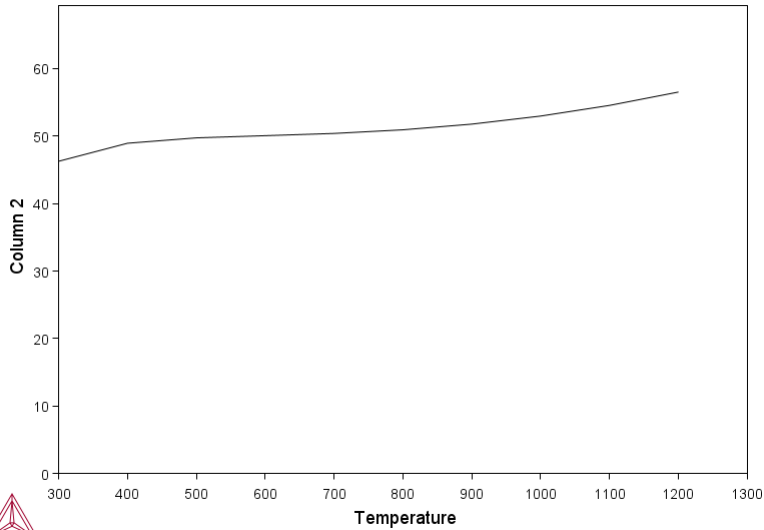
Column 6: fef          (G-H298 )/T

Phase : IN1P1_S          Pressure :      100000.00
Specie: IN1P1

*****
      T          Cp          H          S          G          fef
      (K)        (Joule/K)    (Joule)    (Joule/K)    (Joule)
*****
300.00  4.62734E+01  -7.44015E+04  6.42060E+01  -9.36633E+04  -6.39209E+01
400.00  4.89412E+01  -6.96137E+04  7.79614E+01  -1.00798E+05  -6.57782E+01
500.00  4.97376E+01  -6.46723E+04  8.89845E+01  -1.09165E+05  -6.93552E+01
600.00  5.00615E+01  -5.96811E+04  9.80837E+01  -1.18531E+05  -7.34072E+01
700.00  5.03923E+01  -5.46595E+04  1.05824E+02  -1.28736E+05  -7.74989E+01
800.00  5.09302E+01  -4.95956E+04  1.12585E+02  -1.39664E+05  -8.14708E+01
900.00  5.17709E+01  -4.44633E+04  1.18629E+02  -1.51229E+05  -8.52694E+01
1000.00 5.29647E+01  -3.92297E+04  1.24142E+02  -1.63372E+05  -8.88848E+01
1100.00 5.45403E+01  -3.38577E+04  1.29261E+02  -1.76045E+05  -9.23252E+01
1200.00 5.65148E+01  -2.83083E+04  1.34088E+02  -1.89214E+05  -9.56061E+01
Temperature range exceeded
... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is PLOT_DIAGRAM

```

example 12b

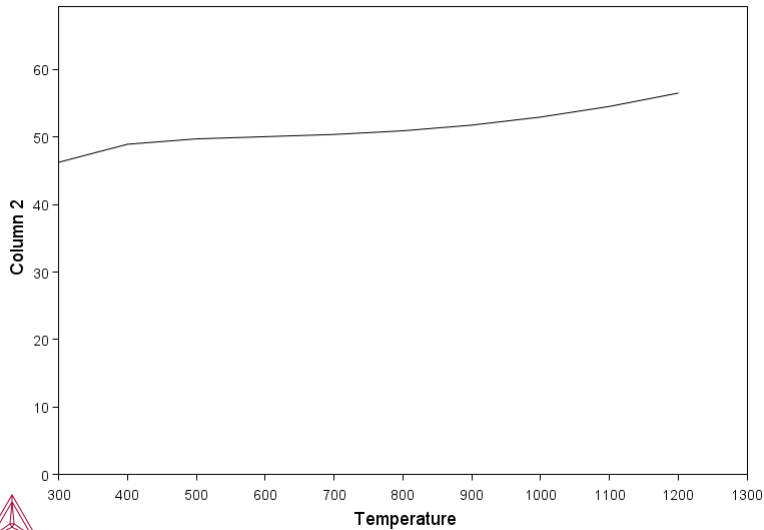


```

POST:Hit RETURN to continue
POST:
POST: set-title example 12c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAPI
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 12c



```

POST:
POST:Hit RETURN to continue
POST: back

TAB: @@ =====
TAB: @@ In order to obtain the partial pressure of a species in
TAB: @@ the gas in its pure condensed state you can enter a reaction
TAB: @@ like this for KOH. The partial pressure is entered as a
TAB: @@ function exp(-G/R/T)
TAB: e-fun
... the command in full is ENTER_FUNCTION
Name: pp
Function: exp(-g/r/t);
TAB:
TAB: tab-r n K101H1=K1H101<g>
... the command in full is TABULATE_REACTION
&
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
H1K101 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Pressure /100000/: 100000
Low temperature limit /300/: 300
High temperature limit /1300/: 2000

```

Step in temperature /100/: 100

Output file /tcex12c/: tcex12d
Grapical output? /Y/: Y
Plot column? /2/: 6

O U T P U T F R O M T H E R M O - C A L C
2025. 5.12 8.52.14

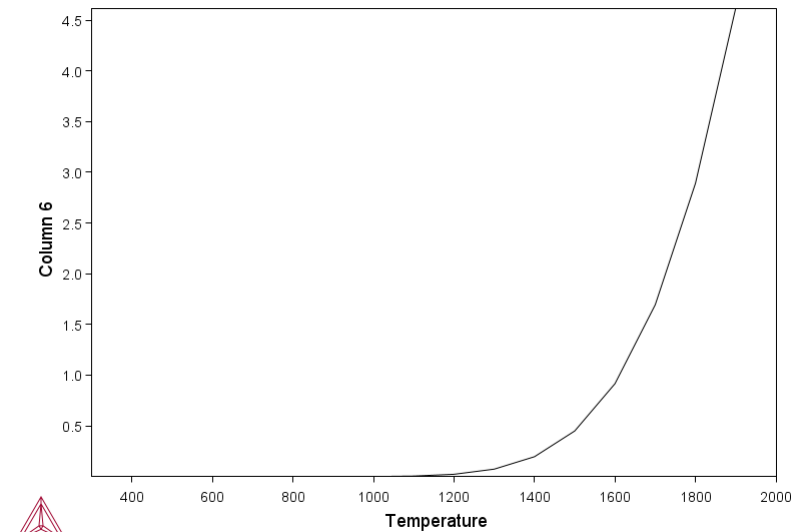
Column 6: pp EXP(-G/R/T)
Reaction: H1K101=H1K101<G>
H1K101 stable as H1K101_S
H1K101<GAS>

T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)	pp
300.00	-1.97899E+01	1.92543E+05	1.56915E+02	1.45469E+05	4.70147E-26
400.00	-2.31294E+01	1.90409E+05	1.50797E+02	1.30090E+05	1.02900E-17
500.00	-2.73216E+01	1.87890E+05	1.45195E+02	1.15293E+05	9.03075E-13
517.	---- H1K101 becomes H1K101_S2 ,delta-H = 5600.00				
600.00	-2.71797E+01	1.79542E+05	1.29351E+02	1.01932E+05	1.33747E-09
680.	---- H1K101 becomes H1K101_L ,delta-H = 7900.00				
700.00	-3.36564E+01	1.68804E+05	1.13354E+02	8.94566E+04	2.11269E-07
800.00	-3.31914E+01	1.65462E+05	1.08890E+02	7.83499E+04	7.66317E-06
900.00	-3.27453E+01	1.62165E+05	1.05007E+02	6.76592E+04	1.18375E-04
1000.00	-3.22973E+01	1.58913E+05	1.01580E+02	5.73333E+04	1.01226E-03
1100.00	-3.18358E+01	1.55706E+05	9.85231E+01	4.73310E+04	5.65583E-03
1200.00	-3.13536E+01	1.52547E+05	9.57735E+01	3.76185E+04	2.30437E-02
1300.00	-3.08482E+01	1.49436E+05	9.32837E+01	2.81676E+04	7.38312E-02
1400.00	-3.03294E+01	1.46378E+05	9.10171E+01	1.89543E+04	1.96257E-01
1500.00	-2.98854E+01	1.43368E+05	8.89402E+01	9.95788E+03	4.50033E-01
1600.00	-2.94990E+01	1.40399E+05	8.70240E+01	1.16091E+03	9.16434E-01
1700.00	-2.91580E+01	1.37467E+05	8.52461E+01	-7.45152E+03	1.69415E+00
1800.00	-2.88535E+01	1.34567E+05	8.35882E+01	-1.58923E+04	2.89182E+00
1900.00	-2.85787E+01	1.31695E+05	8.20357E+01	-2.41727E+04	4.61888E+00

Temperature range exceeded for H1K101

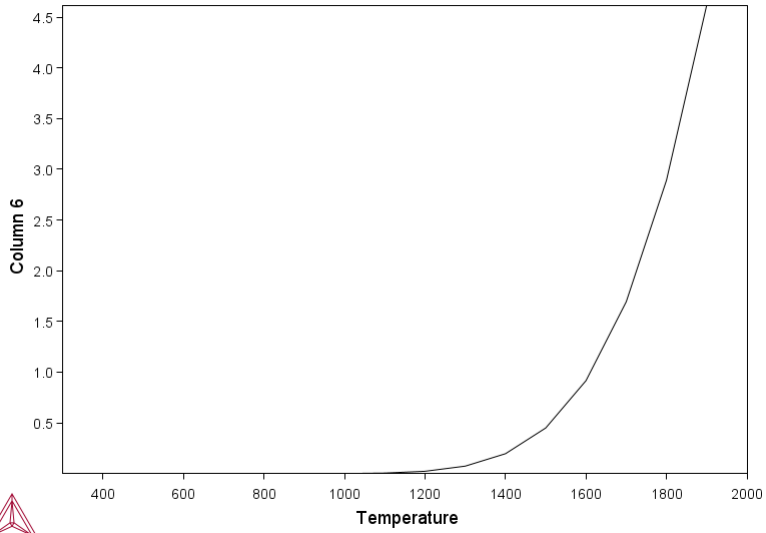
... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is SET_SCALING_STATUS
... the command in full is PLOT_DIAGRAM

example 12c



POST:
POST: set-title example 12d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

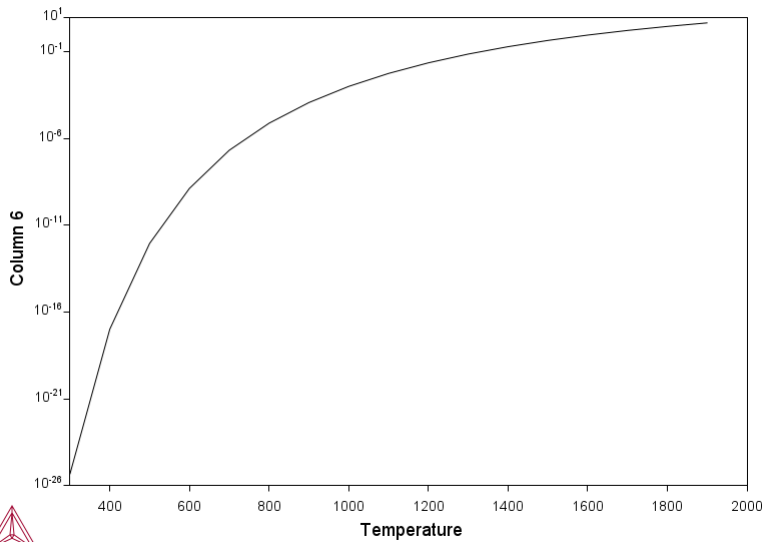
example 12d



```

POST:
POST:Hit RETURN to continue
POST: s-a-ty y
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 12e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
  
```

example 12e



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
  
```

tcex13

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex13\tcex13.TCM"

SYS: set-echo

SYS:

SYS: @@ Calculating the binary Al-Ti phase diagram and its G curve

SYS:

SYS: @@ This example calculates an Al-Ti binary phase diagram and

SYS: @@ G curve using the BINARY module.

SYS:

SYS: set-log ex13,,,

SYS: GO BIN

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED

First element: ?

The following assessed systems

AG-AL AG-AU AG-BI AG-CU AG-GE AG-IN AG-IR AG-MG AG-OS AG-PB AG-PD AG-PT
AG-RH AG-RU AG-SB AG-SI AG-SN AG-TI AG-TL AG-ZN AG-ZR AL-AS AL-AU AL-B
AL-BI AL-C AL-CA AL-CE AL-CO AL-CR AL-CU AL-FE AL-GA AL-GE AL-IN AL-LI
AL-MG AL-MN AL-MO AL-N AL-NB AL-ND AL-NI AL-O AL-P AL-PB AL-SB AL-SI
AL-SN AL-TA AL-TI AL-V AL-W AL-Y AL-ZN AL-ZR AS-AU AS-CU AS-FE AS-GA
AS-GE AS-IN AS-P AS-SB AU-BI AU-C AU-CR AU-CU AU-GE AU-IN AU-PB AU-PD
AU-RH AU-RU AU-SB AU-SI AU-TE AU-TL B-C B-CO B-CR B-FE B-HF B-MG
B-MO B-N B-ND B-NI B-SC B-SI B-TI B-V B-W BA-CU BA-EU BA-SR
BA-Y BI-CU BI-GA BI-GE BI-HG BI-IN BI-K BI-MG BI-O BI-PB BI-SB BI-SI
BI-SN BI-TL BI-ZN C-CO C-CR C-CU C-FE C-HF C-MN C-MO C-NB C-NI
C-PB C-SI C-TA C-TI C-V C-W C-Y C-ZR CA-CU CA-MG CA-PB CA-SI
CA-ZN CD-GA CD-GE CD-HG CD-IN CD-PB CD-SB CD-SN CD-TE CD-ZN CE-MG CO-CR
CO-CU CO-DY CO-FE CO-IN CO-MN CO-MO CO-N CO-NB CO-NI CO-PD CO-PT CO-SI
CO-TA CO-TI CO-V CO-W CR-CU CR-FE CR-MG CR-MN CR-MO CR-N CR-NB CR-NI
CR-P CR-PD CR-PT CR-SI CR-SN CR-TA CR-TI CR-V CR-W CR-ZN CR-ZR CS-K
CS-NA CS-RB CU-FE CU-GE CU-IN CU-LI CU-MG CU-MN CU-N CU-NB CU-NI CU-O
CU-P CU-PB CU-S CU-SB CU-SI CU-SN CU-SR CU-TI CU-TL CU-V CU-Y CU-ZN
CU-ZR DY-ER DY-HO ER-HO ER-TB FE-MG FE-MN FE-MO FE-N FE-NB FE-ND FE-NI
FE-O FE-P FE-PB FE-PD FE-PR FE-PT FE-S FE-SI FE-SN FE-TI FE-V FE-W
FE-ZN FE-ZR GA-GE GA-HG GA-IN GA-P GA-PB GA-SB GA-SN GA-TE GA-ZN GE-IN
GE-PB GE-SB GE-SI GE-SN GE-TE GE-TL GE-ZN H-NB H-ZR HF-TA HF-SI HF-TI
HG-PB HO-TB IN-P IN-PB IN-SB IN-SI IN-SN IN-ZN IR-PD K-RB LA-NI LI-MG
LI-ZR MG-NI MG-O MG-SC MG-SI MG-Y MG-ZN MG-ZR MN-MO MN-N MN-O MN-PB
MN-SI MN-TI MN-V MN-Y MN-ZR MO-N MO-NB MO-NI MO-SI MO-TA MO-TI MO-W
N-NB N-NI N-TA N-TI N-V N-W NA-RB NB-NI NB-O NB-TI NB-V NB-W
NB-ZR ND-PR ND-SB NI-P NI-PD NI-SI NI-TA NI-TI NI-V NI-W NI-Y NI-ZR
O-PB O-SN O-SR O-TI O-Y O-ZR P-SB P-SI PB-PD PB-SB PB-SI PB-SN
PB-TL PB-ZN PD-RU PD-SN PR-SB PT-RH PT-RU RE-TA RE-W SB-SI SB-SN SB-ZN
SE-SN SE-TE SE-TL SI-SN SI-TA SI-TE SI-TI SI-U SI-V SI-W SI-Y SI-ZN
SI-ZR SN-TI SN-ZN SN-ZR TA-TI TA-V TA-W TA-ZR TE-ZN TI-V TI-W TI-ZR
U-ZR V-ZR Y-ZR

First element: AL TI

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:

... the command in full is REJECT

VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
REINITIATING GES

... the command in full is DEFINE_ELEMENTS

AL TI DEFINED
GAS:G LIQUID:L IONIC_LIQUID:Y
FCC_A1 BCC_A2 A2_BCC
HCP_A3 HCP_ZN DIAMOND_A4
BCT_A5 CBCC_A12 CUB_A13
B11_CUT1 B32_ALLI C14_LAVES
C15_LAVES C16_AL2CU C36_LAVES
D019_AL1M3 D019_SNTI3 D022_AL3M1
D1A_CU4TI D513_AL3NI2 D88_SI3TI5
L10_ALTI AL11TI5 AL2TI
AL5FE4 ALCE_AMORPHOUS MTI2

REJECTED
LIQUID:L RESTORED
AL11TI5 RESTORED
AL2TI RESTORED
D022_AL3M1 RESTORED
D019_AL1M3 RESTORED
L10_ALTI RESTORED
A2_BCC RESTORED
BCC_B2 RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED

... the command in full is GET_DATA

08:54:22,392 [Thread=0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION


```
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST_REFERENCES to see the list of references for assessed data

```
-OK-
... the command in full is SET_CONDITION
... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234 created
... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08 created
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```
... the command in full is SET_CONDITION
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
... the command in full is SAVE_WORKSPACES
Version S mapping is selected
```

Organizing start points

```
Generating start point  1
Generating start point  2
```

```
Phase region boundary  1 at:  4.169E-01  1.704E+03
LIQUID
** L10_ALTI
Calculated.              7 equilibria
```

```
Phase region boundary  2 at:  3.454E-01  1.652E+03
LIQUID
** AL11TI5
** L10_ALTI
```

```
Phase region boundary  3 at:  3.153E-01  1.652E+03
LIQUID
** AL11TI5
Calculated.              3 equilibria
```

```
Phase region boundary  4 at:  3.016E-01  1.646E+03
LIQUID
** AL11TI5
** D022_AL3M1
```

```
Phase region boundary  5 at:  2.797E-01  1.646E+03
LIQUID
** D022_AL3M1
Calculated.              36 equilibria
```

```
Phase region boundary  6 at:  1.254E-01  9.380E+02
LIQUID
** D022_AL3M1
** FCC_A1
```

```
Phase region boundary  7 at:  4.025E-03  9.380E+02
LIQUID
** FCC_A1
Calculated              12 equilibria
```

```
Phase region boundary  8 at:  1.287E-01  9.380E+02
D022_AL3M1
** FCC_A1
Calculated..            27 equilibria
Terminating at axis limit.
```

```
Phase region boundary  9 at:  2.981E-01  1.646E+03
AL11TI5
** D022_AL3M1
Calculated.              17 equilibria
```

```
Phase region boundary 10 at:  2.871E-01  1.269E+03
AL11TI5
** AL2TI
** D022_AL3M1
```

```
Phase region boundary 11 at:  3.267E-01  1.269E+03
AL11TI5
** AL2TI
Calculated.              9 equilibria
```

```
Phase region boundary 12 at:  3.267E-01  1.454E+03
AL11TI5
** AL2TI
** L10_ALTI
```

```
Phase region boundary 13 at:  3.539E-01  1.454E+03
AL11TI5
** L10_ALTI
Calculated.              9 equilibria
Terminating at known equilibrium
```

```
Phase region boundary 14 at:  3.605E-01  1.454E+03
AL2TI
** L10_ALTI
Calculated..            48 equilibria
Terminating at axis limit.
```

```
Phase region boundary 15 at:  2.937E-01  1.269E+03
** AL2TI
D022_AL3M1
Calculated..            40 equilibria
Terminating at axis limit.
```

```

Phase region boundary 16 at: 3.454E-01 1.652E+03
LIQUID
** L10_ALTI
Calculated. 9 equilibria

Phase region boundary 17 at: 4.476E-01 1.717E+03
LIQUID
** HCP_A3
** L10_ALTI

Phase region boundary 18 at: 4.672E-01 1.717E+03
LIQUID
** HCP_A3
Calculated. 4 equilibria

Phase region boundary 19 at: 5.157E-01 1.776E+03
LIQUID
** BCC_B2
** HCP_A3

Phase region boundary 20 at: 5.233E-01 1.776E+03
LIQUID
** BCC_B2
Calculated 43 equilibria

Phase region boundary 21 at: 5.477E-01 1.776E+03
** BCC_B2
HCP_A3
Calculated 41 equilibria

Phase region boundary 22 at: 4.784E-01 1.717E+03
** HCP_A3
L10_ALTI
Calculated. 14 equilibria

Phase region boundary 23 at: 5.545E-01 1.399E+03
** D019_AL1M3
** HCP_A3
L10_ALTI

Phase region boundary 24 at: 5.596E-01 1.399E+03
** D019_AL1M3
L10_ALTI
Calculated.. 45 equilibria
Terminating at axis limit.

Phase region boundary 25 at: 5.977E-01 1.399E+03
** D019_AL1M3
HCP_A3
Calculated.. 63 equilibria
Terminating at axis limit.

Phase region boundary 26 at: 4.169E-01 1.704E+03
LIQUID
** L10_ALTI
Calculated. 4 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping 7 seconds
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

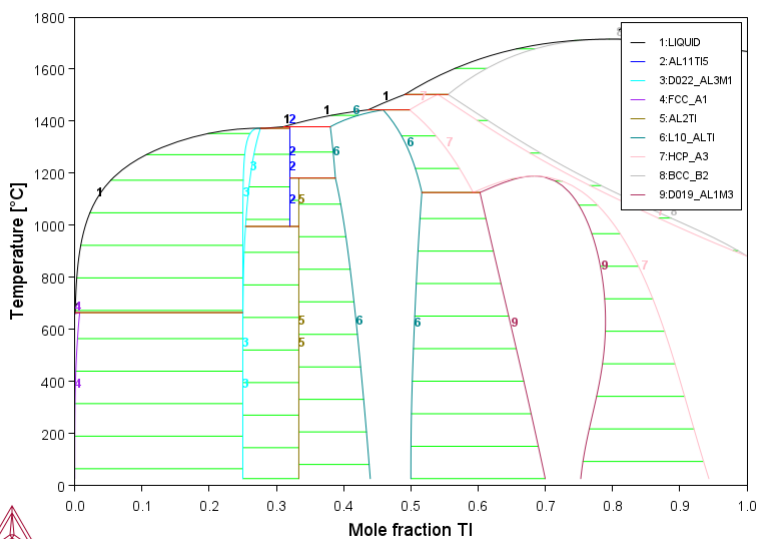
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

```

AL TI



```

POST: @@ Set some phase labels
POST: ADD
... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .7 1400
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 6074 grid points in 0.052 s
Found the set of lowest grid points in 0.003 s
Calculated POLY solution 0.018 s, total time 0.073 s
Stable phases are: BCC_B2
Text size: /.36/:

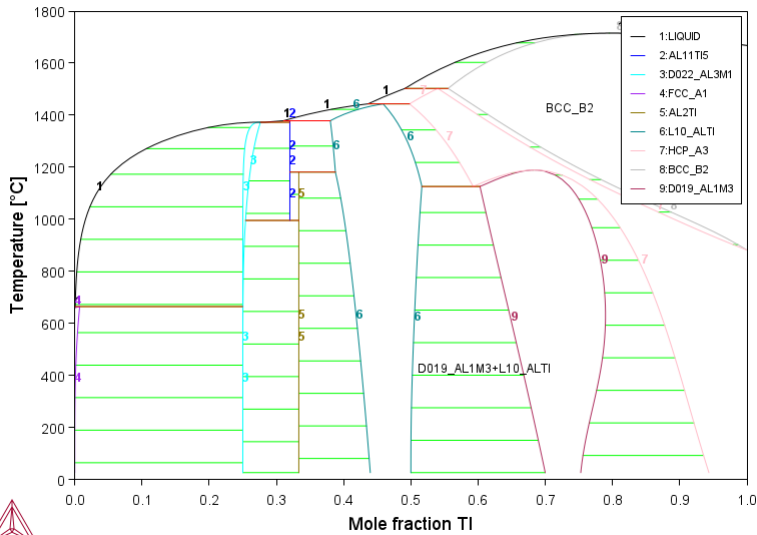
```

```

POST: ADD
... the command in full is ADD_LABEL TEXT
Give X coordinate in axis units: .51 400
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 6074 grid points in 0.032 s
Found the set of lowest grid points in 0.001 s
Calculated POLY solution 0.011 s, total time 0.044 s
Stable phases are: D019_AL1M3+L10_ALTI
Text size: /.36/:
POST: set-title example 13a
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13a

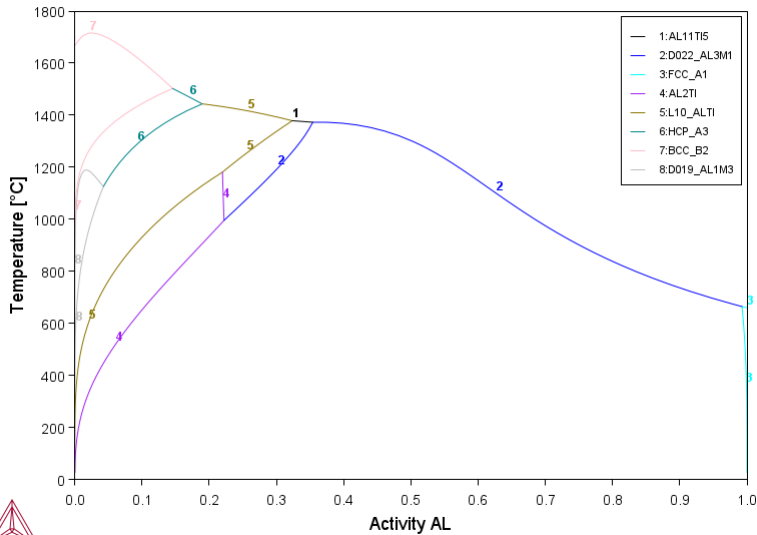


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot the activities, too
POST: S-D-A
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : X
VARIABLE : AC
FOR COMPONENT : AL
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13b

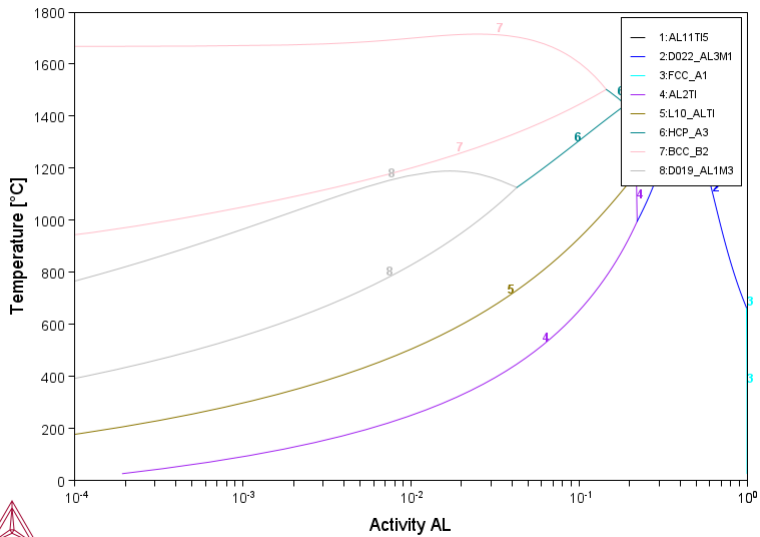


```

POST:
POST:Hit RETURN to continue
POST: S-A-TY X
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: LOG
POST: S-S X N 1E-4 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 13c
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13c

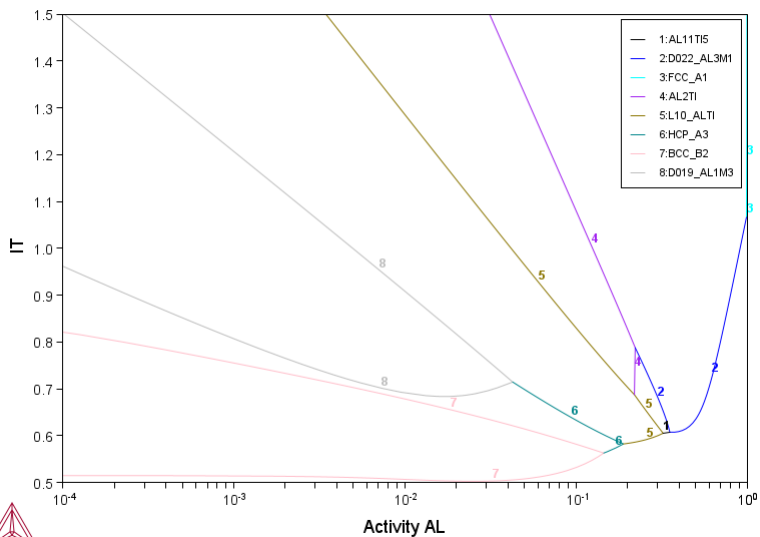


```

POST:
POST:Hit RETURN to continue
POST: @@ Now use inverse of T as y axis
POST: ent fun it=1000/T;
... the command in full is ENTER_SYMBOL
POST: s-d-a y it
... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n .5 1.5
... the command in full is SET_SCALING_STATUS
POST: set-title example 13d
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13d



```

POST:
POST:Hit RETURN to continue
POST: @@ Now the G curves for the same system
POST: BA
... the command in full is BACK
Current database: Steels/Fe-Alloys v11.0

VA                                /- DEFINED
DICTRA FCC_A1 REJECTED
SYS: GO BIN
... the command in full is GOTO_MODULE
Current database: Steels/Fe-Alloys v11.0

VA                                /- DEFINED
DICTRA FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

VA                                /- DEFINED
BCC_B2                            FCC_L12                FCC_L102
D021_HCP REJECTED

First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 1000
... the command in full is REJECT
VA                                /- DEFINED
BCC_B2                            FCC_L12                FCC_L102
D021_HCP REJECTED
REINITIATING GES .....
... the command in full is DEFINE_ELEMENTS
AL                                TI DEFINED
GAS:G                            LIQUID:L                IONIC_LIQUID:Y

```

```

FCC_A1          BCC_A2          A2_BCC
HCP_A3          HCP_ZN          DIAMOND_A4
BCT_A5          CBCC_A12        CUB_A13
B11_CUT1        B32_ALLI        C14_LAVES
C15_LAVES        C16_AL2CU       C36_LAVES
D019_AL1M3      D019_SNTI3      D022_AL3M1
D1A_CU4TI       D513_AL3NI2     D88_SI3TI5
L10_ALTI        AL11TI5         AL2TI
AL5FE4          ALCE_AMORPHOUS   MTI2

```

```

REJECTED
LIQUID:L RESTORED
AL11TI5 RESTORED
AL2TI RESTORED
D022_AL3M1 RESTORED
D019_AL1M3 RESTORED
L10_ALTI RESTORED
A2_BCC RESTORED
BCC_B2 RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

```

Use the command LIST_REFERENCES to see the list of references for assessed data

```

-OK-
... the command in full is SET_CONDITION
... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234 created
... the command in full is SET_CONDITION
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is SAVE_WORKSPACES
... the command in full is STEP_WITH_OPTIONS

```

```

Phase Region from 0.502463 for:
LIQUID
BCC_B2
D019_AL1M3
FCC_A1
HCP_A3
L10_ALTI

```

```

Phase Region from 0.502463 for:
LIQUID
BCC_B2
D019_AL1M3
FCC_A1
HCP_A3
L10_ALTI

```

```

Phase Region from 0.320000 for:
AL11TI5

```

```

Phase Region from 0.333333 for:
AL2TI

```

```

Phase Region from 0.636878 for:
D022_AL3M1

```

```

Phase Region from 0.636878 for:
D022_AL3M1

```

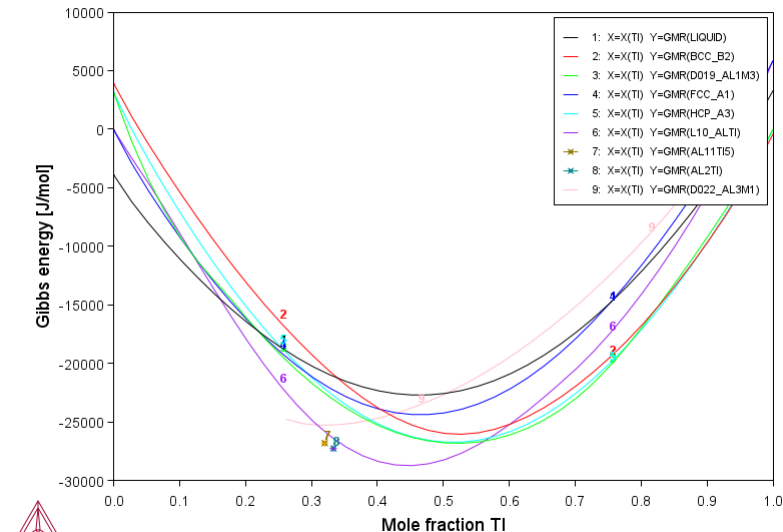
*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\GCURVE_002.POLY3

```

POSTPROCESSOR VERSION 3.2
... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

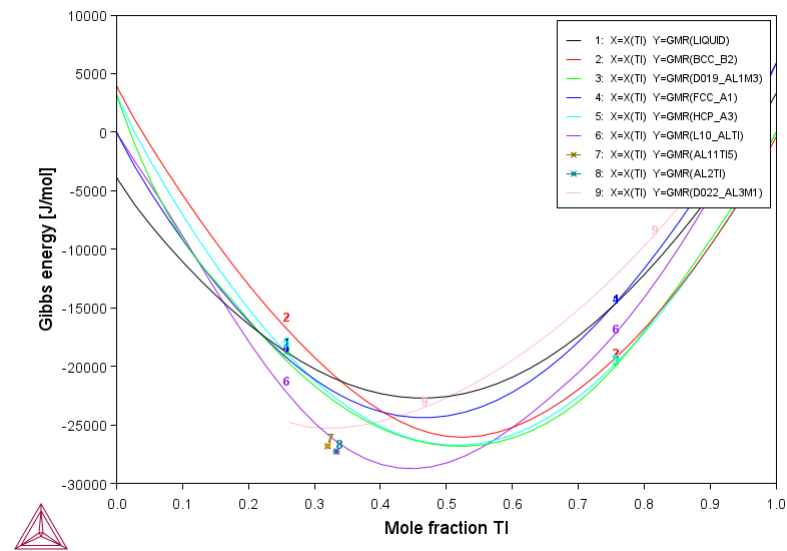
```

AL TI



```
POST:
POST: set-label F
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 13e



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex14

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex14\tcex14.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Variations in solidification of an Al-Mg-Si alloy

SYS:

SYS: @@ This example calculates the heat and heat capacity

SYS: @@ variations during solidification of an Al-Mg-Si alloy.

SYS:

SYS: set-log ex14,,,,,

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw ALDEMO

... the command in full is SWITCH_DATABASE

Current database: Aluminum Demo Database v5.0

VA /- DEFINED

TDB_ALDEMO: d-sys al cu si

... the command in full is DEFINE_SYSTEM

AL CU SI

DEFINED

TDB_ALDEMO: l-s c

... the command in full is LIST_SYSTEM

LIQUID:L :AL CU SI:

AL2CU_C16 :AL:AL CU SI:

ALCU_DEL :AL:CU:

ALCU_EPS :AL CU:CU:

ALCU_ETA :AL CU:CU:

ALCU_ZETA :AL:CU:

ALZR2_B82 :AL VA:VA:

BCC_A2 :AL CU SI VA:VA:

BCC_B2 :AL CU SI VA:AL CU SI VA:VA:

C14_LAVES :AL CU:AL CU:

C15_LAVES :AL CU SI:AL CU SI:

C36_LAVES :AL CU:AL CU:

CU15SI4_EPSILON :CU:AL SI:

CU33SI7_DELTA :CU:SI:

CU56SI11_GAMMA :CU SI:SI:

CUSI_ETA :CU:SI:

DIAMOND_A4 :AL SI:

FCC_A1 :AL CU SI:VA:

GAMMA_D83 :AL SI:AL CU SI:CU:

GAMMA_H :AL:AL CU:CU:

HCP_A3 :AL CU SI:VA:

TDB_ALDEMO: get

... the command in full is GET_DATA

08:55:33,232 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_ALDEMO: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ The composition

POLY: s-c w(si)=.09,w(cu)=.10,t=1000,p=1e5,n=1

... the command in full is SET_CONDITION

POLY: l-c

... the command in full is LIST_CONDITIONS

W(SI)=9E-2, W(CU)=0.1, T=1000, P=100000, N=1

DEGREES OF FREEDOM 0

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 17676 grid points in 0.473 s

Found the set of lowest grid points in 0.003 s

Calculated POLY solution 0.110 s, total time 0.586 s

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: ALDEMO

Conditions:

W(SI)=9E-2, W(CU)=0.1, T=1000, P=100000, N=1

DEGREES OF FREEDOM 0

Temperature 1000.00 K (726.85 C), Pressure 1.000000E+05

Number of moles of components 1.000000E+00, Mass in grams 2.87371E+01

Total Gibbs energy -4.64558E+04, Enthalpy 3.21074E+04, Volume 1.11975E-05

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
AL	8.6269E-01	8.1000E-01	5.0275E-03	-4.4007E+04	SER
CU	4.5223E-02	1.0000E-01	3.2656E-06	-1.0503E+05	SER

```

SI          9.2090E-02  9.0000E-02  7.5475E-03 -4.0629E+04 SER

LIQUID          Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 2.8737E+01, Volume fraction 1.0000E+00  Mass fractions:
AL  8.10000E-01  CU  1.00000E-01  SI  9.00000E-02
POLY:Hit RETURN to continue
POLY: @@ Set temperature as axis
POLY: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: t
Min value /0/: 500
Max value /1/: 1000
Increment /12.5/: 12.5
POLY: save tcex14 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value      1000.00
...OK

Phase Region from      1000.00      for:
LIQUID
Global test at  9.20000E+02 .... OK
Global check of adding phase at  8.41997E+02
Calculated      18 equilibria

Phase Region from      841.997      for:
LIQUID
FCC_A1
Global check of adding phase at  8.28102E+02
Calculated      5 equilibria

Phase Region from      828.102      for:
LIQUID
DIAMOND_A4
FCC_A1
Global check of adding phase at  7.94799E+02
Calculated      6 equilibria

Phase Region from      794.799      for:
LIQUID
AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated      2 equilibria

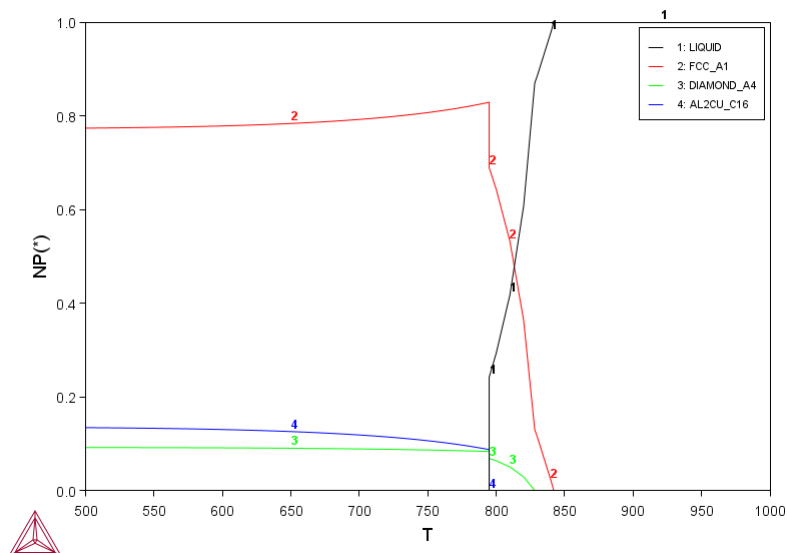
Phase Region from      794.799      for:
AL2CU_C16
DIAMOND_A4
FCC_A1
Global test at  7.20000E+02 .... OK
Global test at  6.20000E+02 .... OK
Global test at  5.20000E+02 .... OK
Terminating at      500.000
Calculated      33 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex14\tcex14.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: @@ Plot phase fractions
POST: S-D-A X T
... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y NP(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: S-LAB D
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 14a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 14a

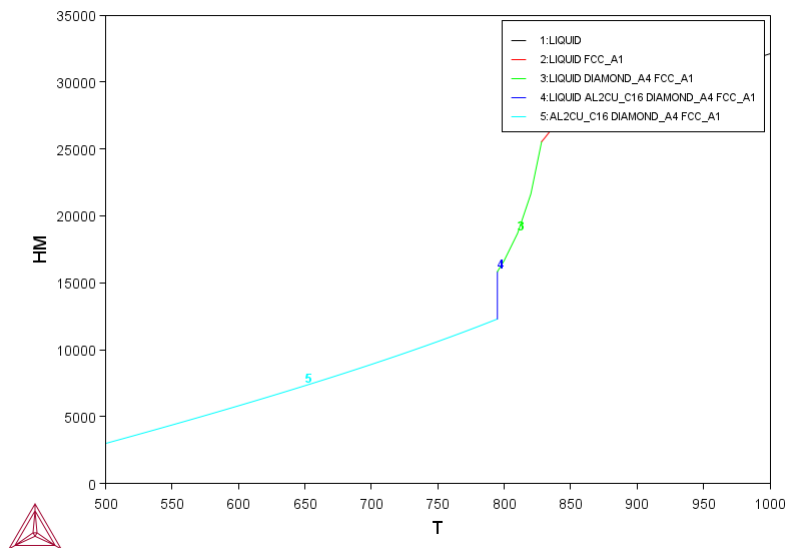



```

POST:
POST:Hit RETURN to continue
POST: @@ Plot the total enthalpy (heat)
POST: S-D-A Y HM
... the command in full is SET_DIAGRAM_AXIS
POST: S-LAB B
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 14b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 14b

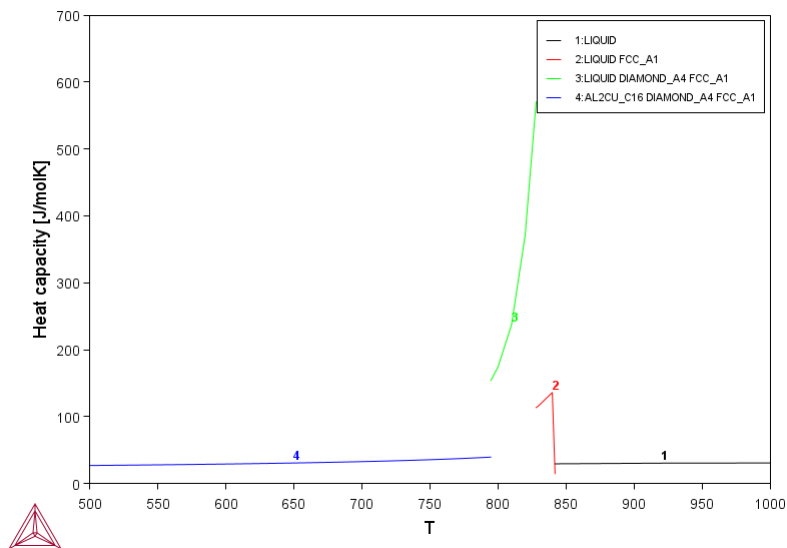


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot the heat capacity. First this must be entered because
POST: @@ a function as derivatives cannot be plotted directly.
POST:
POST: ENT FUN CP=HM.T;
... the command in full is ENTER_SYMBOL
POST: S-D-A Y CP
... the command in full is SET_DIAGRAM_AXIS
POST: S-S
... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC SCALING (Y OR N) /N/: N
MIN VALUE : 0
MAX VALUE : 700
POST: S-A-T-S
... the command in full is SET_AXIS_TEXT_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC AXIS TEXT (Y OR N) /N/: N
AXIS TEXT : Heat capacity [J/molK]
POST: set-title example 14c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 14c



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex15

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex15\tcex15.TCM.test"

SYS: SET_ECHO

SYS:

SYS: @@ Simulating the solidification of a Cr-Ni alloy with

SYS: @@ the Scheil module

SYS:

SYS: @@ This is an example of a solidification simulation

SYS: @@ of a Cr-Ni alloy. There is no back diffusion in the

SYS: @@ solid, i.e. Scheil-Gulliver model is used.

SYS:

SYS: GO SCHEIL

SCHEIL: TEMPERATURE-STEP

Temperature step (C) /1/: 5

SCHEIL: START-WIZARD

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: FEDEMO

Current database: Iron Demo Database v6.0

VA /- DEFINED

Major element or alloy: cr

Composition input in mass (weight) percent? /Y/: n

Composition will be taken to be in mole percent

1st alloying element: ni

Mole percent /1/: 10

2nd alloying element:

Temperature (C) /2000/: 2000

VA /- DEFINED

REINITIATING GES

CR DEFINED

NI DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
C14_LAVES	CBCC_A12	CHI_A12
CUB_A13	FCC_A1	HCP_A3
SIGMA_D8B		

Reject phase(s) /NONE/: *

GAS:G	LIQUID:L	BCC_A2
C14_LAVES	CBCC_A12	CHI_A12
CUB_A13	FCC_A1	HCP_A3
SIGMA_D8B	REJECTED	

Restore phase(s):: liq bcc fcc

LIQUID:L	BCC_A2	FCC_A1
RESTORED		

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

LIQUID:L	BCC_A2	FCC_A1

.....

OK? /Y/: y

08:56:36,927 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/:

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/:

This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.

You must release one of these conditions

T=2273.15, X(NI)=0.1, P=100000, N=1 DEGREES OF FREEDOM 0

PHASE CHANGE AT 2058.59459939

BCC_A2#1 forms

Testing POLY result by global minimization procedure

Calculated 627 grid points in 0.009 s

CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS

...OK

Phase Region from 2058.68 for:

LIQUID

Terminating at 2058.78

Calculated 4 equilibria

Phase Region from 2058.68 for:

LIQUID

Global check of adding phase at 2.05859E+03

Calculated 3 equilibria

Phase Region from 2058.59 for:
LIQUID
BCC_A2
Global test at 2.01868E+03 OK
Global test at 1.96868E+03 OK
Global test at 1.91868E+03 OK
Global check of removing phase at 1.89734E+03
Calculated 35 equilibria

Phase Region from 1897.34 for:
BCC_A2
Calculated 4 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_3680.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_3680.EXP
has been created to store the equilibrium solidification results.

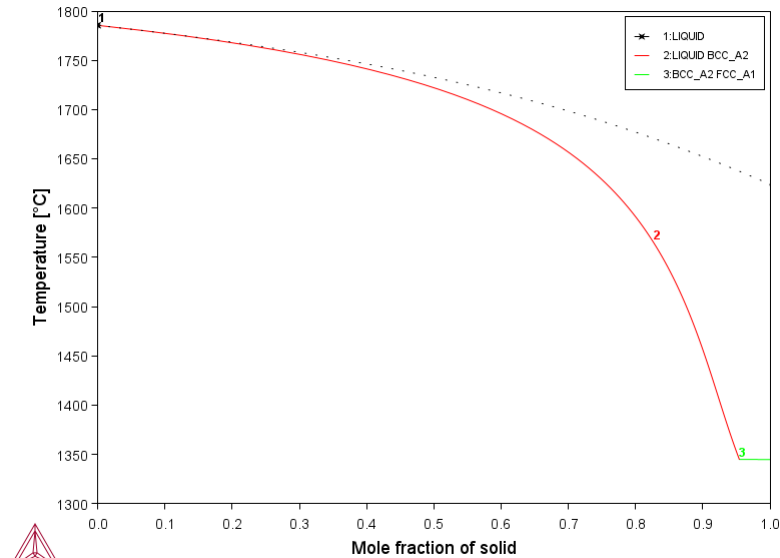
CALCULATING SCHEIL SOLIDIFICATION

T(C)	fraction solid
1785.535	0.000000
PHASE REGION: LIQUID + BCC_A2	
T(C)	fraction solid
1785.375	0.9239971E-03
1780.375	0.6494391E-01
1775.375	0.1226644
1770.375	0.1749130
1765.375	0.2223831
1760.375	0.2656597
1755.375	0.3052393
1750.375	0.3415456
1745.375	0.3749422
1740.375	0.4057426
1735.375	0.4342186
1730.375	0.4606065
1725.375	0.4851127
1720.375	0.5079185
1715.375	0.5291833
1710.375	0.5490480
1705.375	0.5676374
1700.375	0.5850626
1695.375	0.6014224
1690.375	0.6168054
1685.375	0.6312910
1680.375	0.6449504
1675.375	0.6578480
1670.375	0.6700418
1665.375	0.6815843
1660.375	0.6925233
1655.375	0.7029020
1650.375	0.7127599
1645.375	0.7221332
1640.375	0.7310546
1635.375	0.7395545
1630.375	0.7476604
1625.375	0.7553979
1620.375	0.7627903
1615.375	0.7698592
1610.375	0.7766247
1605.375	0.7831051
1600.375	0.7893176
1595.375	0.7952779
1590.375	0.8010009
1585.375	0.8065002
1580.375	0.8117885
1575.375	0.8168779
1570.375	0.8217793
1565.375	0.8265033
1560.375	0.8310595
1555.375	0.8354570
1550.375	0.8397046
1545.375	0.8438103
1540.375	0.8477816
1535.375	0.8516258
1530.375	0.8553497
1525.375	0.8589602
1520.375	0.8624627
1515.375	0.8658633
1510.375	0.8691676
1505.375	0.8723809
1500.375	0.8755083
1495.375	0.8785546
1490.375	0.8815245
1485.375	0.8844227
1480.375	0.8872536
1475.375	0.8900213
1470.375	0.8927303
1465.375	0.8953845
1460.375	0.8979881
1455.375	0.9005451
1450.375	0.9030587
1445.375	0.9055346
1440.375	0.9079761
1435.375	0.9103873
1430.375	0.9127724
1425.375	0.9151359
1420.375	0.9174820
1415.375	0.9198153
1410.375	0.9221406
1405.375	0.9244628
1400.375	0.9267870
1395.375	0.9291184
1390.375	0.9314626
1385.375	0.9338254
1380.375	0.9362126
1375.375	0.9386303
1370.375	0.9410850
1365.375	0.9435828
1360.375	0.9461303
1355.375	0.9487336
1350.375	0.9513987

```

1345.375      0.9541312
1344.897      0.9543838
PHASE REGION:BCC_A2 + FCC_A1
T(C)          fraction solid
1344.738      1.000000
Calculating properties ...
Liquidus temperature: 2058.595 K
Solidus temperature: 1617.888 K

```



```

.....
The following axis variables are available

T - Temperature in Celsius
NL/BL/VL - Mole/mass/volume fraction of liquid
NS/BS/VS - Mole/mass/volume fraction of all solid phases
NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
VS(ph) - Volume fraction of a solid phase
W(ph,el) - Weight fraction of an element in a phase
X(ph,el) - Mole fraction of an element in a phase
Y(ph,el) - Site fraction of an element in a phase
NN(ph,el) - Distribution of an element in a phase
NH/BH - Heat release and Latent heat per mole/gram
CP/BCP - Apparent heat capacity per mole/gram
NV/NV(ph) - Molar volume of the system or a phase
DS/DS(ph) - Average density of the system or a phase
BT - Apparent volumetric TEC of the system
DVIS(ph) - Dynamic viscosity of a phase
KVIS(ph) - Kinematic viscosity of a phase
SURF(ph) - Surface tension of a liquid phase
ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
THCD/THCD(ph) - Thermal conductivity of the system or a phase
THRS/THRS(ph) - Thermal resistivity of the system or a phase
THDF/THDF(ph) - Thermal diffusivity of the system or a phase
DGV - Driving force for evaporation
DHV - Evaporation enthalpy
MMG - Molar mass of gas
XAVG(el) - Mole fraction of an element in solid phases
WAVG(el) - Mass fraction of an element in solid phases

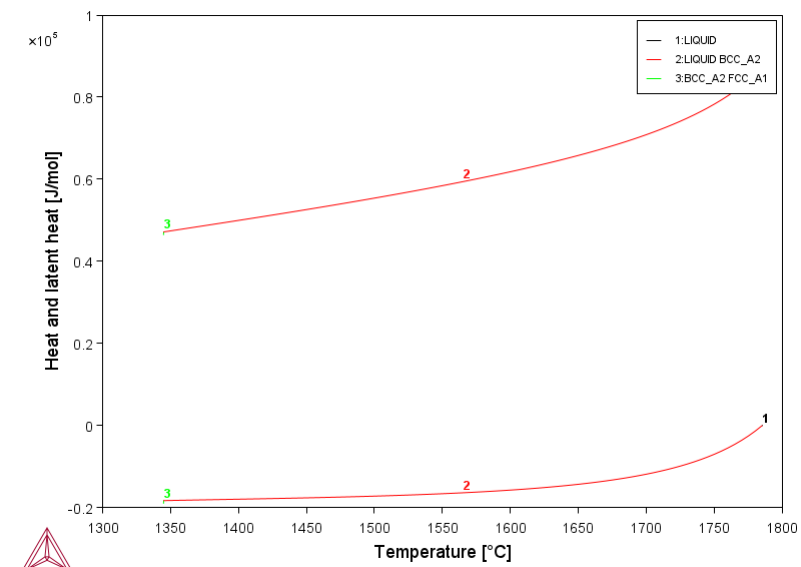
"el" and "ph" are name of element and phase, respectively
"*" can be used as a wild character for "el" and "ph"
.....

```

```

POST:Hit RETURN to continue
POST: s-d-a x t
POST: s-d-a y nh
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,,,,,,,

```



POST: set-inter
POST:

tcex16

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex16\tcex16.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Second order transition of the Al-Fe system

SYS:

SYS: @@ This example calculates the second order transition

SYS: @@ line in the Bcc field of the Al-Fe system.

SYS:

SYS: @@ Note that an SSOL database license is required to run

SYS: @@ the example.

SYS:

SYS: SET-LOG ex16,,

SYS: GO DA

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: SW SSOL7

... the command in full is SWITCH_DATABASE
Current database: SGTE Alloy Solutions v7.0

VA DEFINED

BCC_B2 FCC_L12 FCC_4SL

HCP_ORD GAS:G REJECTED

A2_BCC B2_BCC REJECTED

TDB_SSOL7: D-SYS AL FE

... the command in full is DEFINE_SYSTEM
AL FE DEFINED

TDB_SSOL7: REJ PH /ALL

... the command in full is REJECT

LIQUID:L	FCC_A1	BCC_A2
B2	HCP_A3	HCP_ZN
DHCP	DIAMOND_A4	BCT_A5
TETRAGONAL_U	CBCC_A12	CUB_A13
ORTHORHOMBIC_A20	RHOMBO_C19	LAVES_C14
C14_LAVES	LAVES_C15	LAVES_C36
M4N	ALM_D019	ALCE_AMORPHOUS
ALCR2_C11B	ALCU_THETA	AL2FE
AL5FE2	AL5FE4	AL13FE4
ALLI	AL4MN	AL6MN
AL11MN4	AL12MN	ALNB3
AL3NB	AL3NI2	AL3PD2_D513
ALPD_B2	AL2PD5	ALPD2_C37
ALPT3	ALTI	CR3SI_A15
D_GAMMA	FEPD	FEPD3
FESB	FEU6	FE2U
FE23Y6	FE2Y	FEUZR_DELTA
FEZR2	FEZR3 REJECTED	

TDB_SSOL7: @@ The BCC phase has B2 ordering in this system.

TDB_SSOL7: @@ Note that this is modelled with two sublattices with

TDB_SSOL7: @@ both components in both sublattices

TDB_SSOL7:

TDB_SSOL7: REST PH LIQ BCC_B2 BCC_A2

... the command in full is RESTORE
LIQUID:L BCC_B2 BCC_A2
RESTORED

TDB_SSOL7: LI-SYS

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:

LIQUID:L :AL FE:
BCC_A2 :AL FE:VA:
BCC_B2 :AL FE:AL FE:VA:

TDB_SSOL7: GET

... the command in full is GET_DATA

08:58:02,028 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set BCC_B2#2

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_SSOL7: GO P-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: li-st p

... the command in full is LIST_STATUS

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
BCC_B2#2	ENTERED	0.000000E+00	0.000000E+00
BCC_B2#1	ENTERED	0.000000E+00	0.000000E+00
LIQUID	ENTERED	0.000000E+00	0.000000E+00

POLY:

POLY: advanced global_minimization y 10000

```

... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY:
POLY: @@ Set conditions where the BCC phase should be ordered
POLY: SET-COND P=1E5,N=1,T=400,X(AL)=-.4
... the command in full is SET_CONDITION
POLY: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      10026 grid points in      0.672 s
Found the set of lowest grid points in      0.003 s
Calculated POLY solution      0.104 s, total time      0.779 s
POLY: @@ Use option N in order to see how Al and Fe distribute
POLY: @@ on the sublattices
POLY:
POLY: LIST-EQ
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: N
Output from POLY-3, equilibrium =      1, label A0 , database: SSOL7

Conditions:
P=100000, N=1, T=400, X(AL)=0.4
DEGREES OF FREEDOM 0

Temperature      400.00 K ( 126.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 4.43010E+01
Total Gibbs energy -3.81486E+04, Enthalpy -2.55850E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL      4.0000E-01  2.4362E-01 4.1973E-08 -5.6493E+04 SER
FE      6.0000E-01  7.5638E-01 4.1248E-04 -2.5919E+04 SER

BCC_B2#2      ORD      Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.4301E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 7.56376E-01 AL 2.43624E-01
Constitution:
Sublattice 1, Number of sites 5.0000E-01
AL 7.99996E-01 FE 2.00004E-01
Sublattice 2, Number of sites 5.0000E-01
FE 9.99996E-01 AL 4.22881E-06
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Change the condition of the Al amount so that the
POLY: @@ site-fractions in the two sublattices will have a
POLY: @@ certain difference. If they are the same, the BCC
POLY: @@ phase is disordered. BCC_B2#2 is the default
POLY: @@ ordered phase.
POLY:
POLY: SET-COND X(AL)=NONE
... the command in full is SET_CONDITION
POLY: SET-COND Y(BCC_B2#2,FE#1)-Y(BCC_B2#2,FE#2)=-0.1
... the command in full is SET_CONDITION
POLY: C-S P BCC_B2#1=SUS
... the command in full is CHANGE_STATUS
POLY: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
26 ITS, CPU TIME USED 1 SECONDS
POLY: LIST-EQ
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/:Hit RETURN to continue
Options /VWNS/: @@ Set a smaller difference. This is as close to the
Output from POLY-3, equilibrium =      1, label A0 , database: SSOL7

Conditions:
P=100000, N=1, T=400, Y(BCC_B2#2,FE)-Y(BCC_B2#2,FE#2)=-0.1
DEGREES OF FREEDOM 0

Temperature      400.00 K ( 126.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.36842E+01
Total Gibbs energy -1.86969E+04, Enthalpy -4.69474E+03, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL      7.4926E-02  3.7658E-02 7.3790E-14 -1.0056E+05 SER
FE      9.2507E-01  9.6234E-01 2.6569E-02 -1.2066E+04 SER

BCC_B2#2      ORD      Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.3684E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.62342E-01 AL 3.76585E-02
Constitution:
Sublattice 1, Number of sites 5.0000E-01
FE 8.75074E-01 AL 1.24926E-01
Sublattice 2, Number of sites 5.0000E-01
FE 9.75074E-01 AL 2.49265E-02
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00
POLY: @@ second order transition as it is possible to be
POLY:
POLY: SET-COND Y(BCC_B2#2,FE#1)-Y(BCC_B2#2,FE#2)=1E-4
... the command in full is SET_CONDITION
POLY: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
14 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Now vary the temperature using these conditions
POLY: SET-AXIS-VAR 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: T
Min value /0/: 400
Max value /1/: 2000
Increment /40/: 10
POLY: @@ Always save before STEP or MAP (unless you want to
POLY: @@ overlay the new results on some previous results)
POLY:
POLY: SAVE tcex16 Y
... the command in full is SAVE_WORKSPACES
POLY: STEP NORMAL
... the command in full is STEP_WITH_OPTIONS

```


No initial equilibrium, using default
 Step will start from axis value 400.000
 ...OK

Phase Region from 400.000 for:
 BCC_B2#2
 Global test at 4.80000E+02 OK
 Global test at 5.80000E+02 OK
 Global test at 6.80000E+02 OK
 Global test at 7.80000E+02 OK
 Global test at 8.80000E+02 OK
 Global test at 9.80000E+02 OK
 Global test at 1.08000E+03 OK
 Global test at 1.18000E+03 OK
 Global test at 1.28000E+03 OK
 Global test at 1.38000E+03 OK
 Global test at 1.48000E+03 OK
 Global test at 1.58000E+03 OK
 Global check of adding phase at 1.64515E+03
 Calculated 127 equilibria

Phase Region from 1645.15 for:
 LIQUID
 BCC_B2#2
 Global check of removing phase at 1.64515E+03
 Calculated 3 equilibria

Phase Region from 1645.15 for:
 BCC_B2#2
 Global Check of adding phase at 1.64515E+03
 Calculated 3 equilibria

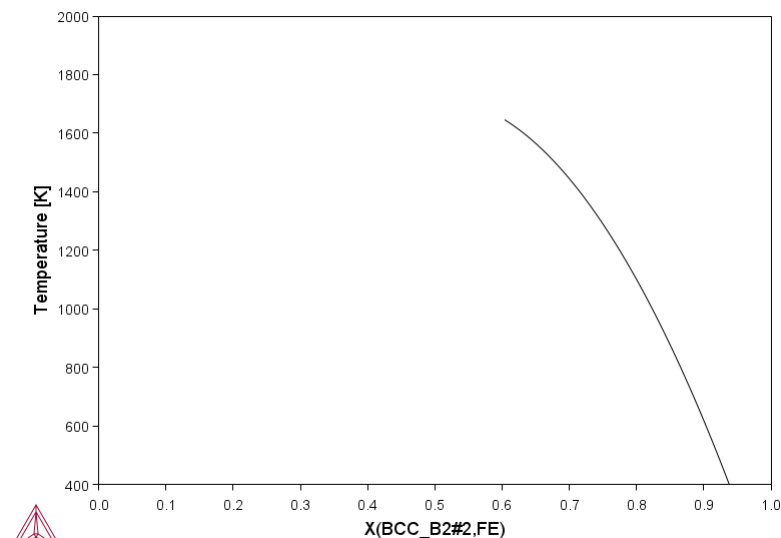
Phase Region from 1645.15 for:
 LIQUID
 BCC_B2#2
 Calculated 3 equilibria
 Sorry cannot continue 0 189 1 1.6451539E+03
 *** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex16\tcex16.POLY3

POLY: POST
 POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: SET-DIA-AXIS X X(BCC_B2#2,FE)
 ... the command in full is SET_DIAGRAM_AXIS
 POST: SET-DIA-AXIS Y T-K
 ... the command in full is SET_DIAGRAM_AXIS
 POST: SET-SCAL X N 0 1
 ... the command in full is SET_SCALING_STATUS
 POST: SET-SCAL Y N 400 2000
 ... the command in full is SET_SCALING_STATUS
 POST:
 POST: set-title example 16a
 POST:
 POST: SET_EXP_FILE FORMAT 5
 POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 POST: SET_EXP_FILE_FORMAT 10
 POST:
 POST: PLOT
 ... the command in full is PLOT_DIAGRAM

example 16a



POST:
 POST:Hit RETURN to continue
 POST: @@ Write on file to plot with a phase diagram
 POST: MAKE TCX16
 ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 POST:
 POST: BACK
 POLY: GO DA
 ... the command in full is GOTO_MODULE
 TDB_SSOL7: @@ Get data for all phases stable in Al-Fe
 TDB_SSOL7: REJ-SYS
 ... the command in full is REJECT
 VA_DEFINED
 BCC_B2 FCC_L12 FCC_4SL
 HCP_ORD GAS:G REJECTED
 A2_BCC B2_BCC REJECTED
 REINITIATING GES
 TDB_SSOL7: D-SYS AL FE
 ... the command in full is DEFINE_SYSTEM
 AL FE_DEFINED

```

TDB_SSOL7: L-SYS
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENT
LIQUID:L      :AL FE:
FCC_A1        :AL FE:VA:
BCC_A2        :AL FE:VA:
B2            :AL:VA:
HCP_A3        :AL FE:VA:
HCP_ZN        :AL FE:VA:
DHCP          :AL:VA:
DIAMOND_A4     :AL:
BCT_A5        :AL:
TETRAGONAL_U  :FE:
CBCC_A12      :AL FE:VA:
CUB_A13       :AL FE:VA:
ORTHORHOMBIC_A20 :FE:
RHOMBO_C19    :AL:
LAVES_C14     :AL FE:AL FE:
C14_LAVES     :FE:FE:
LAVES_C15     :AL FE:AL FE:
LAVES_C36     :AL:AL:
M4N           :FE:VA:
ALM_D019      :AL:AL:
ALCE_AMORPHOUS :AL:
ALCR2_C11B    :AL:AL:
ALCU_THETA    :AL:AL:
AL2FE         :AL:FE:
AL5FE2        :AL:FE:
AL5FE4        :AL FE:
AL13FE4       :AL:FE:AL VA:
ALLI          :AL:VA:
AL4MN         :AL:FE:
AL6MN         :AL:FE:
AL11MN4       :AL:FE:
AL12MN        :AL:FE:
ALNB3         :AL:AL:
AL3NB         :AL:AL:
AL3NI2        :AL:AL:VA:
AL3PD2_D513   :AL:AL:
ALPD_B2       :AL:VA:
AL2PD5        :AL:AL:
ALPD2_C37     :AL:AL:
ALPT3         :AL:AL:
ALTI          :AL:AL:
CR3SI_A15     :FE:AL:VA:
D_GAMMA       :AL:
FEPD          :FE:FE:
FEPD3         :FE:FE:
FESB          :FE:FE:
FEU6          :FE:FE:
FE2U          :FE:FE:
FE23Y6        :FE:FE:
FE2Y          :FE:FE:
FEUZR_DELTA   :FE:FE:
FEZR2         :FE:FE:
FEZR3         :FE:FE:
TDB_SSOL7: REJ PH /ALL
... the command in full is REJECT
LIQUID:L      FCC_A1      BCC_A2
B2            HCP_A3      HCP_ZN
DHCP          DIAMOND_A4   BCT_A5
TETRAGONAL_U  CBCC_A12    CUB_A13
ORTHORHOMBIC_A20 RHOMBO_C19 LAVES_C14
C14_LAVES     LAVES_C15   LAVES_C36
M4N           ALM_D019    ALCE_AMORPHOUS
ALCR2_C11B    ALCU_THETA   AL2FE
AL5FE2        AL5FE4     AL13FE4
ALLI          AL4MN      AL6MN
AL11MN4       AL12MN     ALNB3
AL3NB         AL3NI2     AL3PD2_D513
ALPD_B2       AL2PD5     ALPD2_C37
ALPT3         ALTI       CR3SI_A15
D_GAMMA       FEPD       FEPD3
FESB          FEU6       FE2U
FE23Y6        FE2Y       FEUZR_DELTA
FEZR2         FEZR3      REJECTED
TDB_SSOL7: REST PH LIQ BCC_B2 FCC_A1 BCC_A2 AL13FE4 AL2FE AL5FE2 AL5FE4
... the command in full is RESTORE
LIQUID:L      BCC_B2      FCC_A1
BCC_A2        AL13FE4     AL2FE
AL5FE2        AL5FE4     RESTORED
TDB_SSOL7: GET
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set BCC_B2#2
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_SSOL7: GO P-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ Calculate an equilibrium where BCC is ordered
POLY: S-C T=1300,P=1E5,N=1,X(AL)=.3
... the command in full is SET_CONDITION
POLY: C-E
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 10655 grid points in 0.161 s
Found the set of lowest grid points in 0.003 s
Calculated POLY solution 0.012 s, total time 0.176 s
POLY: @@ List the equilibrium. Note that option N gives the
POLY: @@ constitution of the BCC phase and this shows that the
POLY: @@ site-fractions are different in the two sublattices,

```

```

POLY: @@ i.e. the BCC is ordered
POLY:
POLY: L-E
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/: N
Output from POLY-3, equilibrium =      1, label A0  , database: SSOL7

Conditions:
T=1300, P=100000, N=1, X(AL)=0.3
DEGREES OF FREEDOM 0

Temperature 1300.00 K ( 1026.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 4.71875E+01
Total Gibbs energy -8.63003E+04, Enthalpy 1.26381E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              3.0000E-01  1.7154E-01 3.1606E-05 -1.1200E+05 SER
FE              7.0000E-01  8.2846E-01 9.4427E-04 -7.5285E+04 SER

BCC_B2#2      ORD      Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.7187E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 8.28459E-01 AL 1.71541E-01
Constitution:
Sublattice 1, Number of sites 5.0000E-01
FE 5.22550E-01 AL 4.77450E-01
Sublattice 2, Number of sites 5.0000E-01
FE 8.77450E-01 AL 1.22550E-01
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Set axis
POLY: S-A-V 1 X(AL)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: S-A-V 2 T
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 400
Max value /1/: 2000
Increment /40/: 25
POLY: SAVE tcex16 Y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: MAP
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Trying global minimization! 3
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Trying global minimization! 3
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 5.828E-01 4.100E+02
** AL2FE
BCC_B2#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 5.829E-01 4.000E+02
** AL2FE
BCC_B2#2
Calculated.. 40 equilibria

Phase region boundary 3 at: 6.023E-01 1.368E+03
** AL2FE
** AL5FE4

```

BCC_B2#2

Phase region boundary 4 at: 5.672E-01 1.368E+03
 ** AL5FE4
 BCC_B2#2
 Calculated. 7 equilibria

Phase region boundary 5 at: 5.452E-01 1.496E+03
 ** LIQUID
 ** AL5FE4
 BCC_B2#2

Phase region boundary 6 at: 5.550E-01 1.496E+03
 ** LIQUID
 BCC_B2#2
 Calculated 50 equilibria

Phase region boundary 7 at: 5.842E-01 1.496E+03
 ** LIQUID
 AL5FE4
 Calculated. 6 equilibria

Phase region boundary 8 at: 6.593E-01 1.430E+03
 ** LIQUID
 ** AL5FE2
 AL5FE4

Phase region boundary 9 at: 6.744E-01 1.430E+03
 ** AL5FE2
 AL5FE4
 Calculated. 2 equilibria

Phase region boundary 10 at: 6.740E-01 1.428E+03
 ** AL2FE
 ** AL5FE2
 AL5FE4

Phase region boundary 11 at: 6.502E-01 1.428E+03
 ** AL2FE
 AL5FE4
 Calculated. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 12 at: 6.905E-01 1.428E+03
 ** AL2FE
 AL5FE2
 Calculated.. 43 equilibria
 Terminating at axis limit.

Phase region boundary 13 at: 6.993E-01 1.430E+03
 LIQUID
 ** AL5FE2
 Calculated. 12 equilibria

Phase region boundary 14 at: 7.362E-01 1.424E+03
 LIQUID
 ** AL13FE4
 ** AL5FE2

Phase region boundary 15 at: 7.556E-01 1.424E+03
 LIQUID
 ** AL13FE4
 Calculated. 24 equilibria

Phase region boundary 16 at: 8.723E-01 9.271E+02
 LIQUID
 ** AL13FE4
 ** FCC_A1

Phase region boundary 17 at: 9.955E-01 9.271E+02
 LIQUID
 ** FCC_A1
 Calculated 10 equilibria

Phase region boundary 18 at: 8.813E-01 9.271E+02
 AL13FE4
 ** FCC_A1
 Calculated.. 23 equilibria
 Terminating at axis limit.

Phase region boundary 19 at: 7.337E-01 1.424E+03
 ** AL13FE4
 AL5FE2
 Calculated.. 42 equilibria
 Terminating at axis limit.

Phase region boundary 20 at: 5.828E-01 4.100E+02
 ** AL2FE
 BCC_B2#2
 Calculated. 40 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 8.364E-03 1.237E+03
 BCC_B2#1
 ** FCC_A1
 Calculated 19 equilibria

Phase region boundary 22 at: 8.364E-03 1.237E+03
 BCC_B2#1
 ** FCC_A1
 Calculated 39 equilibria

Phase region boundary 23 at: 3.562E-01 1.702E+03
 ** LIQUID
 BCC_B2#1
 Calculated 35 equilibria

Phase region boundary 24 at: 3.562E-01 1.702E+03
 ** LIQUID
 BCC_B2#1
 Calculated. 17 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 5.828E-01 4.100E+02
 ** AL2FE
 BCC_B2#2

Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 26 at: 5.828E-01 4.100E+02
 ** AL2FE
 BCC_B2#2
 Calculated.. 40 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 8.825E-01 4.100E+02
 ** AL13FE4
 FCC_A1
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 28 at: 8.825E-01 4.100E+02
 ** AL13FE4
 FCC_A1
 Calculated.. 22 equilibria
 Terminating at known equilibrium

Phase region boundary 29 at: 8.825E-01 4.100E+02
 ** AL13FE4
 FCC_A1
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 30 at: 8.825E-01 4.100E+02
 ** AL13FE4
 FCC_A1
 Calculated.. 22 equilibria
 Terminating at known equilibrium

Phase region boundary 31 at: 5.820E-01 9.367E+02
 ** AL2FE
 BCC_B2#2
 Calculated.. 23 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 32 at: 5.820E-01 9.367E+02
 ** AL2FE
 BCC_B2#2
 Calculated.. 19 equilibria
 Terminating at known equilibrium

Phase region boundary 33 at: 8.765E-01 9.367E+02
 LIQUID
 ** AL13FE4
 Calculated.. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 34 at: 8.765E-01 9.367E+02
 LIQUID
 ** AL13FE4
 Calculated.. 27 equilibria
 Terminating at known equilibrium

Phase region boundary 35 at: 1.862E-02 1.463E+03
 ** BCC_B2#1
 FCC_A1
 Calculated 28 equilibria

Phase region boundary 36 at: 1.862E-02 1.463E+03
 ** BCC_B2#1
 FCC_A1
 Calculated 12 equilibria

Phase region boundary 37 at: 6.298E-01 1.463E+03
 LIQUID
 ** AL5FE4
 Calculated.. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 38 at: 6.298E-01 1.463E+03
 LIQUID
 ** AL5FE4
 Calculated.. 7 equilibria
 Calculated 7 equilibria

Phase region boundary 39 at: 6.298E-01 1.463E+03
 LIQUID
 ** AL5FE4
 Calculated.. 6 equilibria
 Terminating at known equilibrium

Phase region boundary 40 at: 1.032E-02 1.813E+03
 LIQUID
 ** BCC_B2#1
 Calculated 13 equilibria

Phase region boundary 41 at: 1.032E-02 1.813E+03
 LIQUID
 ** BCC_B2#1
 Calculated.. 44 equilibria
 Calculated 44 equilibria

Phase region boundary 42 at: 1.032E-02 1.813E+03
 LIQUID
 ** BCC_B2#1
 Calculated.. 47 equilibria
 Terminating at known equilibrium

Phase region boundary 43 at: 3.201E-01 1.728E+03
 LIQUID
 ** BCC_B2#1
 Calculated 34 equilibria

Phase region boundary 44 at: 3.201E-01 1.728E+03
 LIQUID
 ** BCC_B2#1
 Calculated.. 20 equilibria
 Calculated 20 equilibria

```

Phase region boundary 45 at: 3.201E-01 1.728E+03
  LIQUID
  ** BCC_B2#1
Calculated. 22 equilibria
Terminating at known equilibrium

Phase region boundary 46 at: 6.421E-01 1.451E+03
  LIQUID
  ** AL5FE4
Calculated. 7 equilibria
Calculated. 7 equilibria

Phase region boundary 47 at: 6.421E-01 1.451E+03
  LIQUID
  ** AL5FE4
Calculated. 6 equilibria
Terminating at known equilibrium

Phase region boundary 48 at: 6.421E-01 1.451E+03
  LIQUID
  ** AL5FE4
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 49 at: 8.763E-01 9.396E+02
  LIQUID
  ** AL13FE4
Calculated. 28 equilibria
Terminating at known equilibrium

Phase region boundary 50 at: 8.763E-01 9.396E+02
  LIQUID
  ** AL13FE4
Calculated. 2 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex16\tcex16.POLY3
CPU time for mapping 11 seconds

```

```

POLY:
POLY: POST
      POLY-3 POSTPROCESSOR VERSION 3.2

```

```

Setting automatic diagram axes

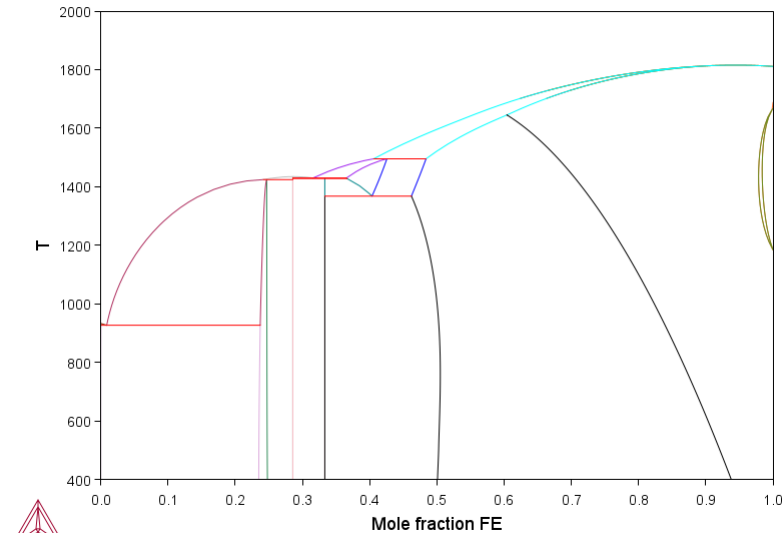
```

```

POST:
POST: S-D-A X M-F FE
      ... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y T
      ... the command in full is SET_DIAGRAM_AXIS
POST: @@ Append the previous line for the 2nd order transition
POST: A-E-D Y TCX16
      ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 16b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
      ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
      ... the command in full is PLOT_DIAGRAM

```

example 16b



```

POST:
POST: set-inter
      ... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex17

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex17\tcex17.TCM.test"

SYS: set-echo

SYS:

SYS: @@ The pseudo-binary system - CaO-SiO2

SYS:

SYS: @@ This example calculates the pseudo-binary system

SYS: @@ CaO-SiO2 using the Oxide Demo database.

SYS:

SYS: set-log ex17,,,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

TDB_TCFe11: REJECTED

TDB_TCFe11: @@ This database can be used both for pseudobinary

TDB_TCFe11: @@ systems like the one in this case, CaO-SiO2, or

TDB_TCFe11: @@ for full ternary systems like Ca-Fe-O.

TDB_TCFe11:

TDB_TCFe11: sw OXDEMO

... the command in full is SWITCH_DATABASE

Current database: Oxide Demo Database v6.0

VA /- DEFINED

TDB_OXDEMO: @@ Note that /- represents the electron.

TDB_OXDEMO: d-sys ca si o

... the command in full is DEFINE_SYSTEM

CA SI O

DEFINED

TDB_OXDEMO: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS

GAS:G :CA CA101 CA2 O 01SI1 02 02SI1 02SI2 03 SI SI2 SI3:

#Gas # # # #6038cfcf41046d48150aa2e6

IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 VA SIO2:

#Liquid # # #Liquid metal and slag mixture. #6038cfda41046d48150aa2e7

BCC A2 :CA SI:O VA:

#Body-Centered Cubic (W, A2, bcc) #cI2 #Im-3m # #602e7f15105f8553a825b4e4

CA2SIO4_ALPHA_A:I :CA+2:CA+2:SIO4-4:

#Ca2SiO4 #hP24 #P6_3/mmc #This is 2CaO.SiO2 and 3CaO.P2O5.

#602eac57674ba8b79b43f865

CA2SIO4_ALPHA_PRIME:I :CA+2:CA+2:SIO4-4:

#K2CoCl4 #oP84 #Pna2_1 #This is Ca2SiO4. #602eaca674ba8b79b43f866

CRISTOBALITE:I :SI+4:SIO4-4:

#Ideal beta-Cristobalite (SiO2, C9) #cF24 #Fd-3m #SiO2 with AlPO4

solubility. #602e7f15105f8553a825b559

DIAMOND FCC_A4 :SI:VA O:

#Diamond (A4) #cF8 #Fd-3m #This is Silicon #602e7f15105f8553a825b4e8

FCC_A1 :CA SI:O VA:

#Face-Centered Cubic (Cu, Al, fcc) #cF4 #Fm-3m #This is FCC_A1 solid

solution and TiO and VO cubic oxides. #602e7f15105f8553a825b4d9

HALITE:I :CA+2 VA:O-2:

#Rock Salt (NaCl, B1) #cF8 #Fm-3m #This is BaO, CaO, CoO, FeO, MgO, MnO

and NiO #602e7f15105f8553a825b4f8

HATRURITE:I :CA+2:SIO4-4:O-2:

#Ca3(SiO4)O-b #hR81 #R3m #This is 3CaO.SiO2 #602eadc3674ba8b79b43f86a

HCP_A3 :CA SI:O VA:

#Hexagonal Close Packed (Mg, A3, hcp) #hP2 #P6_3/mmc #HCP_A3 also

describes hexagonal carbides and nitrides. #602e7f15105f8553a825b4e6

LARNITE:I :CA+2:SI+4:O-2:

#Parawollastonite (CaSiO3, S33(II)) #mP60 #P2_1/c #This is 2CaO.SiO2

(metastable at 1 atm) #602e7f15105f8553a825b68e

OLIVINE:I :CA+2:CA+2:SI+4:O-2:

#Forsterite (Mg2SiO4, S12) #oP28 #Pnma #This is Calcio-olivine (Ca2SiO4)

- Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite

(Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4)

solid solution dissolving Cr and Cu. #602e7f15105f8553a825b684

PROTO_PYROXENE:I :CA+2:SI+4:O-2:

#MgSiO3 #oP40 #Pbcn #This is proto- enstatite (MgSiO3) and proto-diopside

(CaMgSi2O6) dissolving Co, Cr, and Fe. #602ead24674ba8b79b43f867

PSEUDO_WOLLASTONITE:I :CA+2:SI+4:O-2:

#CaSiO3 #mS120 #C2/c #This is CaO.SiO2 with Ba solubility

#602ead45674ba8b79b43f868

QUARTZ:I :SI+4:SIO4-4:

#alpha-Quartz (low Quartz) #hP9 #P3_121 #SiO2 with AlPO4 solubility.

#602e7f15105f8553a825b6e2

RANKINITE:I :CA+2:SI+4:O-2:

#3CaO.2SiO2 #mP48 #P2_1/c # #602eaf3286932e6d2e4f532d

TRIDYMITE:I :SI+4:SIO4-4:

#Monoclinic (Cc) Low Tridymite (SiO2) #mS144 #Cc #SiO2 with AlPO4

solubility. #602e7f15105f8553a825b82e

WOLLASTONITE:I :CA+2:SI+4:O-2:

#Wollastonite (CaSiO3) #aP30 #P-1 #This is CaO.SiO2 with Ba, Fe, Mg and

Mn solubility #602e7f15105f8553a825b913

TDB_OXDEMO: @@ If we want to calculate a pseudobinary system

TDB_OXDEMO: @@ we must take away all phases and constituents that

TDB_OXDEMO: @@ make it possible for the phase to exist outside the

TDB_OXDEMO: @@ composition line from CaO to SiO2.

TDB_OXDEMO:

TDB_OXDEMO: @@ This means that for the IONIC_LIQ phase the

TDB_OXDEMO: @@ constituent Va should be suspended for systems with

TDB_OXDEMO: @@ no degree of freedom with respect to oxygen.

TDB_OXDEMO:

TDB_OXDEMO: rej const

```

... the command in full is REJECT
PHASE: ion
SUBLATTICE NUMBER: 2
CONSTITUENT: va
    VA IN IONIC_LIQ:Y SUBLATTICE    2 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
GAS:G          :CA CA101 CA2 O O1SI1 O2 O2SI1 O2SI2 O3 SI SI2 SI3:
#Gas # # # #6038cfcf41046d48150aa2e6
IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 SIO2:
#Liquid # # #Liquid metal and slag mixture. #6038cfda41046d48150aa2e7
BCC_A2      :CA SI:O VA:
#Body-Centered Cubic (W, A2, bcc) #cI2 #Im-3m # #602e7f15105f8553a825b4e4
CA2SIO4 ALPHA_A:I :CA+2:CA+2:SIO4-4:
#Ca2SIO4 #hP24 #P6_3/mmc #This is 2CaO.SiO2 and 3CaO.P2O5.
#602eac57674ba8b79b43f865
CA2SIO4 ALPHA_PRIME:I :CA+2:CA+2:SIO4-4:
#K2CoCl4 #oP84 #Pna2_1 #This is Ca2SIO4. #602eacaf674ba8b79b43f866
CRISTOBALITE:I :SI+4:SIO4-4:
#Ideal beta-Cristobalite (SiO2, C9) #cF24 #Fd-3m #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b559
DIAMOND FCC_A4 :SI:VA O:
#Diamond (A4) #cF8 #Fd-3m #This is Silicon #602e7f15105f8553a825b4e8
FCC_A1      :CA SI:O VA:
#Face-Centered Cubic (Cu, Al, fcc) #cF4 #Fm-3m #This is FCC_A1 solid
solution and TiO and VO cubic oxides. #602e7f15105f8553a825b54d9
HALITE:I     :CA+2 VA:O-2:
#Rock Salt (NaCl, B1) #cF8 #Fm-3m #This is BaO, CaO, CoO, FeO, MgO, MnO
and NiO #602e7f15105f8553a825b4f8
HATRURITE:I :CA+2:SIO4-4:O-2:
#Ca3(SiO4)O-b #hR81 #R3m #This is 3CaO.SiO2 #602eadc3674ba8b79b43f86a
HCP_A3      :CA SI:O VA:
#Hexagonal Close Packed (Mg, A3, hcp) #hP2 #P6_3/mmc #HCP_A3 also
describes hexagonal carbides and nitrides. #602e7f15105f8553a825b4e6
LARNITE:I    :CA+2:SI+4:O-2:
#Parawollastonite (CaSiO3, S33(II)) #mP60 #P2_1/c #This is 2CaO.SiO2
(metastable at 1 atm) #602e7f15105f8553a825b68e
OLIVINE:I    :CA+2:CA+2:SI+4:O-2:
#Forsterite (Mg2SiO4, S12) #oP28 #Pnma #This is Calcio-olivine (Ca2SiO4)
- Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite
(Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4)
solid solution dissolving Cr and Cu. #602e7f15105f8553a825b684
PROTO_PYROXENE:I :CA+2:SI+4:O-2:
#MgSiO3 #oP40 #Pbcn #This is proto- enstatite (MgSiO3) and proto-diopside
(CaMgSi2O6) dissolving Co, Cr, and Fe. #602ead24674ba8b79b43f867
PSEUDO_WOLLASTONITE:I :CA+2:SI+4:O-2:
#CaSiO3 #mS120 #C2/c #This is CaO.SiO2 with Ba solubility
#602ead45674ba8b79b43f868
QUARTZ:I     :SI+4:SIO4-4:
#alpha-Quartz (low Quartz) #hP9 #P3_121 #SiO2 with AlPO4 solubility.
#602e7f15105f8553a825b6e2
RANKINITE:I :CA+2:SI+4:O-2:
#3CaO.2SiO2 #mP48 #P2_1/c # #602eaf3286932e6d2e4f532d
TRIDYMITTE:I :SI+4:SIO4-4:
#Monoclinic (Cc) Low Tridymite (SiO2) #mS144 #Cc #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b82e
WOLLASTONITE:I :CA+2:SI+4:O-2:
#Wollastonite (CaSiO3) #aP30 #P-1 #This is CaO.SiO2 with Ba, Fe, Mg and
Mn solubility #602e7f15105f8553a825b913
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO: @@ The phase names may seem unfamiliar but this is due
TDB_OXDEMO: @@ to the attempt to create a general database. Thus lime
TDB_OXDEMO: @@ (CaO) is called HALITE which is the generic phase name
TDB_OXDEMO: @@ for this structure. HALITE is also the wudstite phase
TDB_OXDEMO: @@ (FeO) and the periclase phase (MgO).
TDB_OXDEMO:
TDB_OXDEMO: @@ Note also that many phases are modelled with
TDB_OXDEMO: @@ sublattices and vacancies in order to allow for
TDB_OXDEMO: @@ non-stoichiometry in higher order systems.
TDB_OXDEMO:
TDB_OXDEMO: @@ For simplicity reject all phases except those we know
TDB_OXDEMO: @@ should be stable in this system.
TDB_OXDEMO:
TDB_OXDEMO: rej ph /all
... the command in full is REJECT
GAS:G          IONIC_LIQ:Y          BCC_A2
CA2SIO4_ALPHA_A:I    CA2SIO4_ALPHA_PRIME:I    CRISTOBALITE:I
DIAMOND_FCC_A4      FCC_A1          HALITE:I
HATRURITE:I         HCP_A3          LARNITE:I
OLIVINE:I           PROTO_PYROXENE:I    PSEUDO_WOLLASTONITE:I
QUARTZ:I            RANKINITE:I        TRIDYMITTE:I
WOLLASTONITE:I    REJECTED
TDB_OXDEMO: rest ph ionic_liq ca2sio4_alpha ca2sio4_alpha_prime cristobalite halite hatrurite
... the command in full is RESTORE
*** ERROR CA2SIO4_ALPHA INPUT IGNORED
IONIC_LIQ:Y          CA2SIO4_ALPHA_PRIME:I    CRISTOBALITE:I
HALITE:I             HATRURITE:I    RESTORED
TDB_OXDEMO: rest ph larnite olivine pseudo_wollastonite quartz rankinite
... the command in full is RESTORE
LARNITE:I           OLIVINE:I          PSEUDO_WOLLASTONITE:I
QUARTZ:I            RANKINITE:I    RESTORED
TDB_OXDEMO: rest ph tridymite wollastonite
... the command in full is RESTORE
TRIDYMITTE:I        WOLLASTONITE:I    RESTORED
TDB_OXDEMO: @@ To avoid complications also reject the Si+4 in the
TDB_OXDEMO: @@ first sublattice in the liquid phase. When there is
TDB_OXDEMO: @@ oxygen present all Si will form SiO2 or SiO4/-4.
TDB_OXDEMO: @@ The Si+4 ion is needed only for the liquid in systems
TDB_OXDEMO: @@ without oxygen.
TDB_OXDEMO:
TDB_OXDEMO: rej const ionic_liq
... the command in full is REJECT
SUBLATTICE NUMBER: 1
CONSTITUENT: si+4
    SI+4 IN IONIC_LIQ:Y SUBLATTICE    1 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
IONIC_LIQ:Y :CA+2:O-2 SIO4-4 SIO2:
#Liquid # # #Liquid metal and slag mixture. #6038cfda41046d48150aa2e7
CA2SIO4_ALPHA_PRIME:I :CA+2:CA+2:SIO4-4:

```



```

#K2CoCl4 #oP84 #Pna2_1 #This is Ca2SiO4. #602eacaf674ba8b79b43f866
CRISTOBALITE:I :SI+4:SiO4-4:
#Ideal beta-Cristobalite (SiO2, C9) #cF24 #Fd-3m #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b559
HALITE:I :CA+2 VA:O-2:
#Rock Salt (NaCl, B1) #cF8 #Fm-3m #This is BaO, CaO, CoO, FeO, MgO, MnO
and NiO #602e7f15105f8553a825b4f8
HATRURITE:I :CA+2:SiO4-4:O-2:
#Ca3(SiO4)O-b #hR81 #R3m #This is 3CaO.SiO2 #602eadc3674ba8b79b43f86a
LARNITE:I :CA+2:Si+4:O-2:
#Parawollastonite (CaSiO3, S33(II)) #mP60 #P2 1/c #This is 2CaO.SiO2
(metastable at 1 atm) #602e7f15105f8553a825b68e
OLIVINE:I :CA+2:CA+2:Si+4:O-2:
#Forsterite (Mg2SiO4, S12) #oP28 #Pnma #This is Calcio-olivine (Ca2SiO4)
- Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite
(Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4)
solid solution dissolving Cr and Cu. #602e7f15105f8553a825b684
PSEUDO_WOLLASTONITE:I :CA+2:Si+4:O-2:
#CaSiO3 #mS120 #C2/c #This is CaO.SiO2 with Ba solubility
#602ead45674ba8b79b43f868
QUARTZ:I :SI+4:SiO4-4:
#alpha-Quartz (low Quartz) #hP9 #P3_121 #SiO2 with AlPO4 solubility.
#602e7f15105f8553a825b6e2
RANKINITE:I :CA+2:Si+4:O-2:
#3CaO.2SiO2 #mP48 #P2 1/c # #602eaf3286932e6d2e4f532d
TRIDYMITE:I :SI+4:SiO4-4:
#Monoclinic (Cc) Low Tridymite (SiO2) #mS144 #Cc #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b82e
WOLLASTONITE:I :CA+2:Si+4:O-2:
#Wollastonite (CaSiO3) #aP30 #P-1 #This is CaO.SiO2 with Ba, Fe, Mg and
Mn solubility #602e7f15105f8553a825b913
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO:
TDB_OXDEMO: get
... the command in full is GET_DATA
08:59:16,069 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set IONIC_LIQ#2
VA IN HALITE:I SUBLATTICE 1 REJECTED
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_OXDEMO: @@ There is a miscibility gap in the ionic liquid close to SiO2.
TDB_OXDEMO: @@ In this database two composition sets are created
TDB_OXDEMO: @@ automatically and one has SiO2 as a major constituent
TDB_OXDEMO:
TDB_OXDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:
POLY: @@ Define more convenient components than the elements
POLY:
POLY: list-stat cps
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CA ENTERED SER
O ENTERED SER
SI ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
WOLLASTONITE ENTERED 0.000000E+00 0.000000E+00
TRIDYMITE ENTERED 0.000000E+00 0.000000E+00
RANKINITE ENTERED 0.000000E+00 0.000000E+00
QUARTZ ENTERED 0.000000E+00 0.000000E+00
PSEUDO_WOLLASTONITE ENTERED 0.000000E+00 0.000000E+00
OLIVINE ENTERED 0.000000E+00 0.000000E+00
LARNITE ENTERED 0.000000E+00 0.000000E+00
HATRURITE ENTERED 0.000000E+00 0.000000E+00
HALITE ENTERED 0.000000E+00 0.000000E+00
CRISTOBALITE ENTERED 0.000000E+00 0.000000E+00
CA2SiO4_ALPHA_PRIME ENTERED 0.000000E+00 0.000000E+00
IONIC_LIQ#2 ENTERED 0.000000E+00 0.000000E+00
IONIC_LIQ#1 ENTERED 0.000000E+00 0.000000E+00
*** STATUS FOR ALL SPECIES
CA ENTERED O-2 ENTERED O3 ENTERED SiO2 ENTERED
CA+2 ENTERED O1Si1 ENTERED SI ENTERED SiO4-4 ENTERED
CA1O1 ENTERED O2 ENTERED SI+4 ENTERED VA ENTERED
CA2 ENTERED O2Si1 ENTERED SI2 ENTERED
O ENTERED O2Si2 ENTERED SI3 ENTERED
POLY: def-com cao sio2 o
... the command in full is DEFINE_COMPONENTS
POLY: l-st cps
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CAO ENTERED SER
SiO2 ENTERED SER
O ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
WOLLASTONITE ENTERED 0.000000E+00 0.000000E+00
TRIDYMITE ENTERED 0.000000E+00 0.000000E+00
RANKINITE ENTERED 0.000000E+00 0.000000E+00
QUARTZ ENTERED 0.000000E+00 0.000000E+00
PSEUDO_WOLLASTONITE ENTERED 0.000000E+00 0.000000E+00
OLIVINE ENTERED 0.000000E+00 0.000000E+00
LARNITE ENTERED 0.000000E+00 0.000000E+00
HATRURITE ENTERED 0.000000E+00 0.000000E+00
HALITE ENTERED 0.000000E+00 0.000000E+00
CRISTOBALITE ENTERED 0.000000E+00 0.000000E+00
CA2SiO4_ALPHA_PRIME ENTERED 0.000000E+00 0.000000E+00
IONIC_LIQ#2 ENTERED 0.000000E+00 0.000000E+00
IONIC_LIQ#1 ENTERED 0.000000E+00 0.000000E+00
*** STATUS FOR ALL SPECIES

```

```

CA      ENTERED      O      ENTERED      O2SI2  ENTERED      SI3      ENTERED
CA+2    ENTERED      O-2    ENTERED      O3      ENTERED      SIO2     ENTERED
CA101   ENTERED      O1SI1  ENTERED      SI      ENTERED      SIO4-4   ENTERED
CA2      ENTERED      O2     ENTERED      SI+4    ENTERED      VA      ENTERED
CAO      ENTERED      O2SI1  ENTERED      SI2     ENTERED
POLY:Hit RETURN to continue
POLY: s-c t=2000,p=1e5,n=1,w(sio2)=.9
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=2000, P=100000, N=1, W(SIO2)=0.9
DEGREES OF FREEDOM 1
POLY: @@ There is one degree of freedom due to the oxygen. As the
POLY: @@ oxygen content is determined by the Ca/Si ration there is no
POLY: @@ possibility to vary the oxygen content in this system
POLY: @@ independently. Thus the oxygen potential can be set to any
POLY: @@ value (larger than zero).
POLY:
POLY: s-c ac(o)=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
08:59:17,741 [Thread-0] INFO Database: Preparing system for use: OXDEMO_MODIFIED_174704035707216
08:59:19,628 [Thread-0] INFO Phase: Preparing phase for use: IONIC_LIQ
08:59:20,264 [Thread-0] INFO Phase: Preparing phase for use: CA2SIO4_ALPHA_PRIME
08:59:20,784 [Thread-0] INFO Phase: Preparing phase for use: CRISTOBALITE
08:59:21,115 [Thread-0] INFO Phase: Preparing phase for use: HALITE
08:59:21,414 [Thread-0] INFO Phase: Preparing phase for use: HATRURITE
08:59:21,755 [Thread-0] INFO Phase: Preparing phase for use: LARNITE
08:59:22,056 [Thread-0] INFO Phase: Preparing phase for use: OLIVINE
08:59:22,384 [Thread-0] INFO Phase: Preparing phase for use: PSEUDO_WOLLASTONITE
08:59:22,750 [Thread-0] INFO Phase: Preparing phase for use: QUARTZ
08:59:23,108 [Thread-0] INFO Phase: Preparing phase for use: RANKINITE
08:59:23,392 [Thread-0] INFO Phase: Preparing phase for use: TRIDYMITE
08:59:23,671 [Thread-0] INFO Phase: Preparing phase for use: WOLLASTONITE
Testing POLY result by global minimization procedure
Calculated 1976 grid points in 0.078 s
35 ITS, CPU TIME USED 21 SECONDS
POLY:
POLY: @@ Option N is used to include information on the
POLY: @@ constitution of the phases.
POLY: l-e screen
... the command in full is LIST_EQUILIBRIUM
Options /VWCS/: n
Output from POLY-3, equilibrium = 1, label A0 , database: OXDEMO

Conditions:
T=2000, P=100000, N=1, W(SIO2)=0.9, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 2000.00 K ( 1726.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.96568E+01
Total Gibbs energy -1.10541E+06, Enthalpy -7.53273E+05, Volume 2.62576E-05

Component      Moles      W-Fraction Activity Potential Ref.stat
CAO             1.0638E-01  1.0000E-01 6.4224E-25 -9.2632E+05 SER
SIO2            8.9362E-01  9.0000E-01 3.7467E-30 -1.1267E+06 SER
O               0.0000E+00  0.0000E+00 1.0000E+00 0.0000E+00 SER

IONIC_LIQ#1      Status ENTERED Driving force 0.0000E+00
Moles 6.7244E-01, Mass 4.0313E+01, Volume fraction 6.9347E-01 Mass fractions:
SIO2 9.69165E-01 CAO 3.08355E-02 O 0.00000E+00
Constitution:
Sublattice 1, Number of sites 6.8156E-02
CA+2 1.00000E+00
Sublattice 2, Number of sites 2.0000E+00
SIO2 9.82793E-01 SIO4-4 1.68709E-02 O-2 3.36172E-04

IONIC_LIQ#2      Status ENTERED Driving force 0.0000E+00
Moles 3.2756E-01, Mass 1.9344E+01, Volume fraction 3.0653E-01 Mass fractions:
SIO2 7.55858E-01 CAO 2.44142E-01 O 0.00000E+00
Constitution:
Sublattice 1, Number of sites 6.9176E-01
CA+2 1.00000E+00
Sublattice 2, Number of sites 2.0000E+00
SIO2 8.26780E-01 SIO4-4 1.72662E-01 O-2 5.57209E-04
POLY:Hit RETURN to continue
POLY: @@ The result shows the expected miscibility gap. However,
POLY: @@ in some cases the first calculation may fail. In such
POLY: @@ cases try to simplify the calculation by suspending
POLY: @@ all phases but the important ones. Save the results.
POLY:
POLY: save tcex17 y
... the command in full is SAVE_WORKSPACES
POLY: @@ Set the axis
POLY: s-a-v 1 w(sio2)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: s-a-v 2 t
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1500
Max value /1/: 3500
Increment /50/: 20
POLY: save tcex17 Y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11

Organizing start points

```

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26

Phase region boundary 1 at: 1.765E-01 1.510E+03
** CA2SiO4_ALPHA_PRIME
HALITE
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 1.765E-01 1.500E+03
** CA2SiO4_ALPHA_PRIME
HALITE
Calculated. 3 equilibria

Phase region boundary 3 at: 1.765E-01 1.525E+03
** CA2SiO4_ALPHA_PRIME
HALITE
** HATRURITE

Phase region boundary 4 at: 1.327E-01 1.525E+03
HALITE
** HATRURITE
Calculated. 46 equilibria

Phase region boundary 5 at: 1.327E-01 2.422E+03
** IONIC_LIQ#1
HALITE
** HATRURITE

Phase region boundary 6 at: 1.433E-01 2.422E+03
** IONIC_LIQ#1
HALITE
Calculated 53 equilibria

Phase region boundary 7 at: 2.736E-01 2.422E+03
** IONIC_LIQ#1
HATRURITE
Calculated. 7 equilibria

Phase region boundary 8 at: 2.946E-01 2.321E+03
** IONIC_LIQ#1
** CA2SiO4_ALPHA_PRIME
HATRURITE

Phase region boundary 9 at: 3.061E-01 2.321E+03
** CA2SiO4_ALPHA_PRIME
HATRURITE
Calculated. 41 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 3.336E-01 2.321E+03
IONIC_LIQ#1
** CA2SiO4_ALPHA_PRIME
Calculated. 54 equilibria

Phase region boundary 11 at: 3.953E-01 1.732E+03
IONIC_LIQ#1
** CA2SiO4_ALPHA_PRIME
** RANKINITE

Phase region boundary 12 at: 4.291E-01 1.732E+03
IONIC_LIQ#1
** RANKINITE
Calculated. 2 equilibria

Phase region boundary 13 at: 4.309E-01 1.727E+03
IONIC_LIQ#1
** PSEUDO_WOLLASTONITE
** RANKINITE

Phase region boundary 14 at: 4.813E-01 1.727E+03
IONIC_LIQ#1
** PSEUDO_WOLLASTONITE
Calculated. 29 equilibria

Phase region boundary 15 at: 5.740E-01 1.714E+03
IONIC_LIQ#1
** PSEUDO_WOLLASTONITE
** TRIDYMITE

Phase region boundary 16 at: 8.175E-01 1.714E+03
IONIC_LIQ#1
** TRIDYMITE
Calculated. 3 equilibria

Phase region boundary 17 at: 8.222E-01 1.744E+03
IONIC_LIQ#1
** CRISTOBALITE

```

** TRIDYMITE

Phase region boundary 18 at: 8.222E-01 1.744E+03
  IONIC_LIQ#1
** CRISTOBALITE
Calculated. 12 equilibria

Phase region boundary 19 at: 8.695E-01 1.959E+03
  IONIC_LIQ#1
** IONIC_LIQ#2
** CRISTOBALITE

Phase region boundary 20 at: 8.575E-01 1.959E+03
  IONIC_LIQ#1
** IONIC_LIQ#2
Calculated 30 equilibria

Phase region boundary 21 at: 9.882E-01 1.959E+03
** IONIC_LIQ#2
  CRISTOBALITE
Calculated 24 equilibria

Phase region boundary 22 at: 1.000E+00 1.744E+03
** CRISTOBALITE
  TRIDYMITE

Phase region boundary 23 at: 7.627E-01 1.714E+03
  PSEUDO_WOLLASTONITE
** TRIDYMITE
Calculated.. 12 equilibria
Terminating at axis limit.

Phase region boundary 24 at: 4.671E-01 1.727E+03
** PSEUDO_WOLLASTONITE
  RANKINITE
Calculated.. 13 equilibria
Terminating at axis limit.

Phase region boundary 25 at: 3.828E-01 1.732E+03
  CA2SIO4_ALPHA_PRIME
** RANKINITE
Calculated.. 13 equilibria
Terminating at axis limit.

Phase region boundary 26 at: 1.765E-01 1.510E+03
** CA2SIO4_ALPHA_PRIME
  HALITE
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 1.765E-01 1.510E+03
** CA2SIO4_ALPHA_PRIME
  HALITE
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at: 1.765E-01 1.510E+03
** CA2SIO4_ALPHA_PRIME
  HALITE
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 29 at: 1.765E-01 1.510E+03
** CA2SIO4_ALPHA_PRIME
  HALITE
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 30 at: 1.765E-01 1.510E+03
** CA2SIO4_ALPHA_PRIME
  HALITE
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
  TRIDYMITE
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 32 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
  TRIDYMITE
Calculated. 13 equilibria
Calculated 13 equilibria

Phase region boundary 33 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
  TRIDYMITE
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
  TRIDYMITE
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 35 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
  TRIDYMITE
Calculated. 13 equilibria
Calculated 13 equilibria

Phase region boundary 36 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
  TRIDYMITE
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE

```

```

TRIDYMIT
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 38 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
TRIDYMIT
Calculated. 13 equilibria
Calculated 13 equilibria

Phase region boundary 39 at: 7.627E-01 1.510E+03
** PSEUDO_WOLLASTONITE
TRIDYMIT
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 3.705E-01 2.170E+03
IONIC_LIQ#1
** CA2SiO4_ALPHA_PRIME
Calculated. 23 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 3.705E-01 2.170E+03
IONIC_LIQ#1
** CA2SiO4_ALPHA_PRIME
Calculated. 39 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.886E-02 2.830E+03
IONIC_LIQ#1
** HALITE
Calculated. 22 equilibria
Terminating at known equilibrium

Phase region boundary 43 at: 9.886E-02 2.830E+03
IONIC_LIQ#1
** HALITE
Calculated 30 equilibria

Phase region boundary 44 at: 9.886E-02 2.830E+03
IONIC_LIQ#1
** HALITE
Calculated. 22 equilibria
Terminating at known equilibrium

Phase region boundary 45 at: 9.886E-02 2.830E+03
IONIC_LIQ#1
** HALITE
Calculated 30 equilibria

Phase region boundary 46 at: 5.002E-03 3.162E+03
IONIC_LIQ#1
** HALITE
Calculated 9 equilibria

Phase region boundary 47 at: 5.002E-03 3.162E+03
IONIC_LIQ#1
** HALITE
Calculated. 40 equilibria
Terminating at known equilibrium

Phase region boundary 48 at: 3.428E-01 2.374E+03
IONIC_LIQ#1
** CA2SiO4_ALPHA_PRIME
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 49 at: 3.428E-01 2.374E+03
IONIC_LIQ#1
** CA2SiO4_ALPHA_PRIME
Calculated. 58 equilibria
Terminating at known equilibrium

Phase region boundary 50 at: 8.337E-01 1.812E+03
IONIC_LIQ#1
** CRISTOBALITE
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 51 at: 8.337E-01 1.812E+03
IONIC_LIQ#1
** CRISTOBALITE
Calculated 10 equilibria

Phase region boundary 52 at: 8.337E-01 1.812E+03
IONIC_LIQ#1
** CRISTOBALITE
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 53 at: 9.950E-01 1.978E+03
IONIC_LIQ#1
** CRISTOBALITE
Calculated 10 equilibria

Phase region boundary 54 at: 9.950E-01 1.978E+03
IONIC_LIQ#1
** CRISTOBALITE
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 55 at: 9.950E-01 1.978E+03
IONIC_LIQ#1
** CRISTOBALITE
Calculated 18 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex17\tcex17.POLY3
CPU time for mapping 8 seconds
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

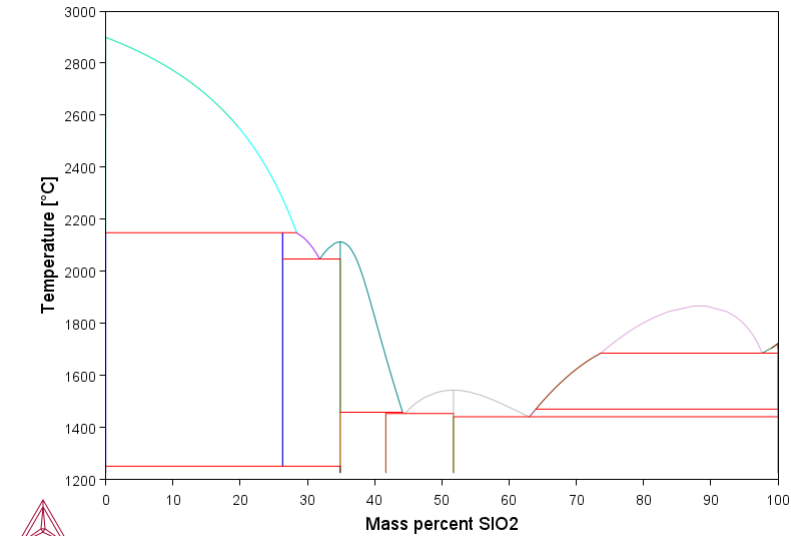
Setting automatic diagram axes

POST: s-d-a x w-p sio2
... the command in full is SET_DIAGRAM_AXIS

```

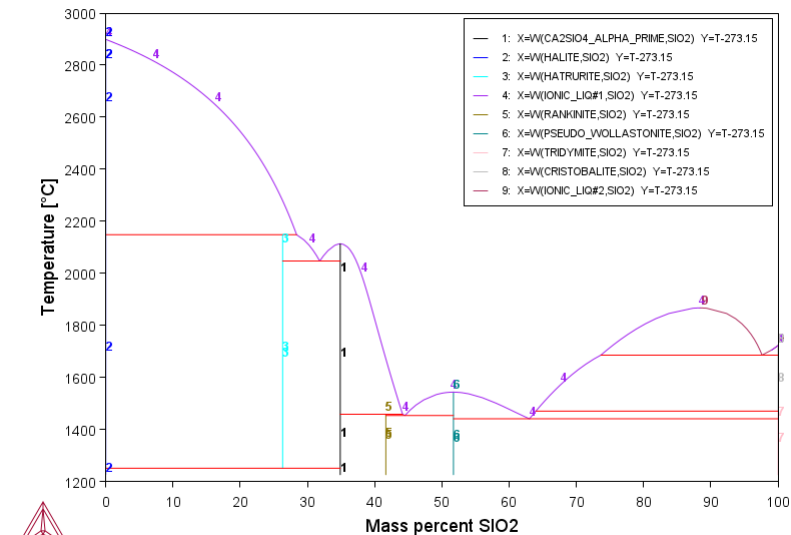
```
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 17a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 17a



```
POST:
POST:Hit RETURN to continue
POST: @@ Indentify the phases with labels
POST: s-lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: f
POST:
POST: set-title example 17b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 17b



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex18

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex18\tcex18.TCM.test"

SYS: set-echo

SYS:

SYS: @@ A3 temperature of a steel

SYS:

SYS: @@ This example calculates the A3 temperature of a steel

SYS: @@ and the influence of each alloying element on

SYS: @@ this temperature

SYS:

SYS: @@ A3 temperature is the temperature where ferrite starts to

SYS: @@ form from austenite. You can easily read A3 from an Fe-C

SYS: @@ phase diagram. But for complex multicomponent steels, no

SYS: @@ simple diagram can be used.

SYS:

SYS: @@ Using POLY, it is easy to find out the influence of each

SYS: @@ alloying element on A3 temperature. This information is

SYS: @@ useful if you want to modify the compositions of a steel

SYS: @@ but keep A3 unchanged.

SYS:

SYS: @@ Note that a TCFE database license is required to run

SYS: @@ the example.

SYS:

SYS: set-log exl8,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfell

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/:

1st alloying element: cr 1.5 mn .5 c .3 si .3 nb .1

Next alloying element:

Temperature (C) /1000/: 1100

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

NB DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	KSI_CARBIDE	Z_PHASE
FE4N_LP1	SIGMA_D8B	HIGH_SIGMA
MU_D85	CHI_A12	C14_LAVES
C15_LAVES	M36I	MN9SI2
MN11SI19	MN6SI	G_PHASE
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NB3SI	NB5SI3_D8L	NB5SI3_D8M
MSI2_C40	CRNBSI	M11SI8
M6SI5	FENBSI2	FE4NB4SI7
FENBSI_C23	FE3NB4SI5	FENB2SI2
FENB4SI	AL4C3_D71	FE8SI2C
SIC_B3	MN5SIC	CRZN17
CUZN_EPSILON	AL5FE4	MNP_B31
M2P_C22	NI31SI12	CO2SI_C37
M2SI_TETA	NISI_B31	NI3SI2
CR5SI3_D8M	DELTA_TIH2	NBH_BETA

Reject phase(s) /NONE/: ?

FILE SYSTEM ERROR IN FILHLP

ERROR 1717 READING HELP FILE

Reject phase(s) /NONE/: *

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	KSI_CARBIDE	Z_PHASE
FE4N_LP1	SIGMA_D8B	HIGH_SIGMA
MU_D85	CHI_A12	C14_LAVES

```

C15_LAVES          M3SI          MN9SI2
MN11SI19          MN6SI          G_PHASE
CR3SI_A15          FESI2_H          FESI2_L
MSI_B20           M5SI3_D88        NBNi3_D0A
NB3SI            NB5SI3_D8L        NB5SI3_D8M
MSI2_C40          CRNBSI          M11SI8
M6SI5            FENBSI2         FE4NB4SI7
FENBSI_C23        FE3NB4SI5        FENB2SI2
FENB4SI          AL4C3_D71        FE8SI2C
SIC_B3           MN5SIC          CRZN17
CUZN_EPSILON     AL5FE4          MNP_B31
M2P_C22          NI3SI12         CO2SI_C37
M2SI_TETA        NISI_B31        NI3SI2
CR5SI3_D8M       DELTA_TIH2      NBH_BETA
REJECTED

Restore phase(s):: liq fcc_a1 bcc_a2 hcp_a3 graphite cementite m23 m7
LIQUID:L          FCC_A1          BCC_A2
HCP_A3            GRAPHITE_A9        CEMENTITE_D011
*** ERROR M7 INPUT IGNORED
M23C6_D84 RESTORED
Restore phase(s): /NONE/:

.....

The following phases are retained in this system:

LIQUID:L          BCC_A2          FCC_A1
HCP_A3            GRAPHITE_A9        CEMENTITE_D011
M23C6_D84

.....

OK? /Y/: Y
09:00:29,084 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Should any phase have a miscibility gap check? /N/: N
Using global minimization procedure
Calculated          9014 grid points in          0.615 s
Found the set of lowest grid points in          0.010 s
Calculated POLY solution          0.553 s, total time          1.178 s
POLY:
POLY: @@ In the TCFE database the number of phases is very large.
POLY: @@ It is strongly recommended that you reject all phases
POLY: @@ that you know should not be stable
POLY:
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =          1, label A0 , database: TCFE11

Conditions:
T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1373.15 K ( 1100.00 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.50374E+01
Total Gibbs energy -7.21959E+04, Enthalpy 4.05733E+04, Volume 7.32300E-06

Component          Moles          W-Fraction Activity Potential Ref.stat
C          1.3747E-02          3.0000E-03 1.0856E-02 -5.1639E+04 SER
CR          1.5877E-02          1.5000E-02 1.3440E-04 -1.0178E+05 SER
FE          9.5890E-01          9.7300E-01 2.0383E-03 -7.0736E+04 SER
MN          5.0091E-03          5.0000E-03 4.2390E-06 -1.4124E+05 SER
NB          5.9240E-04          1.0000E-03 1.3165E-07 -1.8088E+05 SER
SI          5.8790E-03          3.0000E-03 1.1486E-08 -2.0873E+05 SER

FCC_A1#1          Status ENTERED          Driving force 0.0000E+00
Moles 9.9897E-01, Mass 5.4983E+01, Volume fraction 9.9902E-01 Mass fractions:
FE 9.73957E-01 MN 5.00491E-03 C 2.89335E-03
CR 1.50123E-02 SI 3.00297E-03 NB 1.29814E-04

FCC_A1#2          Status ENTERED          Driving force 0.0000E+00
Moles 1.0273E-03, Mass 5.4472E-02, Volume fraction 9.8186E-04 Mass fractions:
NB 8.79352E-01 FE 7.32744E-03 MN 4.50186E-05
C 1.10654E-01 CR 2.62187E-03 SI 1.29638E-09
POLY:Hit RETURN to continue
POLY: @@ Two FCC phases are stable, one with mainly Fe and
POLY: @@ one with mainly Nb and C, which is the NbC carbide.
POLY: @@ The second fcc is called FCC#2. The number after # is
POLY: @@ called composition set but can be ignored if it is unity.
POLY:
POLY: li-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT          STATUS          REF. STATE          T(K)          P(Pa)
VA          ENTERED          SER
C          ENTERED          SER
CR          ENTERED          SER
FE          ENTERED          SER
MN          ENTERED          SER
NB          ENTERED          SER
SI          ENTERED          SER
*** STATUS FOR ALL PHASES
PHASE          STATUS          DRIVING FORCE          MOLES
FCC_A1#2          ENTERED          0.000000E+00          1.027344E-03
FCC_A1#1          ENTERED          0.000000E+00          9.989727E-01
BCC_A2          ENTERED          -1.865997E-02          0.000000E+00
LIQUID          ENTERED          -2.122724E-01          0.000000E+00
HCP_A3#1          ENTERED          -3.255375E-01          0.000000E+00
HCP_A3#2          ENTERED          -3.255375E-01          0.000000E+00

```



```

M23C6_D84          ENTERED      -4.182898E-01    0.000000E+00
CEMENTITE_D011     ENTERED      -4.735993E-01    0.000000E+00
GRAPHITE_A9        ENTERED      -2.493896E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
C   ENTERED      C60   ENTERED      FE+2 ENTERED      MN+3 ENTERED      SI   ENTERED
C2  ENTERED      CR   ENTERED      FE+3 ENTERED      MN+4 ENTERED      SI+4 ENTERED
C3  ENTERED      CR+2 ENTERED      FE+4 ENTERED      NB   ENTERED      VA   ENTERED
C4  ENTERED      CR+3 ENTERED      MN   ENTERED      NB+2 ENTERED
C5  ENTERED      FE   ENTERED      MN+2 ENTERED      NB+4 ENTERED
POLY:
POLY: @@ Fcc appears twice in the list. The HCP phase also has
POLY: @@ two composition sets.
POLY:
POLY: @@ This result looks reasonable; save it to file
POLY: save tcexl8 y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: @@ Now calculate when bcc (ferrite) begins to form
POLY: @@ using the COMPUTE-TRANSITION command
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
You must release One of these conditions
T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated      9014 grid points in      0.057 s
To form BCC_A2 the condition is set to T=1071.58417272
POLY:Hit RETURN to continue
POLY: @@ We may expect BCC to form at a lower temperature, because
POLY: @@ sometimes a higher temperature is found as there is a
POLY: @@ delta-ferrite stable at high temperatures.
POLY:
POLY: @@ Calculate the equilibrium at lower temperature again. You
POLY: @@ can do this with a SET-COND T=... command but then the
POLY: @@ temperature must be given in Kelvin. You can use the
POLY: @@ DEF-MAT command to do this in Celsius
POLY:
POLY: def-mat
... the command in full is DEFINE_MATERIAL
Same elements as before? /Y/: Y
Mass (weight) percent of C /.3/: .3
Mass (weight) percent of CR /1.5/: 1.5
Mass (weight) percent of MN /.5/: .5
Mass (weight) percent of NB /.1/: .1
Mass (weight) percent of SI /.3/: .3
Temperature (C) /798/: 800
Using global minimization procedure
Calculated      9014 grid points in      0.090 s
Found the set of lowest grid points in      0.009 s
Calculated POLY solution      0.185 s, total time      0.284 s
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1073.15 K ( 800.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.50374E+01
Total Gibbs energy -4.87853E+04, Enthalpy 3.03165E+04, Volume 7.17930E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C      1.3747E-02      3.0000E-03 4.4628E-02 -2.7744E+04 SER
CR      1.5877E-02      1.5000E-02 3.6747E-04 -7.0568E+04 SER
FE      9.5890E-01      9.7300E-01 4.8655E-03 -4.7519E+04 SER
MN      5.0091E-03      5.0000E-03 8.1198E-06 -1.0458E+05 SER
NB      5.9240E-04      1.0000E-03 2.9346E-09 -1.7530E+05 SER
SI      5.8790E-03      3.0000E-03 9.3983E-10 -1.8546E+05 SER

FCC_A1#1      Status ENTERED      Driving force 0.0000E+00
Moles 9.9869E-01, Mass 5.4971E+01, Volume fraction 9.9877E-01 Mass fractions:
FE 9.74162E-01 MN 5.00593E-03 C 2.86276E-03
CR 1.49637E-02 SI 3.00363E-03 NB 1.46017E-06

FCC_A1#2      Status ENTERED      Driving force 0.0000E+00
Moles 1.3082E-03, Mass 6.6495E-02, Volume fraction 1.2288E-03 Mass fractions:
NB 8.26485E-01 CR 4.49696E-02 MN 9.44662E-05
C 1.16454E-01 FE 1.19978E-02 SI 1.91601E-10
POLY:
POLY: @@ Try a slightly different COMPUTE-TRANSITION command.
POLY: @@ This finds the first phase change in the specified
POLY: @@ direction.
POLY:
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: any
You must release one of these conditions
T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Estimated change (with sign) /1/: ?
FILE SYSTEM ERROR IN FILHLP
Estimated change (with sign) /1/: -1
Lowering smallest site-fraction from 0.10000E-11 to 0.10000E-12
and recalculating equilibrium
PHASE CHANGE AT 1071.5841681
BCC_A2#1 forms
Testing POLY result by global minimization procedure
Calculated      9014 grid points in      0.042 s
POLY: show t
... the command in full is SHOW_VALUE
T=1071.5842
POLY: @@ The transition temperature to form BCC is the same.
POLY: @@ If we want it in Celsius enter a function.
POLY: enter fun tc=t-273;

```

```

... the command in full is ENTER_SYMBOL
POLY: show tc
... the command in full is SHOW_VALUE
TC=798.58417
POLY:
POLY:Hit RETURN to continue
POLY: @@ This is the minimum temperature for hardening because
POLY: @@ below this temperature ferrite will form from austenite.
POLY: @@ Check how a small change of the composition can change
POLY: @@ this temperature. We must then set bcc as Fix and
POLY: @@ release the condition on the temperature.
POLY:
POLY: c-st p bcc_a2=fix 0
... the command in full is CHANGE_STATUS
POLY: s-c t=none
... the command in full is SET_CONDITION
POLY: @@ The change of the calculated temperature for a small
POLY: @@ change of the amount of a component can be calculated
POLY: @@ as a derivative using the dot "." between the
POLY: @@ calculated variable and the condition.
POLY:
POLY: sh t.w(mn)
... the command in full is SHOW_VALUE
T.W(MN)=-2584.6297
POLY: sh t.w(cr)
... the command in full is SHOW_VALUE
T.W(CR)=-784.00263
POLY: sh t.w(nb)
... the command in full is SHOW_VALUE
T.W(NB)=3035.5587
POLY: sh t.w(c)
... the command in full is SHOW_VALUE
T.W(C)=-21859.659
POLY: sh t.w(si)
... the command in full is SHOW_VALUE
T.W(SI)=3012.5853
POLY:Hit RETURN to continue
POLY: @@ A negative value means the temperature decreases
POLY: @@ if the amount is increased. Check for Mn
POLY:
POLY: s-c w(mn)
... the command in full is SET_CONDITION
Value /.005000000172/: .01
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          9014 grid points in      0.056 s
      9 ITS, CPU TIME USED  0 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=1058.9736
POLY:Hit RETURN to continue
POLY: @@ The temperature decreased from 1072 to 1059
POLY: @@ i.e. 13 degrees. According to the derivatives calculated
POLY: @@ above, you can increase the temperature the same
POLY: @@ amount by increasing the amount of Si
POLY: @@ 2592/2990=0.8669 times of the change in Mn
POLY: @@ i.e. from 0.3 to 0.733 %
POLY:
POLY: s-c w(si)
... the command in full is SET_CONDITION
Value /.003/: .00733
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          9014 grid points in      0.044 s
     10 ITS, CPU TIME USED  1 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=1070.8718
POLY: @@ Being able to calculate these derivatives is a powerful
POLY: @@ feature in order to find the best way to obtain a
POLY: @@ specific property of a material.
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```

tcex19A

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex19A\tcex19A.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si

SYS:

SYS: @@ This is the first part of a two part example showing how

SYS: @@ to map univariant equilibria with the liquid in Al-Cu-Si.

SYS: @@ Part A. Step-by-step calculation using the POLY-3 module.

SYS:

SYS: set-log ex19a,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw USER tcex19_cost2

... the command in full is SWITCH_DATABASE

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

09:01:34,901 [Thread-0] INFO TDBFileParser: USER_1537738403_21, number of lines read: 470

09:01:35,242 [Thread-0] INFO DatabaseUtils: Parsing of USER_1537738403_21 completed in 430 ms

TDB_USER: d-sys

... the command in full is DEFINE_SYSTEM

ELEMENTS: cu al si

CU AL SI

DEFINED

TDB_USER: l-s c

... the command in full is LIST_SYSTEM

LIQUID:L :AL CU SI:
ALCE_AMORPHOUS :AL:
ALCUZN T :AL:CU VA:
ALCU_DELTA :AL:CU:
ALCU_EPSILON :AL CU:CU:
ALCU_ETA :AL CU:CU:
ALCU_PRIME :AL:CU:
ALCU_THETA :AL:AL CU:
ALCU_ZETA :AL:CU:
ALLI :AL:VA:
ALMO :AL:AL:
ALM_D019 :AL:AL:
ALND_AMORPHOUS :AL:
ALTI :AL:AL:
BCC_A2 :AL CU SI:VA:
BCC_B2 :AL CU SI:AL CU SI:VA:
BCT_A5 :AL:
CBCC_A12 :AL SI:VA:
CR3SI_A15 :SI:AL SI:
CRSI2 :SI:SI:
CU19SI6_ETA :CU:SI:
CU33SI7_DELTA :CU:SI:
CU4SI_EPSILON :CU:SI:
CU56SI11_GAMMA :CU:SI:
CU6Y :CU:CU2:
CUB_A13 :AL SI:VA:
CUB_A15 :SI:AL SI:
DIAMOND_A4 :AL SI:
FCC_A1 :AL CU SI:VA:
GAMMA_D83 :AL:AL CU:CU:
GAMMA_H :AL:AL CU:CU:
HCP_A3 :AL CU SI:VA:
HCP_ZN :AL CU SI:VA:
LAVES_C14 :AL CU:AL CU:
LAVES_C15 :AL CU SI:AL CU SI:
LAVES_C36 :AL CU:AL CU:
SIV3 :SI:SI:

TDB_USER: get

... the command in full is GET_DATA

09:01:35,439 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_USER: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: s-c t=1300,p=101325,n=1

... the command in full is SET_CONDITION

POLY: l-c

... the command in full is LIST_CONDITIONS

T=1300, P=101325, N=1

DEGREES OF FREEDOM 2

```

POLY: s-c x(si)=.25,x(al)=.2
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
09:01:36,264 [Thread-0] INFO Database: Preparing system for use: USER_1537738403_21
09:01:37,263 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
09:01:37,713 [Thread-0] INFO Phase: Preparing phase for use: ALCE_AMORPHOUS
09:01:38,065 [Thread-0] INFO Phase: Preparing phase for use: ALCUZN_T
09:01:38,382 [Thread-0] INFO Phase: Preparing phase for use: ALCU_DELTA
09:01:38,707 [Thread-0] INFO Phase: Preparing phase for use: ALCU_EPSILON
09:01:39,053 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ETA
09:01:39,332 [Thread-0] INFO Phase: Preparing phase for use: ALCU_PRIME
09:01:39,684 [Thread-0] INFO Phase: Preparing phase for use: ALCU_THETA
09:01:40,004 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ZETA
09:01:40,258 [Thread-0] INFO Phase: Preparing phase for use: ALLI
09:01:40,544 [Thread-0] INFO Phase: Preparing phase for use: ALMO
09:01:40,817 [Thread-0] INFO Phase: Preparing phase for use: ALM_D019
09:01:41,155 [Thread-0] INFO Phase: Preparing phase for use: ALND_AMORPHOUS
09:01:41,497 [Thread-0] INFO Phase: Preparing phase for use: ALTI
09:01:41,769 [Thread-0] INFO Phase: Preparing phase for use: BCC_B2
09:01:42,021 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2
09:01:42,336 [Thread-0] INFO Phase: Preparing phase for use: BCT_A5
09:01:42,600 [Thread-0] INFO Phase: Preparing phase for use: CBCC_A12
09:01:42,873 [Thread-0] INFO Phase: Preparing phase for use: CR3SI_A15
09:01:43,119 [Thread-0] INFO Phase: Preparing phase for use: CRSI2
09:01:43,433 [Thread-0] INFO Phase: Preparing phase for use: CU19SI6_ETA
09:01:43,753 [Thread-0] INFO Phase: Preparing phase for use: CU33SI7_DELTA
09:01:43,995 [Thread-0] INFO Phase: Preparing phase for use: CU4SI_EPSILON
09:01:44,297 [Thread-0] INFO Phase: Preparing phase for use: CU56SI11_GAMMA
09:01:44,558 [Thread-0] INFO Phase: Preparing phase for use: CU6Y
09:01:44,846 [Thread-0] INFO Phase: Preparing phase for use: CUB_A13
09:01:45,286 [Thread-0] INFO Phase: Preparing phase for use: CUB_A15
09:01:45,541 [Thread-0] INFO Phase: Preparing phase for use: DIAMOND_A4
09:01:45,785 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
09:01:46,087 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_D83
09:01:46,423 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_H
09:01:46,696 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3
09:01:46,947 [Thread-0] INFO Phase: Preparing phase for use: HCP_ZN
09:01:47,210 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C14
09:01:47,492 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C15
09:01:47,781 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C36
09:01:48,092 [Thread-0] INFO Phase: Preparing phase for use: SIV3
Calculated 16744 grid points in 12.176 s
Found the set of lowest grid points in 0.002 s
Calculated POLY solution 0.118 s, total time 12.296 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: vwcs
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
T=1300, P=101325, N=1, X(SI)=0.25, X(AL)=0.2
DEGREES OF FREEDOM 0

Temperature 1300.00 K ( 1026.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 4.73680E+01
Total Gibbs energy -8.02595E+04, Enthalpy 3.22931E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
AL              2.0000E-01  1.1393E-01  5.1836E-05 -1.0666E+05 SER
CU              5.5000E-01  7.3785E-01  4.1349E-04 -8.4211E+04 SER
SI              2.5000E-01  1.4823E-01  9.3957E-03 -5.0450E+04 SER

LIQUID          Status ENTERED   Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.7368E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 7.37847E-01 SI 1.48228E-01 AL 1.13925E-01
POLY:Hit RETURN to continue
POLY: @@ We want to calculate the monovariant lines with liquid.
POLY: @@ Select two compositions and the temperature as the axis.
POLY: s-a-v 1 x(al)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .01
POLY: s-a-v 2 x(si)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .01
POLY: s-a-v 3 t 500 2000 25
... the command in full is SET_AXIS_VARIABLE
POLY: @@ Set liquid as "present", otherwise all monovariant lines
POLY: @@ are calculated.
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: ?
EQUILIBRIUM_CALCUL      NEW_COMPOSITION_SET      STABILITY_CHECK
GLOBAL_MINIMIZATION     OUTPUT_FILE_FOR_SHOW      STEP_AND_MAP
IGNORE_COMPOSITION_SET ORDER PARAEQUILIBRIUM      T-ZERO TEMPERATURE
KEEP_COMP_SET_NUMBERS   PHASE_ADDITION            TOGGLE_ALTERNATE_MODE
LIST_PHASE_ADDITION     PRESENT_PHASE
MAJOR_CONSTITUENTS      SHOW_FOR_T=
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liquid
POLY:
POLY: save tcex19a1 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 8.426E-02 2.500E-01 1.182E+03
LIQUID
** BCC_B2
** DIAMOND_A4
*** Buffer saved on file:
c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex19A\tc

```

```

ex19a1.POLY3
CALCULATED      35 EQUILIBRIA

Phase region boundary  2 at:    4.045E-01  1.269E-01  9.785E+02
  LIQUID
  ALCU_EPSILON
  ** BCC_B2
  ** DIAMOND_A4
  SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary  2 at:    4.045E-01  1.269E-01  9.785E+02
  LIQUID
  ** ALCU_EPSILON
  ** BCC_B2
  Terminating at diagram limit
  CALCULATED      18 EQUILIBRIA

Phase region boundary  2 at:    4.045E-01  1.269E-01  9.785E+02
  LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4
  CALCULATED      20 EQUILIBRIA

Phase region boundary  2 at:    5.755E-01  8.764E-02  8.678E+02
  LIQUID
  ** ALCU_EPSILON
  ALCU_ETA
  ** DIAMOND_A4
  SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary  2 at:    5.755E-01  8.764E-02  8.678E+02
  LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA
  Terminating at diagram limit
  CALCULATED      16 EQUILIBRIA

Phase region boundary  2 at:    5.755E-01  8.764E-02  8.678E+02
  LIQUID
  ** ALCU_ETA
  ** DIAMOND_A4
  CALCULATED       8 EQUILIBRIA

Phase region boundary  2 at:    6.299E-01  7.685E-02  8.291E+02
  LIQUID
  ** ALCU_ETA
  ALCU_THETA
  ** DIAMOND_A4
  SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary  2 at:    6.299E-01  7.685E-02  8.291E+02
  LIQUID
  ** ALCU_ETA
  ** ALCU_THETA
  Terminating at diagram limit
  CALCULATED      13 EQUILIBRIA

Phase region boundary  2 at:    6.299E-01  7.685E-02  8.291E+02
  LIQUID
  ** ALCU_THETA
  ** DIAMOND_A4
  CALCULATED      18 EQUILIBRIA

Phase region boundary  2 at:    7.774E-01  7.282E-02  7.852E+02
  LIQUID
  ** ALCU_THETA
  ** DIAMOND_A4
  FCC_A1
  SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary  2 at:    7.774E-01  7.282E-02  7.852E+02
  LIQUID
  ** ALCU_THETA
  ** FCC_A1
  Terminating at diagram limit
  CALCULATED      12 EQUILIBRIA

Phase region boundary  2 at:    7.774E-01  7.282E-02  7.852E+02
  LIQUID
  ** DIAMOND_A4
  ** FCC_A1
  *** SORRY CANNOT CONTINUE ***    4

CALCULATED      18 EQUILIBRIA

Phase region boundary  2 at:    8.426E-02  2.500E-01  1.182E+03
  LIQUID
  ** BCC_B2
  ** DIAMOND_A4
  CALCULATED       8 EQUILIBRIA

Phase region boundary  2 at:    3.577E-02  2.616E-01  1.025E+03
  LIQUID
  ** BCC_B2
  CU19SI6_ETA
  ** DIAMOND_A4
  SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary  2 at:    3.577E-02  2.616E-01  1.025E+03
  LIQUID
  ** BCC_B2
  ** CU19SI6_ETA
  Terminating at diagram limit
  CALCULATED      12 EQUILIBRIA

Phase region boundary  2 at:    3.577E-02  2.616E-01  1.025E+03
  LIQUID
  ** CU19SI6_ETA
  ** DIAMOND_A4
  Terminating at diagram limit
  CALCULATED       9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex19A\tcex19a1.POLY3
CPU time for mapping          3 seconds
POLY:
POLY: @@ The monovariant line FCC/BCC/LIQ in the Cu corner is not
POLY: @@ connected, so add a start point. This is different from a

```

```

POLY: @@ MAP with two axes, where all connected or non-connected
POLY: @@ lines can be found automatically.
POLY:
POLY: read tcex19a1
... the command in full is READ_WORKSPACES
POLY:
POLY: s-c x(al)=.1 x(si)=.1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0.107 s
Found the set of lowest grid points in 0.006 s
Calculated POLY solution 0.054 s, total time 0.167 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY:
POLY: map
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.390E-02 1.000E-01 1.285E+03
LIQUID
** BCC_B2
** FCC_A1
Terminating at diagram limit
CALCULATED 18 EQUILIBRIA

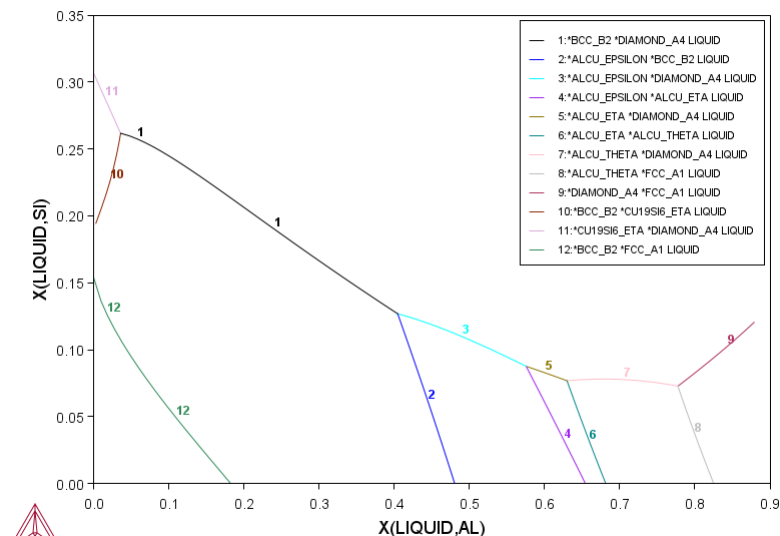
Phase region boundary 2 at: 4.390E-02 1.000E-01 1.285E+03
LIQUID
** BCC_B2
** FCC_A1
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex19A\tcex19a1.POLY3
CPU time for mapping 0 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: @@ We want the liquid compositions only
POST: s-d-a x x(liquid,al)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liquid,si)
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 19Aa
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 19Aa



```

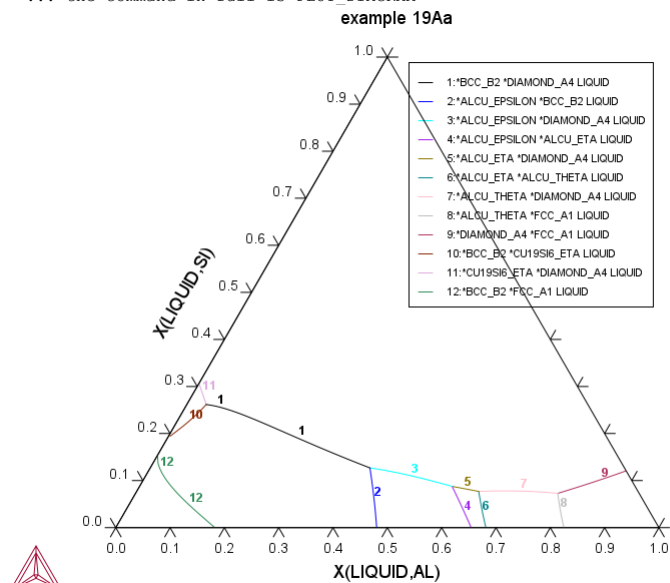
POST:
POST: Hit RETURN to continue
POST: @@ Make it triangular and scale the axis
POST: s-d-t
... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM (Y OR N) /N/: y,,,,,
POST: s-sc y n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-sc x n 0 1
... the command in full is SET_SCALING_STATUS
POST: @@ Plot the phases stable along the lines
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5

```

```

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

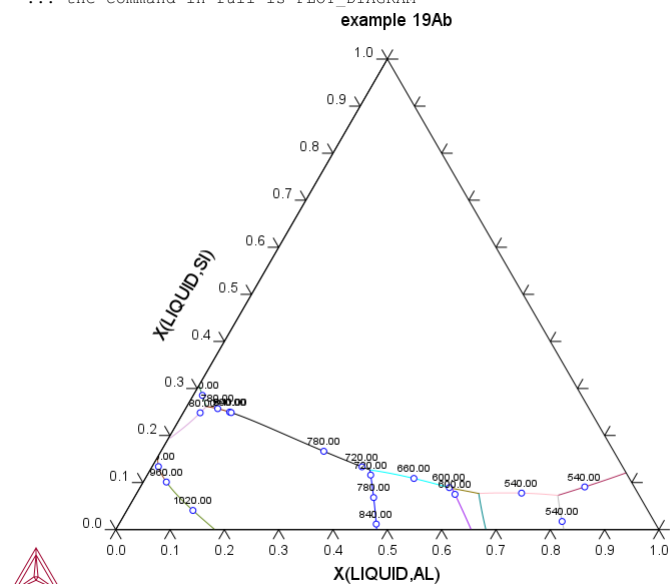
```



```

POST:
POST:Hit RETURN to continue
POST: @@ Take away the phase labels and add tic
POST: @@ marks along the lines (the Z axis)
POST:
POST: s-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a z t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-sc z n 500 1000
... the command in full is SET_SCALING_STATUS
POST: set-title example 19Ab
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



```

POST:
POST:Hit RETURN to continue
POST: @@ Make a new calculation to overlay the monovariant
POST: @@ lines with isothermal calculations
POST:
POST: make tcex19a y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: read tcex19a1
... the command in full is READ_WORKSPACES
POLY:
POLY: s-a-v 3
... the command in full is SET_AXIS_VARIABLE
Condition /T/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0.107 s
Found the set of lowest grid points in 0.003 s
Calculated POLY solution 0.030 s, total time 0.140 s

```

```

POLY: save tcexl9a2 y
... the command in full is SAVE_WORKSPACES
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1300, P=101325, N=1, X(SI)=0.25, X(AL)=0.2
DEGREES OF FREEDOM 0
POLY: s-c x(al)
... the command in full is SET_CONDITION
Value /.2/: .10
POLY: @@ Use ADD to have several start points at different
POLY: @@ temperatures. But do not use default direction as
POLY: @@ that creates many start points. Increasing the Si
POLY: @@ content makes a solid phase stable.
POLY:
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: @@ You can have initial equilibria for different conditions
POLY: @@ at the same time. Just the axis variables have to be
POLY: @@ the same. To make nice isothermal curves is not easy;
POLY: @@ try with several start points to find all curve sections.
POLY:
POLY: s-c t
... the command in full is SET_CONDITION
Value /1300/: 1200
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0.056 s
Found the set of lowest grid points in 0.003 s
Calculated POLY solution 0.074 s, total time 0.133 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: s-c t
... the command in full is SET_CONDITION
Value /1200/: 1100
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0.071 s
Found the set of lowest grid points in 0.002 s
Calculated POLY solution 0.049 s, total time 0.122 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: @@ This line exists only in the Al rich corner
POLY: s-c x(al)=.5 x(si)=.1
... the command in full is SET_CONDITION
POLY: s-c t
... the command in full is SET_CONDITION
Value /1100/: 1000
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0.063 s
Found the set of lowest grid points in 0.003 s
Calculated POLY solution 0.022 s, total time 0.088 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY: @@ A start point in the low melting Al corner too
POLY:
POLY: s-c x(al)=.9 x(si)=.01 t=900
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0.059 s
Found the set of lowest grid points in 0.002 s
Calculated POLY solution 0.017 s, total time 0.078 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: map
Version S mapping is selected

Organizing start points

```


Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard

Phase region boundary 1 at: 5.000E-02 6.891E-01
LIQUID
** DIAMOND_A4
Calculated 10 equilibria

Phase region boundary 2 at: 5.000E-02 6.891E-01
LIQUID
** DIAMOND_A4
Calculated 52 equilibria

Phase region boundary 3 at: 1.004E-01 3.055E-02
LIQUID
** FCC_A1
Calculated 21 equilibria

Phase region boundary 4 at: 1.004E-01 3.055E-02
LIQUID
** FCC_A1
Calculated. 5 equilibria

Phase region boundary 5 at: 1.373E-01 1.932E-02
LIQUID
** BCC_B2
** FCC_A1

Phase region boundary 6 at: 1.463E-01 2.848E-02
LIQUID
** BCC_B2
Calculated 51 equilibria

Phase region boundary 7 at: 1.373E-01 1.932E-02
LIQUID
** FCC_A1
Calculated 27 equilibria

Phase region boundary 8 at: 5.000E-02 6.515E-01
LIQUID
** DIAMOND_A4
Calculated 43 equilibria

Phase region boundary 9 at: 5.000E-02 6.515E-01
LIQUID
** DIAMOND_A4
Calculated 52 equilibria

Phase region boundary 10 at: 1.081E-01 1.639E-01
LIQUID
** BCC_B2
Calculated. 16 equilibria

Phase region boundary 11 at: 2.872E-02 1.169E-01
LIQUID
** BCC_B2
** FCC_A1

Phase region boundary 12 at: 2.764E-02 9.624E-02
LIQUID
** FCC_A1
Calculated 13 equilibria

Phase region boundary 13 at: 2.872E-02 1.169E-01
LIQUID
** BCC_B2
Calculated 70 equilibria

Phase region boundary 14 at: 1.081E-01 1.639E-01
LIQUID
** BCC_B2
Calculated 44 equilibria

Phase region boundary 15 at: 5.000E-02 6.262E-01
LIQUID
** DIAMOND_A4
Calculated 38 equilibria

Phase region boundary 16 at: 5.000E-02 6.262E-01
LIQUID
** DIAMOND_A4
Calculated 56 equilibria

Phase region boundary 17 at: 1.116E-01 1.999E-01
LIQUID
** BCC_B2
Calculated 23 equilibria

Phase region boundary 18 at: 1.116E-01 1.999E-01
LIQUID
** BCC_B2
Calculated. 34 equilibria

```

Phase region boundary 19 at: 4.370E-01 1.765E-02
LIQUID
** ALCU_EPSILON
** BCC_B2

Phase region boundary 20 at: 4.453E-01 1.265E-02
LIQUID
** ALCU_EPSILON
Calculated 18 equilibria

Phase region boundary 21 at: 4.370E-01 1.765E-02
LIQUID
** BCC_B2
Calculated. 43 equilibria

Phase region boundary 22 at: 2.106E-02 1.939E-01
LIQUID
** BCC_B2
** CU19SI6_ETA

Phase region boundary 23 at: 7.190E-03 2.263E-01
LIQUID
** CU19SI6_ETA
Calculated 24 equilibria

Phase region boundary 24 at: 2.500E-01 5.691E-01
LIQUID
** DIAMOND_A4
Calculated. 8 equilibria

Phase region boundary 25 at: 1.890E-01 5.683E-01
LIQUID
** BCC_B2
** DIAMOND_A4

Phase region boundary 26 at: 3.667E-01 1.003E-01
LIQUID
** BCC_B2
Calculated. 5 equilibria

Phase region boundary 27 at: 3.979E-01 7.953E-02
LIQUID
** ALCU_EPSILON
** BCC_B2

Phase region boundary 28 at: 4.219E-01 5.542E-02
LIQUID
** ALCU_EPSILON
Calculated 28 equilibria

Phase region boundary 29 at: 1.890E-01 5.683E-01
LIQUID
** DIAMOND_A4
Calculated 42 equilibria

Phase region boundary 30 at: 2.500E-01 5.691E-01
LIQUID
** DIAMOND_A4
Calculated 49 equilibria

Phase region boundary 31 at: 4.698E-01 3.348E-02
LIQUID
** ALCU_EPSILON
Calculated. 6 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 4.698E-01 3.348E-02
LIQUID
** ALCU_EPSILON
Calculated 27 equilibria

Phase region boundary 33 at: 9.694E-01 5.516E-03
LIQUID
** FCC_A1
Calculated 12 equilibria

Phase region boundary 34 at: 9.694E-01 5.516E-03
LIQUID
** FCC_A1
Calculated 16 equilibria

Phase region boundary 35 at: 5.506E-01 5.000E-03
LIQUID
** ALCU_EPSILON
Calculated 18 equilibria

Phase region boundary 36 at: 5.506E-01 5.000E-03
LIQUID
** ALCU_EPSILON
Calculated. 10 equilibria

Phase region boundary 37 at: 4.954E-01 4.888E-02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4

Phase region boundary 38 at: 2.690E-01 5.489E-01
LIQUID
** DIAMOND_A4
Calculated 35 equilibria

Phase region boundary 39 at: 4.954E-01 4.888E-02
LIQUID
** ALCU_EPSILON
Calculated 22 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex19A\tcex19a2.POLY3
CPU time for mapping 10 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x x(liquid,al)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liquid,si)
... the command in full is SET_DIAGRAM_AXIS

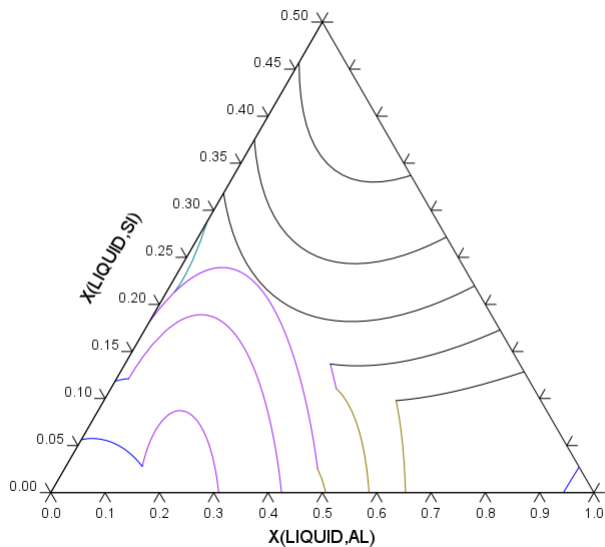
```

```

POST: s-d-ty y,,,,
... the command in full is SET_DIAGRAM_TYPE
POST:
POST:
POST: set-title example 19Ac
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 19Ac

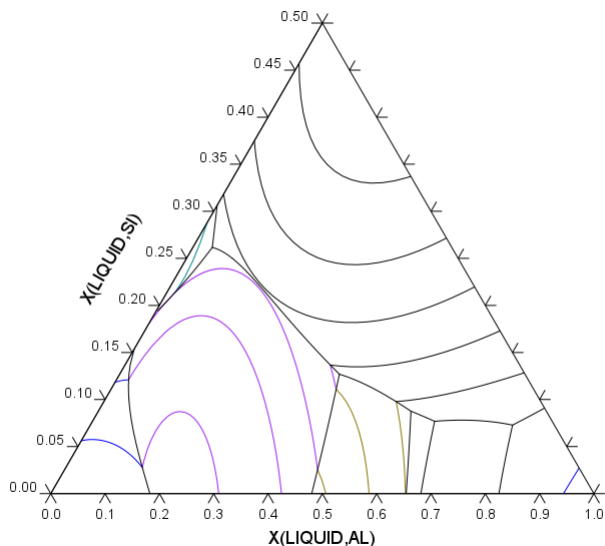


```

POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex19a
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 19Ad
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 19Ad

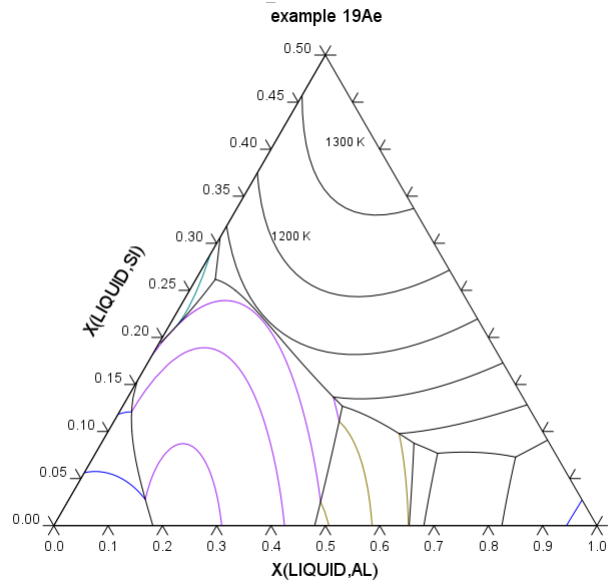


```

POST:
POST:Hit RETURN to continue
POST: add .1 .4 n 1300 K
... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: add .1 .3 n 1200 K
... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: set-title example 19Ae
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10

```

```
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 19Ae
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```



tcex19B

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex19B\tcex19B.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si

SYS:

SYS: @@ This is the second part of a two part example showing how

SYS: @@ to map univariant equilibria with the liquid in Al-Cu-Si.

SYS: @@ Part B. Using the Ternary module, you can get the

SYS: @@ information on invariant reactions, such as temperature

SYS: @@ and compositions.

SYS:

SYS: set-log ex19b,,

SYS: go ter

... the command in full is GOTO_MODULE

Quick ternary phase diagram calculation module

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Current database: Iron Demo Database v6.0

VA /- DEFINED

Database: /FEDEMO/: user tcex19_cost2.TDB

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

09:03:02,727 [Thread-0] INFO TDBFileParser: USER_1760156540_21, number of lines read: 470

09:03:03,083 [Thread-0] INFO DatabaseUtils: Parsing of USER_1760156540_21 completed in 439 ms

First element: al cu si

Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: L

Min temperature, C /25/: 25

Max temperature, C /2500/: 2500

Temperature interval /100/: 100

Global minimization on: /N/: N

VA /- DEFINED

REINITIATING GES

AL CU SI

DEFINED

*** ERROR GAS INPUT IGNORED

* WARNING: This database has no list of assessed systems *

* The diagram may be wrong. *

Quit? /Y/: N

09:03:03,287 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Forcing automatic start values

Automatic start values will be set

09:03:03,712 [Thread-0] INFO Database: Preparing system for use: USER_1760156540_21

09:03:04,720 [Thread-0] INFO Phase: Preparing phase for use: LIQUID

09:03:05,092 [Thread-0] INFO Phase: Preparing phase for use: ALCU_AMORPHOUS

09:03:05,532 [Thread-0] INFO Phase: Preparing phase for use: ALCUZN_T

09:03:05,870 [Thread-0] INFO Phase: Preparing phase for use: ALCU_DELTA

09:03:06,270 [Thread-0] INFO Phase: Preparing phase for use: ALCU_EPSILON

09:03:06,679 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ETA

09:03:06,949 [Thread-0] INFO Phase: Preparing phase for use: ALCU_PRIME

09:03:07,226 [Thread-0] INFO Phase: Preparing phase for use: ALCU_THETA

09:03:07,593 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ZETA

09:03:07,869 [Thread-0] INFO Phase: Preparing phase for use: ALLI

09:03:08,166 [Thread-0] INFO Phase: Preparing phase for use: ALMO

09:03:08,419 [Thread-0] INFO Phase: Preparing phase for use: ALM_D019

09:03:08,694 [Thread-0] INFO Phase: Preparing phase for use: ALND_AMORPHOUS

09:03:09,012 [Thread-0] INFO Phase: Preparing phase for use: ALTI

09:03:09,322 [Thread-0] INFO Phase: Preparing phase for use: BCC_B2

09:03:09,614 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2

09:03:09,859 [Thread-0] INFO Phase: Preparing phase for use: BCT_A5

09:03:10,123 [Thread-0] INFO Phase: Preparing phase for use: CBCC_A12

09:03:10,364 [Thread-0] INFO Phase: Preparing phase for use: CR3SI_A15

09:03:10,635 [Thread-0] INFO Phase: Preparing phase for use: CRSI2

09:03:10,890 [Thread-0] INFO Phase: Preparing phase for use: CU19SI6_ETA

09:03:11,223 [Thread-0] INFO Phase: Preparing phase for use: CU33SI7_DELTA

09:03:11,546 [Thread-0] INFO Phase: Preparing phase for use: CU4SI_EPSILON

09:03:11,791 [Thread-0] INFO Phase: Preparing phase for use: CU56SI11_GAMMA

09:03:12,070 [Thread-0] INFO Phase: Preparing phase for use: CU6Y

09:03:12,309 [Thread-0] INFO Phase: Preparing phase for use: CUB_A13

09:03:12,549 [Thread-0] INFO Phase: Preparing phase for use: CUB_A15

09:03:12,830 [Thread-0] INFO Phase: Preparing phase for use: DIAMOND_A4

```

09:03:13,067 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
09:03:13,357 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_D83
09:03:13,594 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_H
09:03:13,841 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3
09:03:14,172 [Thread-0] INFO Phase: Preparing phase for use: HCP_ZN
09:03:14,450 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C14
09:03:14,708 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C15
09:03:15,013 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C36
09:03:15,546 [Thread-0] INFO Phase: Preparing phase for use: SIV3
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
T = 1673.15 K
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 7.327E-03 9.853E-01
LIQUID
** DIAMOND_A4
Calculated 15 equilibria

Phase region boundary 2 at: 7.327E-03 9.853E-01
LIQUID
** DIAMOND_A4
Calculated 15 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 2 seconds
T = 1573.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 7.453E-02 8.883E-01
LIQUID
** DIAMOND_A4
Calculated 23 equilibria

Phase region boundary 2 at: 7.453E-02 8.883E-01
LIQUID
** DIAMOND_A4
Calculated 25 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 1 seconds
T = 1473.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.372E-01 7.942E-01
LIQUID
** DIAMOND_A4
Calculated 30 equilibria

Phase region boundary 2 at: 1.372E-01 7.942E-01
LIQUID
** DIAMOND_A4
Calculated 22 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 1 seconds
T = 1373.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.926E-01 7.111E-01
LIQUID
** DIAMOND_A4
Calculated 28 equilibria

Phase region boundary 2 at: 1.926E-01 7.111E-01
LIQUID
** DIAMOND_A4
Calculated 32 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 0 seconds
T = 1273.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy

```

the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 6.652E-01 9.329E-03
LIQUID
** BCC_B2
Calculated. 2 equilibria

Phase region boundary 2 at: 6.645E-01 6.795E-03
LIQUID
** BCC_B2
** GAMMA_H

Phase region boundary 3 at: 6.653E-01 4.077E-03
LIQUID
** GAMMA_H
Calculated 12 equilibria

Phase region boundary 4 at: 6.645E-01 6.795E-03
LIQUID
** BCC_B2
Calculated. 29 equilibria

Phase region boundary 5 at: 8.419E-01 6.666E-02
LIQUID
** BCC_B2
** FCC_A1

Phase region boundary 6 at: 8.633E-01 4.917E-02
LIQUID
** FCC_A1
Calculated 25 equilibria

Phase region boundary 7 at: 6.652E-01 9.329E-03
LIQUID
** BCC_B2
Calculated. 30 equilibria

Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 1 seconds

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 2.311E-01 6.535E-01
LIQUID
** DIAMOND_A4
Calculated 34 equilibria

Phase region boundary 2 at: 2.311E-01 6.535E-01
LIQUID
** DIAMOND_A4
Calculated 40 equilibria

*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 1 seconds
T = 1173.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 5.840E-01 7.591E-03
LIQUID
** BCC_B2
Calculated 9 equilibria

Phase region boundary 2 at: 5.840E-01 7.591E-03
LIQUID
** BCC_B2
Calculated. 39 equilibria

Phase region boundary 3 at: 8.543E-01 1.296E-01
LIQUID
** BCC_B2
** FCC_A1

Phase region boundary 4 at: 8.749E-01 1.099E-01
LIQUID
** FCC_A1
Calculated 24 equilibria

Phase region boundary 5 at: 8.543E-01 1.296E-01
LIQUID
** BCC_B2
Calculated 54 equilibria

*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 2 seconds

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```
Generating start point  1
Generating start point  2

Phase region boundary  1 at:  2.562E-01  6.158E-01
  LIQUID
  ** DIAMOND_A4
Calculated              39 equilibria

Phase region boundary  2 at:  2.562E-01  6.158E-01
  LIQUID
  ** DIAMOND_A4
Calculated              37 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping    0 seconds
T = 1073.15 K
```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```
Generating start point  1
Generating start point  2

Phase region boundary  1 at:  5.198E-01  5.412E-03
  LIQUID
  ** ALCU_EPSILON
Calculated              11 equilibria

Phase region boundary  2 at:  5.198E-01  5.412E-03
  LIQUID
  ** ALCU_EPSILON
Calculated              5 equilibria

Phase region boundary  3 at:  5.361E-01  2.533E-02
  LIQUID
  ** ALCU_EPSILON
  ** BCC_B2
Calculated              12 equilibria

Phase region boundary  4 at:  5.383E-01  3.569E-02
  LIQUID
  ** BCC_B2
Calculated              12 equilibria

Phase region boundary  5 at:  5.962E-01  1.431E-01
  LIQUID
  ** BCC_B2
  ** DIAMOND_A4
Calculated              41 equilibria

Phase region boundary  6 at:  2.789E-01  5.911E-01
  LIQUID
  ** DIAMOND_A4
Calculated              41 equilibria

Phase region boundary  7 at:  5.361E-01  2.533E-02
  LIQUID
  ** ALCU_EPSILON
Calculated              16 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping    0 seconds
```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```
Generating start point  1
Generating start point  2

Phase region boundary  1 at:  7.337E-01  2.597E-01
  LIQUID
  ** CU19SI6_ETA
Calculated              4 equilibria

Phase region boundary  2 at:  7.478E-01  2.387E-01
  LIQUID
  ** BCC_B2
  ** CU19SI6_ETA
Calculated              8 equilibria

Phase region boundary  3 at:  7.525E-01  2.105E-01
  LIQUID
  ** BCC_B2
Calculated              8 equilibria

Phase region boundary  4 at:  6.917E-01  2.112E-01
  LIQUID
  ** BCC_B2
  ** DIAMOND_A4
Calculated              14 equilibria

Phase region boundary  5 at:  3.329E-01  6.250E-01
  LIQUID
  ** DIAMOND_A4
Calculated              14 equilibria

Phase region boundary  6 at:  3.469E-01  6.529E-01
  LIQUID
  ** CU19SI6_ETA
Calculated              14 equilibria
```



```

** DIAMOND_A4

Phase region boundary 7 at: 7.269E-01 2.729E-01
LIQUID
** CU19SI6_ETA
Calculated. 6 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 7.337E-01 2.597E-01
LIQUID
** CU19SI6_ETA
Calculated. 3 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 0 seconds
T = 973.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.736E-01 5.113E-03
LIQUID
** ALCU_EPSILON
Calculated 12 equilibria

Phase region boundary 2 at: 4.736E-01 5.113E-03
LIQUID
** ALCU_EPSILON
Calculated. 12 equilibria

Phase region boundary 3 at: 5.106E-01 6.209E-02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4

Phase region boundary 4 at: 2.273E-01 5.621E-01
LIQUID
** DIAMOND_A4
Calculated 36 equilibria

Phase region boundary 5 at: 5.106E-01 6.209E-02
LIQUID
** ALCU_EPSILON
Calculated 24 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 0 seconds
T = 873.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 3.646E-02 1.803E-02
LIQUID
** FCC_A1
Calculated 15 equilibria

Phase region boundary 2 at: 3.646E-02 1.803E-02
LIQUID
** FCC_A1
Calculated 33 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 1 seconds

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.151E-01 5.493E-03
LIQUID
** ALCU_ETA
Calculated 8 equilibria

Phase region boundary 2 at: 4.151E-01 5.493E-03
LIQUID
** ALCU_ETA
Calculated. 6 equilibria

Phase region boundary 3 at: 4.241E-01 3.756E-02
LIQUID
** ALCU_EPSILON
** ALCU_ETA

Phase region boundary 4 at: 4.398E-01 3.756E-02
LIQUID
** ALCU_EPSILON
Calculated. 2 equilibria

```

```

Phase region boundary 5 at: 4.420E-01 4.464E-02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4

Phase region boundary 6 at: 1.706E-01 5.446E-01
LIQUID
** DIAMOND_A4
Calculated 27 equilibria

Phase region boundary 7 at: 4.241E-01 3.756E-02
LIQUID
** ALCU_ETA
Calculated 17 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 0 seconds
T = 773.15 K

```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

T = 1773.15 K
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 3.379E-01 7.512E-02 8.731E+02
LIQUID
** ALCU_EPSILON
** ALCU_ETA
CALCULATED 4 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_EPSILON
** ALCU_ETA
DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4
CALCULATED 25 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** ALCU_EPSILON
BCC_B2
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** ALCU_EPSILON
** BCC_B2
Terminating at diagram limit
CALCULATED 34 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** BCC_B2
** DIAMOND_A4
CALCULATED 43 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** BCC_B2
CU19SI6_ETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** BCC_B2
** CU19SI6_ETA
Terminating at known equilibrium
CALCULATED 37 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** CU19SI6_ETA
** DIAMOND_A4
*** SORRY CANNOT CONTINUE *** 4

CALCULATED 16 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_ETA
** DIAMOND_A4
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_ETA
ALCU_THETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_ETA
** ALCU_THETA
Terminating at diagram limit
CALCULATED 14 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_THETA

```

[illegible]

Automatic start values will be set

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6

Phase region boundary 1 at: 3.379E-01 7.512E-02 8.731E+02
LIQUID
** ALCU_EPSILON
** ALCU_ETA
CALCULATED 4 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_EPSILON
** ALCU_ETA
DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4
CALCULATED 25 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** ALCU_EPSILON
BCC_B2
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** ALCU_EPSILON
** BCC_B2
Terminating at diagram limit
CALCULATED 34 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** BCC_B2
** DIAMOND_A4
CALCULATED 43 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** BCC_B2
CU19SI6_ETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** BCC_B2
** CU19SI6_ETA
Terminating at known equilibrium
CALCULATED 37 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** CU19SI6_ETA
** DIAMOND_A4
*** SORRY CANNOT CONTINUE *** 4
CALCULATED 16 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_ETA
** DIAMOND_A4
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_ETA
ALCU_THETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_ETA
** ALCU_THETA
Terminating at diagram limit
CALCULATED 14 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_THETA
** DIAMOND_A4
CALCULATED 17 EQUILIBRIA

Phase region boundary 2 at: 1.498E-01 7.282E-02 7.852E+02
LIQUID
** ALCU_THETA
** DIAMOND_A4
FCC_A1
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 1.498E-01 7.282E-02 7.852E+02
LIQUID
** ALCU_THETA

```
FCC_A1
Terminating at diagram limit
CALCULATED      12 EQUILIBRIA

Phase region boundary    2 at:   1.498E-01   7.282E-02   7.852E+02
LIQUID
** DIAMOND_A4
** FCC_A1
Terminating at diagram limit
CALCULATED      21 EQUILIBRIA

Phase region boundary    2 at:   3.379E-01   7.512E-02   8.731E+02
LIQUID
** ALCU_EPSILON
** ALCU_ETA
Terminating at diagram limit
CALCULATED      12 EQUILIBRIA

Phase region boundary    2 at:   8.482E-01   6.736E-02   1.273E+03
LIQUID
** BCC_B2
** FCC_A1
*** SORRY CANNOT CONTINUE ***          9

CALCULATED      46 EQUILIBRIA

Phase region boundary    2 at:   8.482E-01   6.736E-02   1.273E+03
LIQUID
** BCC_B2
** FCC_A1
Terminating at diagram limit
CALCULATED      13 EQUILIBRIA

Phase region boundary    2 at:   6.503E-01   8.154E-03   1.273E+03
LIQUID
** BCC_B2
** GAMMA_H
Terminating at diagram limit
CALCULATED      13 EQUILIBRIA

Phase region boundary    2 at:   6.503E-01   8.154E-03   1.273E+03
LIQUID
** BCC_B2
** GAMMA_H
Terminating at diagram limit
CALCULATED       9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping                      1 seconds
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point    1
Generating start point    2
Generating start point    3
Generating start point    4
Generating start point    5
Generating start point    6
Generating start point    7
Generating start point    8
Generating start point    9
Generating start point   10
Working hard
Generating start point   11
Generating start point   12
Generating start point   13
Generating start point   14
Generating start point   15
Generating start point   16
Generating start point   17
Generating start point   18
Generating start point   19
Generating start point   20
Working hard
Generating start point   21
Generating start point   22
Generating start point   23
Generating start point   24
Generating start point   25
Generating start point   26
Generating start point   27
Generating start point   28
Generating start point   29
Generating start point   30
Generating start point   31
Generating start point   32
Generating start point   33
Generating start point   34
```

```

Generating start point 35
Working hard

Phase region boundary 1 at: 4.398E-01 3.756E-02
LIQUID
** ALCU_EPSILON
Calculated. 2 equilibria

Phase region boundary 2 at: 4.420E-01 4.464E-02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4

Phase region boundary 3 at: 1.706E-01 5.446E-01
LIQUID
** DIAMOND_A4
Calculated. 30 equilibria

Phase region boundary 4 at: 4.420E-01 4.464E-02
LIQUID
** ALCU_EPSILON
Calculated. 2 equilibria

Phase region boundary 5 at: 4.398E-01 3.756E-02
LIQUID
** ALCU_EPSILON
** ALCU_ETA

Phase region boundary 6 at: 4.241E-01 3.756E-02
LIQUID
** ALCU_ETA
Calculated. 19 equilibria

Phase region boundary 7 at: 4.241E-01 3.756E-02
LIQUID
** ALCU_ETA
Calculated. 1 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 8.419E-01 6.666E-02
LIQUID
** BCC_B2
Calculated. 1 equilibria

Phase region boundary 9 at: 8.419E-01 6.666E-02
LIQUID
** BCC_B2
** FCC_A1

Phase region boundary 10 at: 8.633E-01 4.917E-02
LIQUID
** FCC_A1
Calculated. 25 equilibria

Phase region boundary 11 at: 8.419E-01 6.666E-02
LIQUID
** BCC_B2
Calculated. 28 equilibria

Phase region boundary 12 at: 6.645E-01 6.795E-03
LIQUID
** BCC_B2
** GAMMA_H

Phase region boundary 13 at: 6.653E-01 4.077E-03
LIQUID
** GAMMA_H
Calculated. 12 equilibria

Phase region boundary 14 at: 8.633E-01 4.917E-02
LIQUID
** FCC_A1
Calculated. 25 equilibria

Phase region boundary 15 at: 6.645E-01 6.795E-03
LIQUID
** BCC_B2
Calculated. 26 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 6.653E-01 4.077E-03
LIQUID
** GAMMA_H
Calculated. 12 equilibria

Phase region boundary 17 at: 7.327E-03 9.853E-01
LIQUID
** DIAMOND_A4
Calculated. 15 equilibria

Phase region boundary 18 at: 7.327E-03 9.853E-01
LIQUID
** DIAMOND_A4
Calculated. 15 equilibria

Phase region boundary 19 at: 7.453E-02 8.883E-01
LIQUID
** DIAMOND_A4
Calculated. 23 equilibria

Phase region boundary 20 at: 7.453E-02 8.883E-01
LIQUID
** DIAMOND_A4
Calculated. 25 equilibria

Phase region boundary 21 at: 1.372E-01 7.942E-01
LIQUID
** DIAMOND_A4
Calculated. 30 equilibria

Phase region boundary 22 at: 1.372E-01 7.942E-01
LIQUID
** DIAMOND_A4
Calculated. 22 equilibria

Phase region boundary 23 at: 1.926E-01 7.111E-01

```

```

    LIQUID
    ** DIAMOND_A4
Calculated                28  equilibria

Phase region boundary 24 at:  1.926E-01  7.111E-01
    LIQUID
    ** DIAMOND_A4
Calculated                32  equilibria

Phase region boundary 25 at:  6.652E-01  9.329E-03
    LIQUID
    ** BCC_B2
Calculated.                2  equilibria
Terminating at known equilibrium

Phase region boundary 26 at:  6.652E-01  9.329E-03
    LIQUID
    ** BCC_B2
Calculated.               30  equilibria
Terminating at known equilibrium

Phase region boundary 27 at:  2.311E-01  6.535E-01
    LIQUID
    ** DIAMOND_A4
Calculated                34  equilibria

Phase region boundary 28 at:  2.311E-01  6.535E-01
    LIQUID
    ** DIAMOND_A4
Calculated                40  equilibria

Phase region boundary 29 at:  5.840E-01  7.591E-03
    LIQUID
    ** BCC_B2
Calculated                9  equilibria

Phase region boundary 30 at:  5.840E-01  7.591E-03
    LIQUID
    ** BCC_B2
Calculated.               39  equilibria

Phase region boundary 31 at:  8.543E-01  1.296E-01
    LIQUID
    ** BCC_B2
    ** FCC_A1

Phase region boundary 32 at:  8.749E-01  1.099E-01
    LIQUID
    ** FCC_A1
Calculated                24  equilibria

Phase region boundary 33 at:  8.543E-01  1.296E-01
    LIQUID
    ** BCC_B2
Calculated                54  equilibria

Phase region boundary 34 at:  2.562E-01  6.158E-01
    LIQUID
    ** DIAMOND_A4
Calculated                39  equilibria

Phase region boundary 35 at:  2.562E-01  6.158E-01
    LIQUID
    ** DIAMOND_A4
Calculated                37  equilibria

Phase region boundary 36 at:  5.198E-01  5.412E-03
    LIQUID
    ** ALCU_EPSILON
Calculated                11  equilibria

Phase region boundary 37 at:  5.198E-01  5.412E-03
    LIQUID
    ** ALCU_EPSILON
Calculated.                5  equilibria

Phase region boundary 38 at:  5.361E-01  2.533E-02
    LIQUID
    ** ALCU_EPSILON
    ** BCC_B2

Phase region boundary 39 at:  5.383E-01  3.569E-02
    LIQUID
    ** BCC_B2
Calculated.               12  equilibria

Phase region boundary 40 at:  5.962E-01  1.431E-01
    LIQUID
    ** BCC_B2
    ** DIAMOND_A4

Phase region boundary 41 at:  2.789E-01  5.911E-01
    LIQUID
    ** DIAMOND_A4
Calculated                41  equilibria

Phase region boundary 42 at:  5.361E-01  2.533E-02
    LIQUID
    ** ALCU_EPSILON
Calculated                16  equilibria

Phase region boundary 43 at:  7.337E-01  2.597E-01
    LIQUID
    ** CU19SI6_ETA
Calculated.                4  equilibria

Phase region boundary 44 at:  7.478E-01  2.387E-01
    LIQUID
    ** BCC_B2
    ** CU19SI6_ETA

Phase region boundary 45 at:  7.525E-01  2.105E-01
    LIQUID
    ** BCC_B2
Calculated.                8  equilibria

```

```

Phase region boundary 46 at: 6.917E-01 2.112E-01
LIQUID
** BCC_B2
** DIAMOND_A4

Phase region boundary 47 at: 3.329E-01 6.250E-01
LIQUID
** DIAMOND_A4
Calculated. 14 equilibria

Phase region boundary 48 at: 3.469E-01 6.529E-01
LIQUID
** CU19SI6_ETA
** DIAMOND_A4

Phase region boundary 49 at: 7.269E-01 2.729E-01
LIQUID
** CU19SI6_ETA
Calculated. 6 equilibria
Terminating at known equilibrium

Phase region boundary 50 at: 7.337E-01 2.597E-01
LIQUID
** CU19SI6_ETA
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 51 at: 4.736E-01 5.113E-03
LIQUID
** ALCU_EPSILON
Calculated. 12 equilibria

Phase region boundary 52 at: 4.736E-01 5.113E-03
LIQUID
** ALCU_EPSILON
Calculated. 12 equilibria

Phase region boundary 53 at: 5.106E-01 6.209E-02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4

Phase region boundary 54 at: 2.273E-01 5.621E-01
LIQUID
** DIAMOND_A4
Calculated. 36 equilibria

Phase region boundary 55 at: 5.106E-01 6.209E-02
LIQUID
** ALCU_EPSILON
Calculated. 24 equilibria

Phase region boundary 56 at: 3.646E-02 1.803E-02
LIQUID
** FCC_A1
Calculated. 15 equilibria

Phase region boundary 57 at: 3.646E-02 1.803E-02
LIQUID
** FCC_A1
Calculated. 33 equilibria

Phase region boundary 58 at: 4.151E-01 5.493E-03
LIQUID
** ALCU_ETA
Calculated. 8 equilibria

Phase region boundary 59 at: 4.151E-01 5.493E-03
LIQUID
** ALCU_ETA
Calculated. 6 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping 8 seconds
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

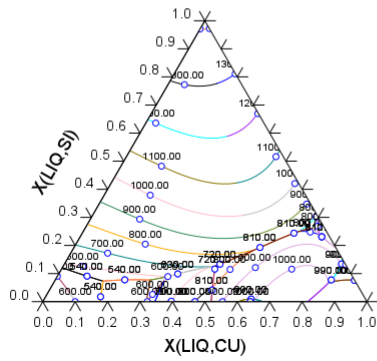
INVARIANT REACTIONS:

```

E 1: 751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1: 705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2: 594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3: 555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2: 512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1

```


AL-CU-SI (600C/1400C/100C)

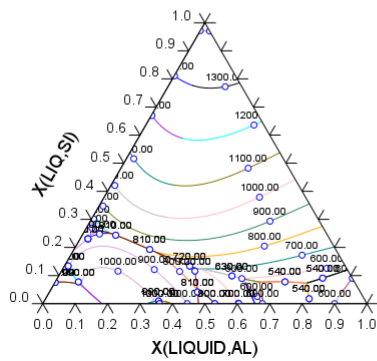


INVARIANT REACTIONS:

E 1 : 751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
 U 1 : 705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
 U 2 : 594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
 U 3 : 555.98 C: LIQUID + ALCU_ETA -> ALCU_THETA + DIAMOND
 E 2 : 512.07 C: LIQUID -> ALCU_THETA + DIAMOND + FCC_A1



```
POST: s-d-a x x(liquid,al)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 19B
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 19B
```



INVARIANT REACTIONS:

E 1 : 751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
 U 1 : 705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
 U 2 : 594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
 U 3 : 555.98 C: LIQUID + ALCU_ETA -> ALCU_THETA + DIAMOND
 E 2 : 512.07 C: LIQUID -> ALCU_THETA + DIAMOND + FCC_A1



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex20

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex20\tcex20.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Adiabatic decompression in a geological system

SYS:

SYS: @@ This example calculates the adiabatic decompression

SYS: @@ in a geological system using the geochemical

SYS: @@ database (PGEO.TDB)

SYS:

SYS: set-log ex20,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw user PGEO.TDB

... the command in full is SWITCH_DATABASE

Current database: User defined Database

O VA DEFINED
STEAM OXYGEN HYDROGEN

REJECTED
CARBON MONOXIDE CARBON_DIOXIDE METHANE
REJECTED

09:05:00,960 [Thread-0] INFO TDBFileParser: USER_2008403235_21, number of lines read: 3095

09:05:02,102 [Thread-0] INFO DatabaseUtils: Parsing of USER_2008403235_21 completed in 1248 ms

TDB_USER: d-sys mg si

... the command in full is DEFINE_SYSTEM

MG SI DEFINED

TDB_USER: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:

GAS:G :O2:
> Gaseous Mixture with C-H-O species, using ideal gas model

A_QUARTZ :Si1O2:
B_QUARTZ :Si1O2:
CRISTOBALITE :Si1O2:
TRIDYMIT :Si1O2:
COESITE :Si1O2:
STISHOVITE :Si1O2:
PERICLASE :MG1O1:
FORSTERITE :Si1MG2O4:
BETA_FORSTERITE :Si1MG2O4:
GAMMA_FORSTERITE :Si1MG2O4:
ILMENITE_MG :Si1MG1O3:
MG_PEROVSKITE :Si1MG1O3:
CLINOENSTATITE :Si1MG1O3:
ORTHOENSTATITE :Si1MG1O3:
PROTOENSTATITE :Si1MG1O3:
CLINOENSTHP :Si1MG1O3:
GARNET_MG :Si1MG1O3:

TDB_USER: rej ph gas proto

... the command in full is REJECT

GAS:G PROTOENSTATITE REJECTED

TDB_USER: get

... the command in full is GET_DATA

09:05:02,871 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

-OK-

TDB_USER: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Define more convenient components

POLY: def-com mgo o sio2

... the command in full is DEFINE_COMPONENTS

POLY: l-st

... the command in full is LIST_STATUS

Option /CPS/: CPS

*** STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T (K)	P (Pa)
VA	ENTERED	SER		
MGO	ENTERED	SER		
O	ENTERED	SER		
SIO2	ENTERED	SER		

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
TRIDYMIT	ENTERED	0.000000E+00	0.000000E+00
STISHOVITE	ENTERED	0.000000E+00	0.000000E+00
PERICLASE	ENTERED	0.000000E+00	0.000000E+00
ORTHOENSTATITE	ENTERED	0.000000E+00	0.000000E+00
MG_PEROVSKITE	ENTERED	0.000000E+00	0.000000E+00
ILMENITE_MG	ENTERED	0.000000E+00	0.000000E+00
GARNET_MG	ENTERED	0.000000E+00	0.000000E+00
GAMMA_FORSTERITE	ENTERED	0.000000E+00	0.000000E+00
FORSTERITE	ENTERED	0.000000E+00	0.000000E+00
CRISTOBALITE	ENTERED	0.000000E+00	0.000000E+00
COESITE	ENTERED	0.000000E+00	0.000000E+00
CLINOENSTHP	ENTERED	0.000000E+00	0.000000E+00

```

CLINOENSTATITE      ENTERED      0.000000E+00      0.000000E+00
B_QUARTZ            ENTERED      0.000000E+00      0.000000E+00
BETA_FORSTERITE     ENTERED      0.000000E+00      0.000000E+00
A_QUARTZ            ENTERED      0.000000E+00      0.000000E+00
*** STATUS FOR ALL SPECIES
MG      ENTERED      0      ENTERED      SI1MG103 ENTERED      SIO2      ENTERED
MG101   ENTERED      O2      ENTERED      SI1MG204 ENTERED      VA      ENTERED
MGO      ENTERED      SI      ENTERED      SIO2      ENTERED
POLY:Hit RETURN to continue
POLY: @@ and specify a composition assumed
POLY: @@ to be present in the Earth's mantle
POLY:
POLY: s-i-a n(mgo)=80
... the command in full is SET_INPUT_AMOUNTS
POLY: s-i-a n(silmg103)=100
... the command in full is SET_INPUT_AMOUNTS
POLY: l-c
... the command in full is LIST_CONDITIONS
N(MGO)=180, N(SIO2)=100
DEGREES OF FREEDOM 3
POLY:Hit RETURN to continue
POLY: @@ There is an error if MgSiO3 is used instead of the
POLY: @@ defined Si1Mg103, since MgSiO3 is not defined as
POLY: @@ a species.
POLY:
POLY: s-c t=2200,p=2e10
... the command in full is SET_CONDITION
POLY: save tcex20 y
... the command in full is SAVE_WORKSPACES
POLY: @@ There is no degree of freedom with respect
POLY: @@ to oxygen so set its activity to unity (or
POLY: @@ any positive number)
POLY:
POLY: s-c ac(o)=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
09:05:04,673 [Thread-0] INFO Database: Preparing system for use: USER_2008403235_21_MODIFIED_174704070363216
09:05:07,772 [Thread-0] INFO Phase: Preparing phase for use: A_QUARTZ
09:05:08,300 [Thread-0] INFO Phase: Preparing phase for use: BETA_FORSTERITE
09:05:08,661 [Thread-0] INFO Phase: Preparing phase for use: B_QUARTZ
09:05:08,983 [Thread-0] INFO Phase: Preparing phase for use: CLINOENSTATITE
09:05:09,265 [Thread-0] INFO Phase: Preparing phase for use: CLINOENSTHP
09:05:09,611 [Thread-0] INFO Phase: Preparing phase for use: COESITE
09:05:09,890 [Thread-0] INFO Phase: Preparing phase for use: CRISTOBALITE
09:05:10,265 [Thread-0] INFO Phase: Preparing phase for use: FORSTERITE
09:05:10,535 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_FORSTERITE
09:05:10,858 [Thread-0] INFO Phase: Preparing phase for use: GARNET_MG
09:05:11,214 [Thread-0] INFO Phase: Preparing phase for use: ILMENITE_MG
09:05:11,508 [Thread-0] INFO Phase: Preparing phase for use: MG_PEROVSKITE
09:05:11,764 [Thread-0] INFO Phase: Preparing phase for use: ORTHOENSTATITE
09:05:12,075 [Thread-0] INFO Phase: Preparing phase for use: PERICLASE
09:05:12,379 [Thread-0] INFO Phase: Preparing phase for use: STISHOVITE
09:05:12,636 [Thread-0] INFO Phase: Preparing phase for use: TRIDYHITE
Testing POLY result by global minimization procedure
Calculated      16 grid points in      0.000 s
31 ITS, CPU TIME USED 23 SECONDS
POLY: save tcex20 y
... the command in full is SAVE_WORKSPACES
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
GARNET_MG   ENTERED      0.000000E+00      4.000000E+01
BETA_FORSTERITE ENTERED      0.000000E+00      2.400000E+02
GAMMA_FORSTERITE ENTERED      -5.946730E-03      0.000000E+00
MG_PEROVSKITE ENTERED      -2.558352E-02      0.000000E+00
ILMENITE_MG ENTERED      -4.828445E-02      0.000000E+00
PERICLASE   ENTERED      -9.575143E-02      0.000000E+00
CLINOENSTHP ENTERED      -1.541632E-01      0.000000E+00
ORTHOENSTATITE ENTERED      -2.197450E-01      0.000000E+00
CLINOENSTATITE ENTERED      -2.394369E-01      0.000000E+00
FORSTERITE   ENTERED      -2.417190E-01      0.000000E+00
STISHOVITE   ENTERED      -3.053984E-01      0.000000E+00
COESITE       ENTERED      -3.775316E+00      0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -7.835592E+00
A_QUARTZ B_QUARTZ TRIDYHITE CRISTOBALITE
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: X
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(MGO)=180, N(SIO2)=100, T=2200, P=2E10, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 2200.00 K ( 1926.85 C), Pressure 2.000000E+10
Number of moles of components 2.800000E+02, Mass in grams 1.32632E+04
Total Gibbs energy -1.80863E+08, Enthalpy -9.91578E+07, Volume 3.55512E-03

Component      Moles      M-Fraction Activity Potential Ref.stat
MGO      1.8000E+02      6.4286E-01 7.6674E-14 -5.5240E+05 SER
O      0.0000E+00      0.0000E+00 1.0000E+00 0.0000E+00 SER
SIO2     1.0000E+02      3.5714E-01 4.6393E-20 -8.1430E+05 SER

BETA_FORSTERITE      Status ENTERED      Driving force 0.0000E+00
Moles 2.4000E+02, Mass 1.1255E+04, Volume fraction 8.5320E-01 Mole fractions:
MGO 6.6667E-01 SIO2 3.3333E-01 O 0.000000E+00

GARNET_MG      Status ENTERED      Driving force 0.0000E+00
Moles 4.0000E+01, Mass 2.0078E+03, Volume fraction 1.4680E-01 Mole fractions:
MGO 5.0000E-01 SIO2 5.0000E-01 O 0.000000E+00
POLY:Hit RETURN to continue
POLY:
POLY: ent fun dens=1e-3*bm/vm;
... the command in full is ENTER_SYMBOL
POLY: sh dens
... the command in full is SHOW_VALUE
DENS=3730.7358
POLY: @@ We have found the equilibrium at this pressue.
POLY: @@ Now assume this system is decompressed
POLY: @@ adiabatically. What will the new temperature become?

```

```

POLY:
POLY: s-c h
... the command in full is SET_CONDITION
Value /-99157833.21/:
POLY: s-c t
... the command in full is SET_CONDITION
Value /2200/: none
POLY: l-c
... the command in full is LIST_CONDITIONS
N(MGO)=180, N(SIO2)=100, P=2E10, AC(O)=1, H=-99157833.21
DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ Now t is independent, calculate the equilibrium and get t
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=2200.
POLY:Hit RETURN to continue
POLY: @@ It's the same temperature. Now change pressure
POLY:
POLY: s-c p
... the command in full is SET_CONDITION
Value /2E+10/: 150e8
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 16 grid points in 0.004 s
17 ITS, CPU TIME USED 1 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=2977.6276
POLY:Hit RETURN to continue
POLY: @@ We will also have a new density and another set of
POLY: @@ stable phases.
POLY:
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(MGO)=180, N(SIO2)=100, P=1.5E10, AC(O)=1, H=-99157833.21
DEGREES OF FREEDOM 0

Temperature 2977.63 K ( 2704.48 C), Pressure 1.500000E+10
Number of moles of components 2.800000E+02, Mass in grams 1.32632E+04
Total Gibbs energy -2.30661E+08, Enthalpy -9.91578E+07, Volume 3.59115E-03

Component      Moles      M-Fraction  Activity   Potential  Ref.stat
MGO             1.8000E+02  6.4286E-01  4.6875E-13 -7.0283E+05 SER
O               0.0000E+00  0.0000E+00  1.0000E+00  0.0000E+00 SER
SIO2            1.0000E+02  3.5714E-01  5.3688E-19 -1.0415E+06 SER

GARNET_MG      Status ENTERED      Driving force  0.0000E+00
Moles 2.0000E+02, Mass 1.0039E+04, Volume fraction 7.4847E-01 Mole fractions:
MGO 5.00000E-01 SIO2 5.00000E-01 O 0.00000E+00

PERICLASE      Status ENTERED      Driving force  0.0000E+00
Moles 8.0000E+01, Mass 3.2244E+03, Volume fraction 2.5153E-01 Mole fractions:
MGO 1.00000E+00 SIO2 0.00000E+00 O 0.00000E+00
POLY: sh dens
... the command in full is SHOW_VALUE
DENS=3693.3029
POLY: sh v
... the command in full is SHOW_VALUE
V=3.5911547E-3
POLY: sh vm
... the command in full is SHOW_VALUE
VM=1.2825553E-5
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```

tcex21

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex21\tcex21.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a ternary isotherm in Fe-Cr-Ni

SYS:

SYS: @@ This example calculates a ternary isotherm

SYS: @@ in Fe-Cr-Ni with a user-defined database.

SYS:

SYS: set-log ex21,,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw user tcex21

... the command in full is SWITCH_DATABASE

Current database: User defined DataBase

This database does not support the DATABASE_INFORMATION command

VA DEFINED

09:06:12,072 [Thread-0] INFO TDBFileParser: USER_121842300_21, number of lines read: 195

09:06:12,317 [Thread-0] INFO DatabaseUtils: Parsing of USER_121842300_21 completed in 336 ms

TDB_USER: def-sys *

... the command in full is DEFINE_SYSTEM

/- VA CR

FE NI DEFINED

TDB_USER: li-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:

LIQUID:L :CR FE NI:

BCC_A2 :CR FE NI:VA:

FCC_A1 :CR FE NI:VA:

HCP_A3 :CR FE NI:VA:

SIGMA :FE NI:CR:CR FE NI:

TDB_USER:Hit RETURN to continue

TDB_USER: get

... the command in full is GET_DATA

09:06:12,479 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_USER: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ With 3 components we must set 5 conditions

POLY: s-c t=1073 p=1e5 n=1 x(cr)=.2 x(ni)=.2

... the command in full is SET_CONDITION

POLY: l-c

... the command in full is LIST_CONDITIONS

T=1073, P=100000, N=1, X(CR)=0.2, X(NI)=0.2

DEGREES OF FREEDOM 0

POLY:

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

09:06:13,136 [Thread-0] INFO Database: Preparing system for use: USER_121842300_21

09:06:14,149 [Thread-0] INFO Phase: Preparing phase for use: LIQUID

09:06:14,578 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2

09:06:14,987 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1

09:06:15,298 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3

09:06:15,635 [Thread-0] INFO Phase: Preparing phase for use: SIGMA

Calculated 9684 grid points in 2.910 s

Found the set of lowest grid points in 0.010 s

Calculated POLY solution 0.169 s, total time 3.089 s

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/:

Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:

T=1073, P=100000, N=1, X(CR)=0.2, X(NI)=0.2

DEGREES OF FREEDOM 0

Temperature 1073.00 K (799.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.56454E+01

Total Gibbs energy -5.39559E+04, Enthalpy 3.01555E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
CR	2.0000E-01	1.8688E-01	5.8626E-03	-4.5849E+04	SER
FE	6.0000E-01	6.0217E-01	3.1002E-03	-5.1533E+04	SER
NI	2.0000E-01	2.1094E-01	4.2164E-04	-6.9332E+04	SER

FCC_A1 Status ENTERED Driving force 0.0000E+00

Moles 1.0000E+00, Mass 5.5645E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 6.02174E-01 NI 2.10943E-01 CR 1.86883E-01

POLY:Hit RETURN to continue

POLY: @@ Define axis

POLY: s-a-v 1 x(cr) 0 1,,,

... the command in full is SET_AXIS_VARIABLE

POLY: s-a-v 2 x(ni) 0 1,,,

... the command in full is SET_AXIS_VARIABLE

POLY: save tcex21 y

... the command in full is SAVE_WORKSPACES

POLY: map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

ERROR 1611 when calculating equilibrium

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Phase region boundary 1 at: 3.521E-02 1.510E-02

BCC_A2

** FCC_A1

Calculated. 20 equilibria

Phase region boundary 2 at: 2.615E-01 6.190E-02

BCC_A2

** FCC_A1

** SIGMA

Phase region boundary 3 at: 3.723E-01 3.566E-02

BCC_A2

** SIGMA

Calculated 21 equilibria

Phase region boundary 4 at: 3.168E-01 6.107E-02

FCC_A1

** SIGMA

Calculated. 20 equilibria

Phase region boundary 5 at: 4.140E-01 2.295E-01

** BCC_A2

FCC_A1

** SIGMA

Phase region boundary 6 at: 5.304E-01 1.820E-01

** BCC_A2

FCC_A1

Calculated 43 equilibria

Phase region boundary 7 at: 6.616E-01 7.178E-02

** BCC_A2

SIGMA

Calculated 31 equilibria

Phase region boundary 8 at: 2.615E-01 6.190E-02

BCC_A2

** FCC_A1

Calculated 33 equilibria

Phase region boundary 9 at: 3.521E-02 1.510E-02

BCC_A2

** FCC_A1

Calculated 15 equilibria

Phase region boundary 10 at: 1.095E-02 2.044E-02

BCC_A2

** FCC_A1

Calculated 18 equilibria

Phase region boundary 11 at: 1.095E-02 2.044E-02

BCC_A2

** FCC_A1

Calculated. 22 equilibria

Terminating at known equilibrium

Phase region boundary 12 at: 3.838E-01 1.780E-02

BCC_A2

** SIGMA

Calculated. 2 equilibria

Terminating at known equilibrium

Phase region boundary 13 at: 3.838E-01 1.780E-02

BCC_A2

** SIGMA

Calculated 21 equilibria

Phase region boundary 14 at: 5.848E-01 2.838E-02

BCC_A2

```

** SIGMA
Calculated                      32  equilibria

Phase region boundary 15 at:    5.848E-01  2.838E-02
  BCC_A2
** SIGMA
Calculated.                     8  equilibria
Terminating at known equilibrium

Phase region boundary 16 at:    5.404E-01  9.033E-03
  BCC_A2
** SIGMA
Calculated                      12  equilibria

Phase region boundary 17 at:    5.404E-01  9.033E-03
  BCC_A2
** SIGMA
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary 18 at:    4.123E-01  2.273E-01
  FCC_A1
** SIGMA
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary 19 at:    4.123E-01  2.273E-01
  FCC_A1
** SIGMA
Calculated.                     2  equilibria
Terminating at known equilibrium

Phase region boundary 20 at:    9.183E-03  2.090E-02
  BCC_A2
  FCC_A1
Calculated                      13  equilibria

Phase region boundary 21 at:    9.183E-03  2.090E-02
  BCC_A2
  FCC_A1
Calculated.                     22  equilibria
Terminating at known equilibrium

Phase region boundary 22 at:    6.363E-01  2.710E-01
  BCC_A2
  FCC_A1
Calculated.                     16  equilibria
Terminating at known equilibrium

Phase region boundary 23 at:    6.363E-01  2.710E-01
  BCC_A2
  FCC_A1
Calculated                      26  equilibria

Phase region boundary 24 at:    6.789E-01  3.114E-01
  BCC_A2
  FCC_A1
Calculated.                     22  equilibria
Terminating at known equilibrium

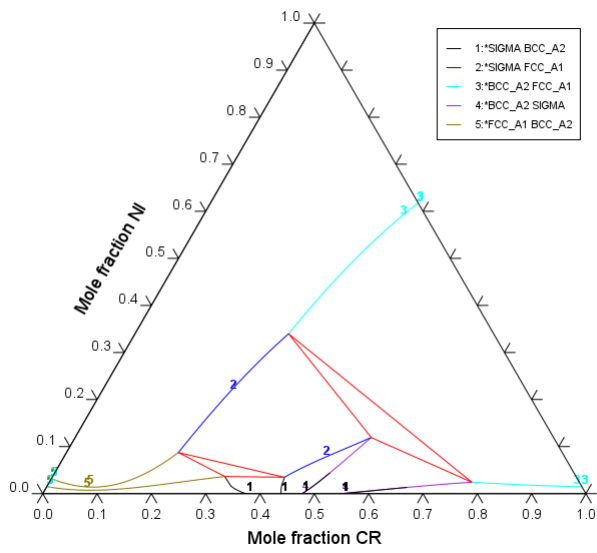
Phase region boundary 25 at:    6.789E-01  3.114E-01
  BCC_A2
  FCC_A1
Calculated                      16  equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex21\tcex21.POLY3
CPU time for mapping              6  seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: set-title example 21a
POST: se-d-ty y,,,
... the command in full is SET_DIAGRAM_TYPE
POST: s-l b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 21a



POST:
 POST:Hit RETURN to continue
 POST: set-inter
 ... the command in full is SET_INTERACTIVE_MODE
 POST:

tcex22

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex22\tcex22.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating an adiabatic flame temperature

SYS:

SYS: @@ This example examines a heat balance when C3H8 is burned

SYS: @@ in oxygen by calculating the adiabatic flame temperature.

SYS: @@ Note that a SSUB database license is required to run

SYS: @@ the example.

SYS:

SYS: set-log ex22,,

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw ssub6

... the command in full is SWITCH_DATABASE

Current database: SGTE Substances v6.0

VA DEFINED

TDB_SSUB6: def-sys c o h

... the command in full is DEFINE_SYSTEM

C O H

DEFINED

TDB_SSUB6: get

... the command in full is GET_DATA

09:07:18,502 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_SSUB6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: l-st

... the command in full is LIST_STATUS

Option /CPS/:

*** STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
C	ENTERED	SER		
H	ENTERED	SER		
O	ENTERED	SER		

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
H2O2_L	ENTERED	0.000000E+00	0.000000E+00
H2O1_L	ENTERED	0.000000E+00	0.000000E+00
DIAMOND	ENTERED	0.000000E+00	0.000000E+00
C_S	ENTERED	0.000000E+00	0.000000E+00
C_L	ENTERED	0.000000E+00	0.000000E+00
C6H6_L	ENTERED	0.000000E+00	0.000000E+00
C60_S	ENTERED	0.000000E+00	0.000000E+00
C4H8_L	ENTERED	0.000000E+00	0.000000E+00
C3H8_L	ENTERED	0.000000E+00	0.000000E+00
C3H6_L	ENTERED	0.000000E+00	0.000000E+00
C2H6_L	ENTERED	0.000000E+00	0.000000E+00
C2H6O2_L	ENTERED	0.000000E+00	0.000000E+00
C2H6O1_L	ENTERED	0.000000E+00	0.000000E+00
C2H4O2_L	ENTERED	0.000000E+00	0.000000E+00
C1H4_L	ENTERED	0.000000E+00	0.000000E+00
C1H4O1_L	ENTERED	0.000000E+00	0.000000E+00
C1H2O2_L	ENTERED	0.000000E+00	0.000000E+00
GAS	ENTERED	0.000000E+00	0.000000E+00

*** STATUS FOR ALL SPECIES

C	ENTERED	C3H6	ENTERED
C1H1	ENTERED	C3H6O1_1	ENTERED
C1H1O1	ENTERED	C3H6O1_2	ENTERED
C1H1O2	ENTERED	C3H6_1	ENTERED
C1H2	ENTERED	C3H6_2	ENTERED
C1H2O1	ENTERED	C3H8	ENTERED
C1H2O2	ENTERED	C3O2	ENTERED
C1H2O2_CIS	ENTERED	C4	ENTERED
C1H2O2_DIOXIRANE	ENTERED	C4H1	ENTERED
C1H2O2_TRANS	ENTERED	C4H10_1	ENTERED
C1H3	ENTERED	C4H10_2	ENTERED
C1H3O1_CH2OH	ENTERED	C4H2_1	ENTERED
C1H3O1_CH3O	ENTERED	C4H2_2	ENTERED
C1H4	ENTERED	C4H4_1	ENTERED
C1H4O1	ENTERED	C4H4_2	ENTERED
C1O1	ENTERED	C4H6_1	ENTERED
C1O2	ENTERED	C4H6_2	ENTERED
C2	ENTERED	C4H6_3	ENTERED
C2H1	ENTERED	C4H6_4	ENTERED
C2H2	ENTERED	C4H6_5	ENTERED
C2H2O1	ENTERED	C4H8	ENTERED
C2H3	ENTERED	C4H8_1	ENTERED

```

C2H4          ENTERED      C4H8_2          ENTERED
C2H4O1_ACETALDEHYDE ENTERED      C4H8_3          ENTERED
C2H4O1_OXIRANE ENTERED      C4H8_4          ENTERED
C2H4O2        ENTERED      C4H8_5          ENTERED
C2H4O2_ACETICACID ENTERED      C4H8_6          ENTERED
C2H4O2_DIOXETANE ENTERED      C5            ENTERED
C2H4O3_123TRIOXOLANE ENTERED      C60          ENTERED
C2H4O3_124TRIOXOLANE ENTERED      C6H6         ENTERED
C2H5          ENTERED      C6H6O1        ENTERED
C2H6          ENTERED      H            ENTERED
C2H6O1        ENTERED      H1O1          ENTERED
C2H6O1_1      ENTERED      H1O2          ENTERED
C2H6O1_2      ENTERED      H2            ENTERED
C2H6O2        ENTERED      H2O1          ENTERED
C2O1          ENTERED      H2O2          ENTERED
C3            ENTERED      O            ENTERED
C3H1          ENTERED      O2           ENTERED
C3H4_1        ENTERED      O3           ENTERED
C3H4_2        ENTERED      VA           ENTERED
POLY: @@ We need to know the heat content of C3H8<G> at room
POLY: @@ temperature. This is a simple number to look up in a
POLY: @@ table but actually quite tricky to calculate as pure
POLY: @@ C3H8 at room temperature does not represent an
POLY: @@ equilibrium state. However, you can get it as follows.
POLY:
POLY: s-c t=298.15,p=1e5,n(o)=1e-10
... the command in full is SET_CONDITION
POLY: s-i-a n(c3h8)=1
... the command in full is SET_INPUT_AMOUNTS
POLY: c-s p *=sus
... the command in full is CHANGE_STATUS
POLY: c-s p gas
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 76 grid points in 0.016 s
Found the set of lowest grid points in 0.003 s
Calculated POLY solution 0.112 s, total time 0.131 s
POLY: @@ The equilibrium state at room temperature is listed
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:
T=298.15, P=100000, N(O)=1E-10, N(C)=3, N(H)=8
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 1.10000E+01, Mass in grams 4.40962E+01
Total Gibbs energy -2.20108E+05, Enthalpy -1.06064E+05, Volume 4.99502E-02

Component      Moles      W-Fraction Activity Potential Ref.stat
C              3.0000E+00  8.1715E-01 1.1356E+07 4.0271E+04 SER
H              8.0000E+00  1.8285E-01 3.4211E-08 -4.2615E+04 SER
O              1.0000E-10  3.6282E-11 1.2651E-49 -2.7911E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.1000E+01, Mass 4.4096E+01, Volume fraction 1.0000E+00 Mass fractions:
C 8.17145E-01 H 1.82855E-01 O 3.62820E-11
Constitution:
C1H4          9.90348E-01 C1H2O1          4.96084E-27 C4H6_3          1.00000E-30
C60           8.16678E-03 C1H2O2_CIS 4.88436E-27 C2H4O1_OXIRA 1.00000E-30
C6H6          1.38456E-03 C4H6_4          3.94602E-28 C4H6_5          1.00000E-30
C2H6          1.00313E-04 C3H4_2          6.04110E-29 C5            1.00000E-30
C3H8          5.44582E-07 C2H5           1.32230E-29 C2H3          1.00000E-30
C4H10_2       3.84975E-08 C1H2O2_TRANS 6.61825E-30 C2H2O1        1.00000E-30
H2            7.83769E-09 C3H4_1          2.45341E-30 C2H2          1.00000E-30
C4H10_1       6.16323E-09 C4H6_1          2.07866E-30 C2H1          1.00000E-30
C1O2          2.32090E-11 C            1.00000E-30 C2            1.00000E-30
H2O1          2.50979E-12 C3O2           1.00000E-30 H            1.00000E-30
C1O1          7.01016E-13 C4            1.00000E-30 H1O1         1.00000E-30
C4H8_5        6.29486E-14 C3H6O1_2       1.00000E-30 H1O2         1.00000E-30
C3H6_2        5.52670E-14 C3H6O1_1       1.00000E-30 H2O2         1.00000E-30
C2H4          3.33175E-14 C4H1           1.00000E-30 C1H3O1_CH3O 1.00000E-30
C4H8_2        7.83367E-15 C4H2_1         1.00000E-30 C1H3O1_CH2OH 1.00000E-30
C4H8_3        3.33692E-15 C3H1           1.00000E-30 C1H3         1.00000E-30
C4H8_1        4.53470E-16 C3            1.00000E-30 O            1.00000E-30
C6H6O1        1.02341E-18 C2O1           1.00000E-30 C1H2O2_DIOXI 1.00000E-30
C3H6_1        2.70389E-21 C2H6O2         1.00000E-30 O2           1.00000E-30
C4H8_6        1.07592E-21 C2H6O1_2       1.00000E-30 O3           1.00000E-30
C4H6_2        4.91032E-22 C4H2_2         1.00000E-30 C1H2         1.00000E-30
C2H4O1_ACETA 1.25014E-22 C4H4_1         1.00000E-30 C1H1O2       1.00000E-30
C4H8_4        2.10624E-23 C4H4_2         1.00000E-30 C1H1O1       1.00000E-30
C2H4O2_ACETI 9.64309E-24 C2H4O3_124TR 1.00000E-30 C1H1         1.00000E-30
C2H6O1_1      1.76369E-24 C2H4O3_123TR 1.00000E-30
C1H4O1        1.08754E-24 C2H4O2_DIOXE 1.00000E-30
POLY: @@ The enthalpy for the system is
POLY: sh h
... the command in full is SHOW_VALUE
H=-106064.27
POLY:Hit RETURN to continue
POLY: @@ But we want a gas with just C3H8.
POLY: @@ Use the Set-All-Startvalues command.
POLY: s-a-s
... the command in full is SET_ALL_START_VALUES
Automatic start values for phase constituents? /N/: n
Should GAS be stable? /Y/: 1
Major constituent(s): C3H8
POLY: sh h
... the command in full is SHOW_VALUE
H=-99431.45
POLY: @@ The difference in H for the two calculations is actually
POLY: @@ not very large. The value is approximate but good as the
POLY: @@ enthalpy is calculated for the following gas constitution
POLY:
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:
T=298.15, P=100000, N(O)=1E-10, N(C)=3, N(H)=8

```

DEGREES OF FREEDOM 0

Temperature 298.15 K (25.00 C), Pressure 1.000000E+05
Number of moles of components 1.07458E+01, Mass in grams 4.32993E+01
Total Gibbs energy -1.78580E+05, Enthalpy -9.94314E+04, Volume 2.43005E-02

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	2.9417E+00	8.1602E-01	1.1356E+07	4.0271E+04	SER
H	7.7974E+00	1.8150E-01	3.4211E-08	-4.2615E+04	SER
O	6.7105E-03	2.4795E-03	1.2651E-49	-2.7911E+05	SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.0746E+01, Mass 4.3299E+01, Volume fraction 1.0000E+00 Mass fractions:
C 8.16017E-01 H 1.81504E-01 O 2.47953E-03

Constitution:

C3H8	9.70396E-01	C4H4_1	1.31579E-04	C2H4O2_ACETI	1.31579E-04
C	1.31579E-04	C4H2_2	1.31579E-04	C2H4O1_OXIRA	1.31579E-04
O2	1.31579E-04	C4H2_1	1.31579E-04	C2H4O1_ACETA	1.31579E-04
O	1.31579E-04	C4H10_2	1.31579E-04	C2H4	1.31579E-04
H2O2	1.31579E-04	C4H10_1	1.31579E-04	C2H3	1.31579E-04
H2O1	1.31579E-04	C4H1_	1.31579E-04	C2H2O1	1.31579E-04
H2	1.31579E-04	C4	1.31579E-04	C2H2	1.31579E-04
H1O2	1.31579E-04	C3O2	1.31579E-04	C2H1	1.31579E-04
H1O1	1.31579E-04	O3	1.31579E-04	C2	1.31579E-04
H	1.31579E-04	C3H6_2	1.31579E-04	C1O2	1.31579E-04
C6H6O1	1.31579E-04	C3H6_1	1.31579E-04	C1O1	1.31579E-04
C6H6	1.31579E-04	C3H6O1_2	1.31579E-04	C1H4O1	1.31579E-04
C6O	1.31579E-04	C3H6O1_1	1.31579E-04	C1H4	1.31579E-04
C5	1.31579E-04	C3H4_2	1.31579E-04	C1H3O1_CH3O	1.31579E-04
C4H8_6	1.31579E-04	C3H4_1	1.31579E-04	C1H3O1_CH2OH	1.31579E-04
C4H8_5	1.31579E-04	C3H1_	1.31579E-04	C1H3	1.31579E-04
C4H8_4	1.31579E-04	C3	1.31579E-04	C1H2O2_TRANS	1.31579E-04
C4H8_3	1.31579E-04	C2O1	1.31579E-04	C1H2O2_DIOXI	1.31579E-04
C4H8_2	1.31579E-04	C2H6O2	1.31579E-04	C1H2O2_CIS	1.31579E-04
C4H8_1	1.31579E-04	C2H6O1_2	1.31579E-04	C1H2O1	1.31579E-04
C4H6_5	1.31579E-04	C2H6O1_1	1.31579E-04	C1H2	1.31579E-04
C4H6_4	1.31579E-04	C2H6	1.31579E-04	C1H1O2	1.31579E-04
C4H6_3	1.31579E-04	C2H5	1.31579E-04	C1H1O1	1.31579E-04
C4H6_2	1.31579E-04	C2H4O3_124TR	1.31579E-04	C1H1	1.31579E-04
C4H6_1	1.31579E-04	C2H4O3_123TR	1.31579E-04		
C4H4_2	1.31579E-04	C2H4O2_DIOXE	1.31579E-04		

POLY:Hit RETURN to continue

POLY: @@ We now have the initial amount of heat. Assuming an excess

POLY: @@ of oxygen we can calculate the temperature where the

POLY: @@ heat content would be the same

POLY:

POLY: sh h

... the command in full is SHOW_VALUE

H=-99431.45

POLY: @@ H is just 11 times HM as there are 11 atoms in C3H8.

POLY: @@ Save that value in a variable

POLY:

POLY: enter var h298=h;

... the command in full is ENTER_SYMBOL

POLY: sh h298

... the command in full is SHOW_VALUE

H298=-99431.45

POLY: @@ If all carbon and hydrogen react with oxygen we need 7

POLY: @@ oxygen atoms to form 3 moles C1O and 4 moles of H2O.

POLY: @@ Add some oxygen in excess

POLY:

POLY: s-c n(o)=9

... the command in full is SET_CONDITION

POLY: @@ Set the heat content as a condition and remove the

POLY: @@ condition on t

POLY:

POLY: s-c h=h298

... the command in full is SET_CONDITION

POLY: s-c t

... the command in full is SET_CONDITION

Value /298.15/: none

POLY: l-c

... the command in full is LIST_CONDITIONS

P=100000, N(O)=9, N(C)=3, N(H)=8, H=H298

DEGREES OF FREEDOM 0

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 76 grid points in 0.004 s

152 ITS, CPU TIME USED 2 SECONDS

POLY: l-e,,,

... the command in full is LIST_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:

P=100000, N(O)=9, N(C)=3, N(H)=8, H=H298

DEGREES OF FREEDOM 0

Temperature 3103.37 K (2830.22 C), Pressure 1.000000E+05
Number of moles of components 2.00000E+01, Mass in grams 1.88087E+02
Total Gibbs energy -7.70691E+06, Enthalpy -9.94314E+04, Volume 2.20472E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	3.0000E+00	1.9158E-01	9.3982E-09	-4.7691E+05	SER
H	8.0000E+00	4.2869E-02	7.7626E-06	-3.0360E+05	SER
O	9.0000E+00	7.6555E-01	6.3815E-08	-4.2748E+05	SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 2.0000E+01, Mass 1.8809E+02, Volume fraction 1.0000E+00 Mass fractions:
O 7.65554E-01 C 1.91576E-01 H 4.28695E-02

Constitution:

H2O1	3.17918E-01	C1H2O2_DIOXI	7.89694E-16	C3H6O1_2	1.00000E-30
C1O1	2.27799E-01	C2H1	8.90508E-17	C3H6_1	1.00000E-30
C1O2	1.23305E-01	C3O2	8.73154E-17	C3H6_2	1.00000E-30
H1O1	8.75243E-02	C2	1.57966E-17	C3H8	1.00000E-30
H2	7.66545E-02	C2H2O1	2.52104E-18	C4	1.00000E-30
O2	6.61854E-02	C2H3	2.72613E-19	C4H1	1.00000E-30
H	5.95645E-02	C2H4O1_ACETA	1.22421E-20	C4H10_1	1.00000E-30
O	4.10043E-02	C2H4	1.12666E-20	C4H10_2	1.00000E-30
H1O2	4.23460E-05	C2H4O2_ACETI	7.64173E-21	C4H4_1	1.00000E-30
H2O2	1.60571E-06	C3H1	9.69741E-23	C4H8_4	1.00000E-30
C1H1O1	9.35079E-07	C3	6.41061E-23	C4H8_5	1.00000E-30
C1H1O2	6.80240E-07	C2H4O1_OXIRA	1.10545E-23	C4H4_2	1.00000E-30
O3	3.00641E-08	C2H5	2.16426E-24	C4H6_1	1.00000E-30

ClH2O2_CIS	1.60533E-08	C2H6	2.32872E-26	C4H6_2	1.00000E-30
ClH2O2_TRANS	8.97486E-09	C2H6O1_1	6.05817E-27	C4H6_3	1.00000E-30
ClH2O1	7.25807E-09	C2H6O2	8.46558E-28	C4H6_4	1.00000E-30
C	5.41880E-11	C3H4_2	5.36473E-28	C4H8_6	1.00000E-30
ClH1	5.71334E-12	C3H4_1	2.88191E-28	C4H6_5	1.00000E-30
ClH2	2.82748E-12	C2H6O1_2	7.51593E-29	C5	1.00000E-30
ClH3	2.09122E-12	C2H4O2_DIOXE	1.26866E-29	C60	1.00000E-30
C2O1	1.16897E-12	C2H4O3_124TR	2.44145E-30	C4H8_1	1.00000E-30
ClH3O1_CH2OH	8.94424E-13	C4H2_1	2.38485E-30	C6H6	1.00000E-30
ClH4	1.80436E-13	C4H2_2	2.37831E-30	C6H6O1	1.00000E-30
ClH3O1_CH3O	1.92548E-14	C4H8_3	1.00000E-30	C4H8_2	1.00000E-30
ClH4O1	9.77820E-15	C2H4O3_123TR	1.00000E-30		
C2H2	1.14657E-15	C3H6O1_1	1.00000E-30		

POLY: @@ The adiabatic temperature is

POLY: sh t

... the command in full is SHOW_VALUE

T=3103.3658

POLY:Hit RETURN to continue

POLY: @@ Now calculate how the adiabatic temperature varies

POLY: @@ with the amount of oxygen

POLY:

POLY: s-a-v 1 n(o) 5 10

... the command in full is SET_AXIS_VARIABLE

Increment /.125/:

POLY: save tcex22 y

... the command in full is SAVE_WORKSPACES

POLY: step normal

... the command in full is STEP_WITH_OPTIONS

No initial equilibrium, using default

Step will start from axis value 9.00000

...OK

Phase Region from 9.00000 for:

GAS

Global test at 1.00000E+01 OK

Terminating at 10.0000

Calculated 11 equilibria

Phase Region from 9.00000 for:

GAS

Global test at 8.00000E+00 OK

Global test at 6.75000E+00 OK

Global test at 5.50000E+00 OK

Terminating at 5.00000

Calculated 35 equilibria

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex22\tcex22.POLY3

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST:

POST: s-d-a x n(o)

... the command in full is SET_DIAGRAM_AXIS

POST: s-d-a y t

... the command in full is SET_DIAGRAM_AXIS

POST: set-title example 22a

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

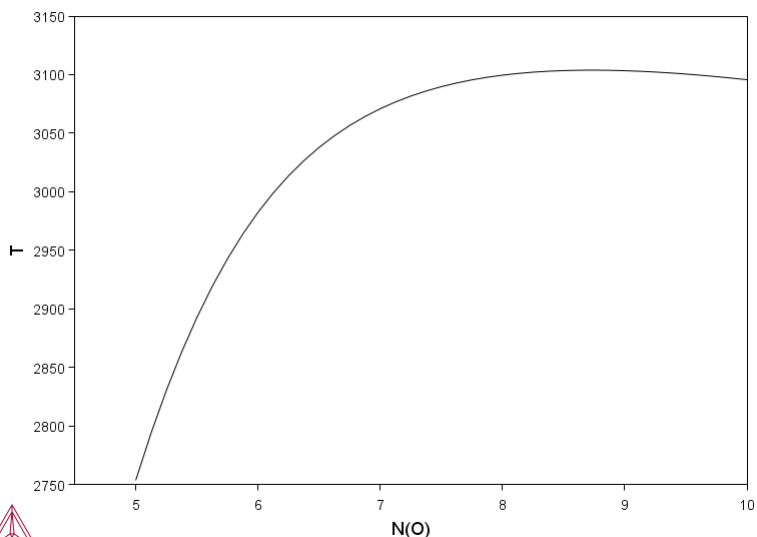
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 22a



POST:

POST:Hit RETURN to continue

POST: @@ Plot how the gas constitution changes

POST: s-d-a y y(gas,*)

... the command in full is SET_DIAGRAM_AXIS

COLUMN NUMBER /*/:

POST: set-title example 22b

POST:

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

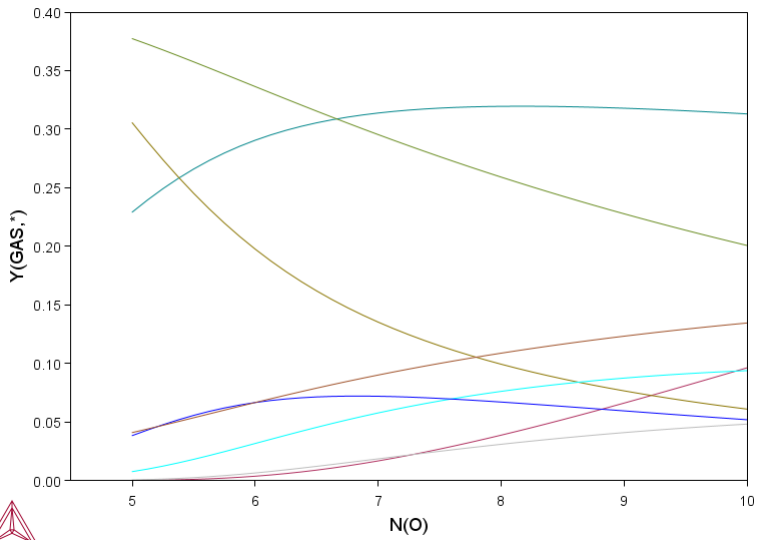
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 22b

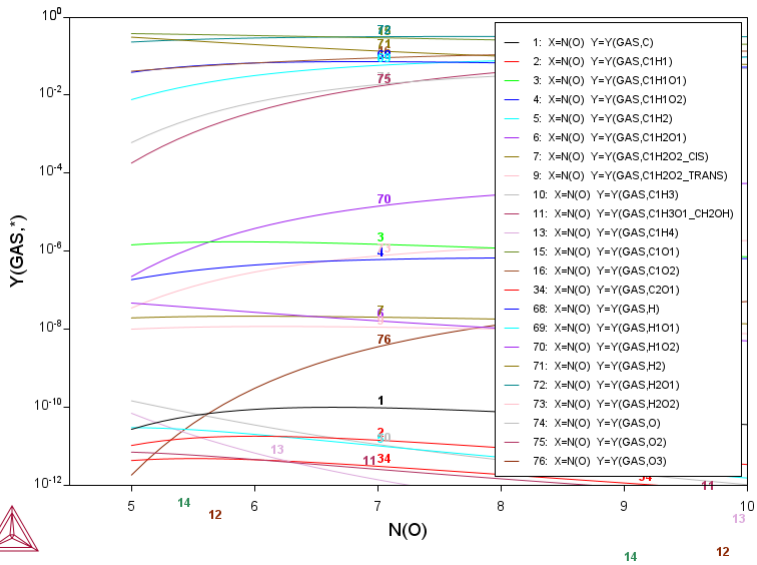


```

POST:
POST:Hit RETURN to continue
POST: @@ Add labels and a logarithmic fraction scale
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 22c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 22c

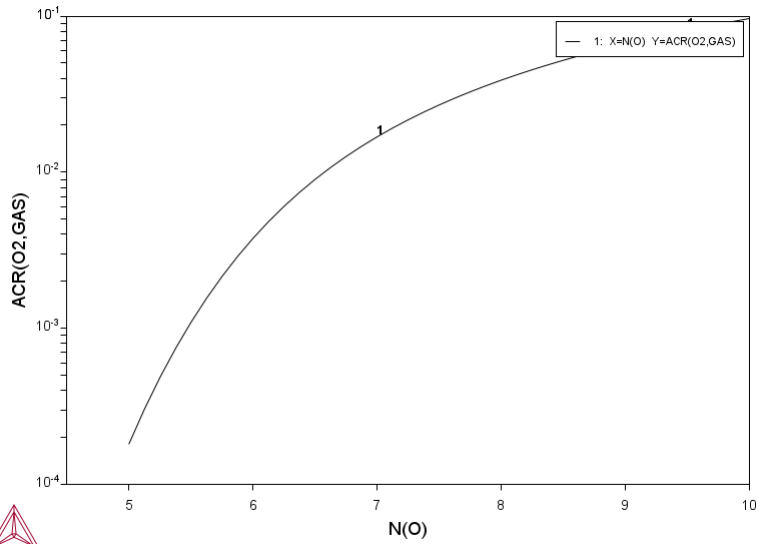


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot how the oxygen partial pressure changes
POST: s-d-a y acr(o2,gas)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 22d

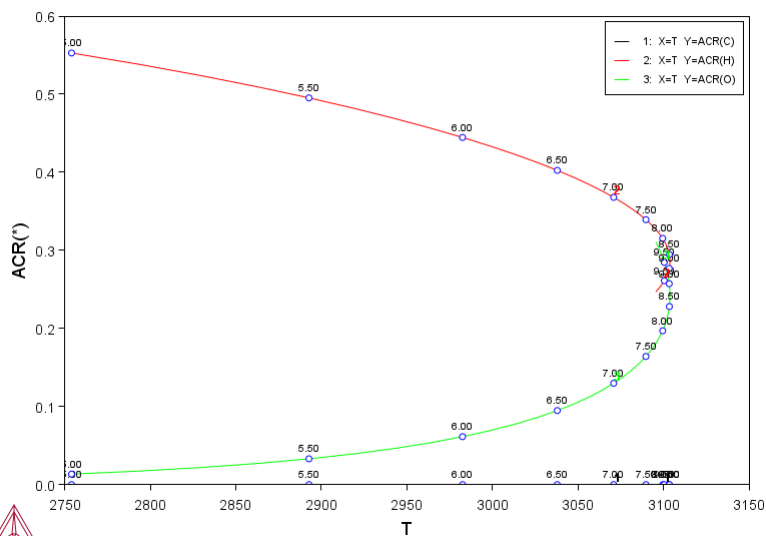


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot how the activities of the components change
POST: @@ with temperature. Note that the oxygen content
POST: @@ also changes. Set the reference states
POST:
POST: set-ref-state o gas * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state h gas * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state c c_s * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: s-d-a x t
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y lin
... the command in full is SET_AXIS_TYPE
POST: s-d-a z n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 5 10
... the command in full is SET_SCALING_STATUS
POST: s-d-a y acr(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 22e



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex23

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex23\tcex23.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a paraequilibrium and the

SYS: @@ T0 temperature in a low alloyed steel

SYS:

SYS: @@ Note that a TCFE database license is required to run

SYS: @@ the example.

SYS:

SYS: set-log ex23,,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Define the material

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfel1

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: mn 1.5

2nd alloying element: si .3

Next alloying element: c .3

Next alloying element:

Temperature (C) /1000/: 700

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M5C2	KSI_CARBIIDE
FE4N_LP1	C14_LAVES	C15_LAVES
M3SI	MN9SI2	MN11SI19
MN6SI	G_PHASE	CR3SI_A15
FESI2_H	FESI2_L	MSI_B20
M5SI3_D88	NBNI3_D0A	AL4C3_D71
FE8SI2C	SIC_B3	MN5SiC
CUZN_EPSILON	AL5FE4	MNP_B31
M2P_C22	NI3SI12	CO2SI_C37
M2SI_TETA	NISI_B31	NI3SI2
CR5SI3_D8M		

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M5C2	KSI_CARBIIDE
FE4N_LP1	C14_LAVES	C15_LAVES
M3SI	MN9SI2	MN11SI19
MN6SI	G_PHASE	CR3SI_A15
FESI2_H	FESI2_L	MSI_B20
M5SI3_D88	NBNI3_D0A	AL4C3_D71
FE8SI2C	SIC_B3	MN5SiC
CUZN_EPSILON	AL5FE4	MNP_B31
M2P_C22	NI3SI12	CO2SI_C37
M2SI_TETA	NISI_B31	NI3SI2
CR5SI3_D8M		

.....

OK? /Y/: Y

09:08:28,668 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

```

... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
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... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Should any phase have a miscibility gap check? /N/: N
Using global minimization procedure
Calculated          31546 grid points in          0.832 s
Found the set of lowest grid points in          0.006 s
Calculated POLY solution          0.289 s, total time          1.127 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =          1, label A0 , database: TCFE11

Conditions:
T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature          973.15 K (          700.00 C), Pressure          1.000000E+05
Number of moles of components          1.00000E+00, Mass in grams          5.50671E+01
Total Gibbs energy -4.16107E+04, Enthalpy          2.38957E+04, Volume          7.24171E-06

Component           Moles           W-Fraction Activity Potential Ref.stat
C                   1.3754E-02          3.0000E-03 2.2665E-01 -1.2010E+04 SER
FE                   9.6533E-01          9.7900E-01 6.6047E-03 -4.0618E+04 SER
MN                   1.5035E-02          1.5000E-02 6.4361E-05 -7.8089E+04 SER
SI                   5.8822E-03          3.0000E-03 2.0473E-10 -1.8051E+05 SER

BCC_A2              Status ENTERED          Driving force          0.0000E+00
Moles 7.3879E-01, Mass 4.1107E+01, Volume fraction 7.4524E-01 Mass fractions:
FE 9.87914E-01 MN 8.77859E-03 SI 3.19709E-03 C 1.10316E-04

FCC_A1              Status ENTERED          Driving force          0.0000E+00
Moles 2.5523E-01, Mass 1.3888E+01, Volume fraction 2.5031E-01 Mass fractions:
FE 9.57680E-01 MN 3.34919E-02 C 6.39600E-03 SI 2.43217E-03

GRAPHITE_A9         Status ENTERED          Driving force          0.0000E+00
Moles 5.9809E-03, Mass 7.1837E-02, Volume fraction 4.4546E-03 Mass fractions:
C 1.00000E+00 SI 0.00000E+00 MN 0.00000E+00 FE 0.00000E+00
POLY: @@ Suspend some phases that normally never appear
POLY: ch-st p gra m5c2=sus
... the command in full is CHANGE_STATUS
POLY:Hit RETURN to continue
POLY: @@ Set axis for T-w(c) phase diagram
POLY: s-a-v 1 w(c)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .01
Increment /2.5E-04/: 2.5E-04
POLY: s-a-v 2 t
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 800
Max value /1/: 1200
Increment /10/: 30
POLY: save tcex23a y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24

```


Phase region boundary 1 at: 2.500E-04 9.472E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated. 3 equilibria

Phase region boundary 2 at: 6.572E-05 9.454E+02
 BCC_A2
 ** CEMENTITE_D011
 ** FCC_A1

Phase region boundary 3 at: 6.572E-05 9.454E+02
 BCC_A2
 ** FCC_A1
 Calculated 24 equilibria

Phase region boundary 4 at: 6.572E-05 9.454E+02
 BCC_A2
 ** CEMENTITE_D011
 Calculated.. 11 equilibria
 Terminating at axis limit.

Phase region boundary 5 at: 6.572E-05 9.454E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1
 Calculated. 31 equilibria

Phase region boundary 6 at: 7.062E-03 9.920E+02
 ** BCC_A2
 ** CEMENTITE_D011
 FCC_A1

Phase region boundary 7 at: 7.062E-03 9.920E+02
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 17 equilibria
 Terminating at axis limit.

Phase region boundary 8 at: 7.062E-03 9.920E+02
 ** BCC_A2
 FCC_A1
 Calculated 42 equilibria

Phase region boundary 9 at: 7.062E-03 9.920E+02
 ** BCC_A2
 CEMENTITE_D011
 FCC_A1
 Calculated.. 13 equilibria
 Terminating at axis limit.

Phase region boundary 10 at: 6.572E-05 9.454E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 42 equilibria
 Terminating at axis limit.

Phase region boundary 11 at: 2.500E-04 9.472E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 41 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 12 at: 3.417E-03 9.669E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated. 15 equilibria
 Terminating at known equilibrium

Phase region boundary 13 at: 3.417E-03 9.669E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 28 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 14 at: 6.583E-03 9.764E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated. 28 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 6.583E-03 9.764E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 16 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 16 at: 5.319E-06 8.100E+02
 BCC_A2
 ** CEMENTITE_D011
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 17 at: 5.319E-06 8.100E+02
 BCC_A2
 ** CEMENTITE_D011
 Calculated. 10 equilibria
 Terminating at known equilibrium

Phase region boundary 18 at: 9.750E-03 9.821E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated. 40 equilibria
 Terminating at known equilibrium

```

Phase region boundary 19 at: 9.750E-03 9.821E+02
  BCC_A2
  CEMENTITE_D011
  ** FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 5.765E-05 9.367E+02
  BCC_A2
  ** CEMENTITE_D011
Calculated.. 11 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at: 5.765E-05 9.367E+02
  BCC_A2
  ** CEMENTITE_D011
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 2.646E-03 1.063E+03
  ** BCC_A2
  FCC_A1
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 2.646E-03 1.063E+03
  ** BCC_A2
  FCC_A1
Calculated 24 equilibria

Phase region boundary 24 at: 8.894E-03 1.063E+03
  ** CEMENTITE_D011
  FCC_A1
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 8.894E-03 1.063E+03
  ** CEMENTITE_D011
  FCC_A1
Calculated.. 7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 26 at: 2.500E-04 1.128E+03
  ** BCC_A2
  FCC_A1
Calculated 4 equilibria

Phase region boundary 27 at: 2.500E-04 1.128E+03
  ** BCC_A2
  FCC_A1
Calculated. 29 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 3.417E-03 1.048E+03
  ** BCC_A2
  FCC_A1
Calculated 26 equilibria

Phase region boundary 29 at: 3.417E-03 1.048E+03
  ** BCC_A2
  FCC_A1
Calculated. 16 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 6.583E-03 9.982E+02
  ** BCC_A2
  FCC_A1
Calculated 38 equilibria

Phase region boundary 31 at: 6.583E-03 9.982E+02
  ** BCC_A2
  FCC_A1
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 9.750E-03 1.095E+03
  ** CEMENTITE_D011
  FCC_A1
Calculated. 12 equilibria
Terminating at known equilibrium

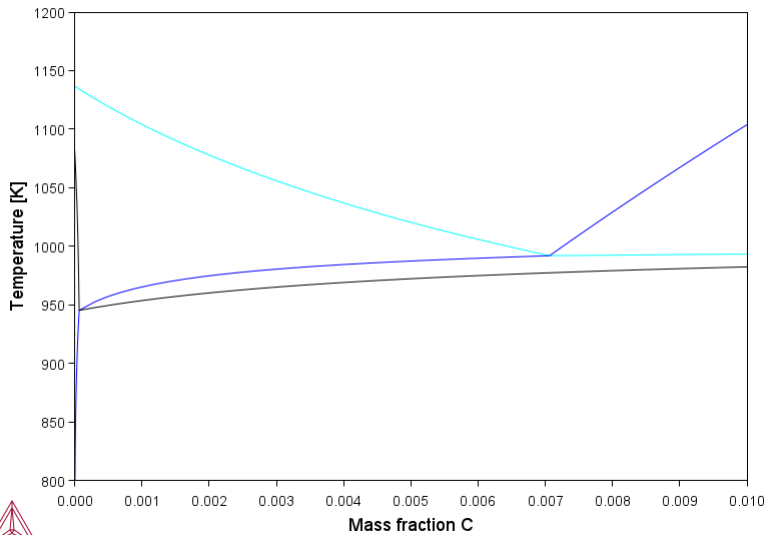
Phase region boundary 33 at: 9.750E-03 1.095E+03
  ** CEMENTITE_D011
  FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex23\tcex23a.POLY3
CPU time for mapping 24 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: set-title example 23a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23a

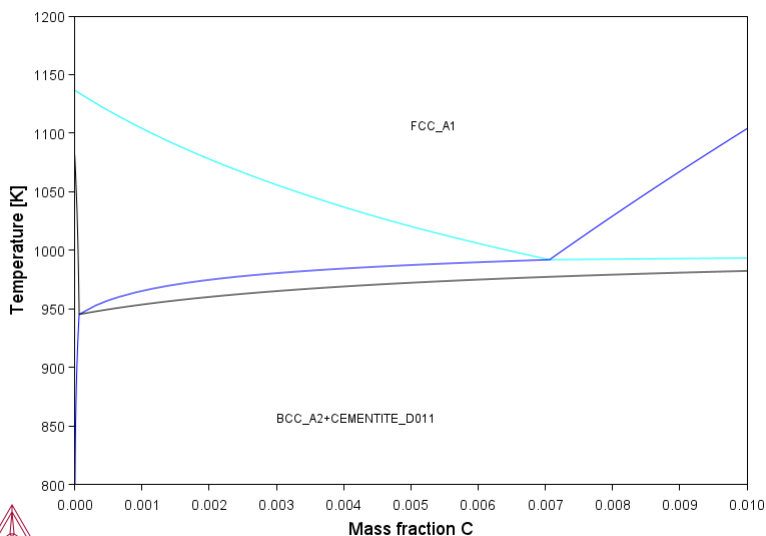


```

POST:
POST:Hit RETURN to continue
POST: @@ Add labels
POST: add
... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .005
Give Y coordinate in axis units: 1100
Automatic phase labels? /Y/: Y
Automatic labelling not always possible
Using global minimization procedure
Calculated 31336 grid points in 0.120 s
Found the set of lowest grid points in 0.005 s
Calculated POLY solution 0.091 s, total time 0.216 s
Stable phases are: FCC_A1
Text size: /.36/. .34
POST: add
... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .003
Give Y coordinate in axis units: 850
Automatic phase labels? /Y/: Y
Automatic labelling not always possible
Using global minimization procedure
Calculated 31336 grid points in 0.118 s
Found the set of lowest grid points in 0.004 s
Calculated POLY solution 0.067 s, total time 0.189 s
Stable phases are: BCC_A2+CEMENTITE_D011
Text size: /.36/. .34
POST: set-title example 23b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23b



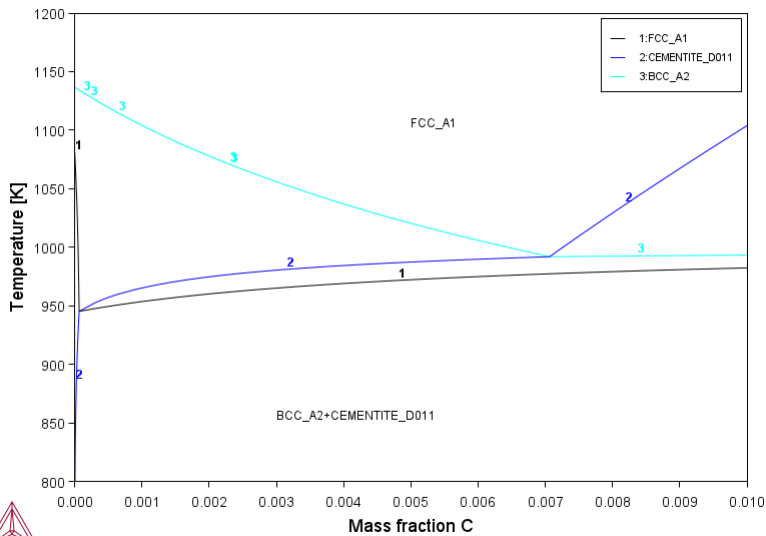
```

POST:
POST:Hit RETURN to continue
POST: s-lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: ?
THE OPTIONS MEANS:
A LIST STABLE PHASES ALONG LINE
B AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
C LIST AXIS QUANTITIES
D AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
E AS B WITH CHANGING COLORS

```

```
F      AS D WITH CHANGING COLORS
N      NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: e
POST:  set-title example 23c
POST:
POST:
POST:  SET_EXP_FILE_FORMAT 5
POST:  MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:  SET_EXP_FILE_FORMAT 10
POST:
POST:  plot
... the command in full is PLOT_DIAGRAM
```

example 23c



```
POST:
POST:Hit RETURN to continue
POST:  ba
... the command in full is BACK
POLY:  @@ Now calculate the T-zero temperature for the steel
POLY:  read tcex23a
... the command in full is READ_WORKSPACES
POLY:  advanced-options
Which option? /STEP_AND_MAP/: ?
EQUILIBRIUM_CALCUL      NEW_COMPOSITION_SET      STABILITY_CHECK
GLOBAL_MINIMIZATION     OUTPUT_FILE_FOR_SHOW    STEP_AND_MAP
IGNORE_COMPOSITION_ORDER PARAEQUILIBRIUM         T-ZERO TEMPERATURE
KEEP_COMP_SET_NUMBERS   PHASE_ADDITION          TOGGLE_ALTERNATE_MODE
LIST_PHASE_ADDITION     PRESENT_PHASE
MAJOR_CONSTITUENTS      SHOW_FOR_T=
Which option? /STEP_AND_MAP/: t-z
```

This command calculates the temperature when two phases have the same Gibbs energy. You must calculate an equilibrium at an estimated temperature first.

```
Name of first phase: fcc_a1
Name of second phase: bcc_a2
```

```
The T0 temperature is 922.16 K
Note: LIST-EQUILIBRIUM is not relevant
POLY:Hit RETURN to continue
POLY:  @@ Calculate the T-zero line, remove the T-axis
POLY:  l-ax
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W(C)      Min: 0      Max: 1E-2      Inc: 2.5E-4
Axis No 2: T         Min: 800     Max: 1200     Inc: 30
```

```
POLY:  s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY:  save tcex23b y
... the command in full is SAVE_WORKSPACES
POLY:  step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: ?
The following options are available:
NORMAL      Stepping with given conditions
INITIAL_EQUILIBRIA An initial equilibrium stored at every step
EVALUATE     Specified variables evaluated after each step
SEPARATE_PHASES Each phase calculated separately
T-ZERO       T0 line calculation
PARAEQUILIBRIUM Paraequilibrium diagram
MIXED_SCHEIL Scheil with fast diffusing elements
ONE_PHASE_AT_TIME One phase at a time
```

```
Option? /NORMAL/: t-z
Name of first phase: fcc_a1
Name of second phase: bcc_a2
```

```
Phase Region from 0.300000E-02 for:
BCC_A2
FCC_A1
3.000000E-03      922.16
2.750000E-03      932.50
2.500000E-03      943.20
2.250000E-03      954.33
2.000000E-03      965.99
1.750000E-03      978.35
1.500000E-03      991.63
1.250000E-03      1006.24
1.000000E-03      1022.92
7.500000E-04      1041.84
5.000000E-04      1063.23
2.500000E-04      1087.64
2.500000E-10      1115.87
```

```
Phase Region from 0.169768E-02 for:
```

```

      BCC_A2
      FCC_A1
1.697680E-03      980.98
1.947680E-03      968.46
2.197680E-03      956.66
2.447680E-03      945.44
2.697680E-03      934.65
2.947680E-03      924.24
3.197680E-03      914.14
3.447680E-03      904.29
3.697680E-03      894.67
3.947680E-03      885.23
4.197680E-03      875.97
4.447680E-03      866.85
4.697680E-03      857.86
4.947680E-03      848.99
5.197680E-03      840.23
5.447680E-03      831.55
5.697680E-03      822.95
5.947680E-03      814.43
6.197680E-03      805.98
6.447680E-03      797.58
6.697680E-03      789.24
6.947680E-03      780.94
7.197680E-03      772.69
7.447680E-03      764.47
7.697680E-03      756.29
7.947680E-03      748.14
8.197680E-03      740.01
8.447680E-03      731.91
8.697680E-03      723.82
8.947680E-03      715.76
9.197680E-03      707.70
9.447680E-03      699.65
9.697680E-03      691.62
9.947680E-03      683.59
1.000000E-02      681.91
*** Buffer savend on file c:\jenkins\WORKSP~1\DEV_PI~1\GENERA~1\examples\tcex23\tcex23b.POLY3

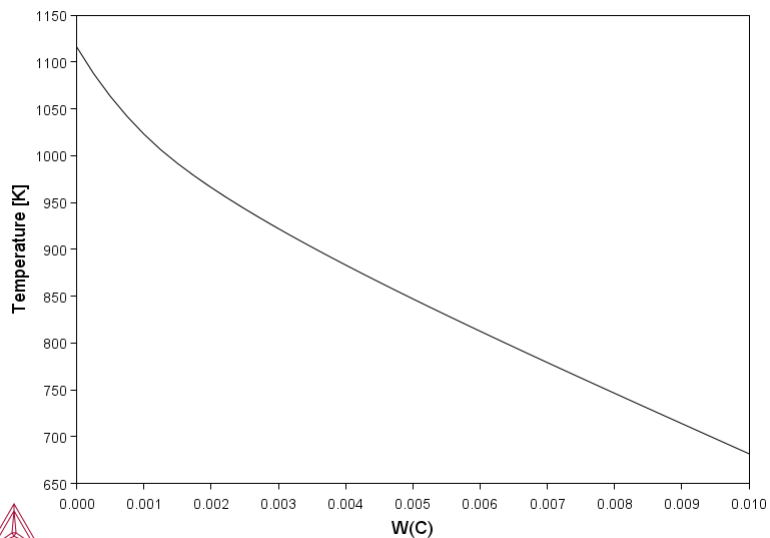
```

```

POLY: post
      POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: set-title example 23d
POST: s-d-a x w(c)
      ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-k
      ... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
      ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
      ... the command in full is PLOT_DIAGRAM

```

example 23d



```

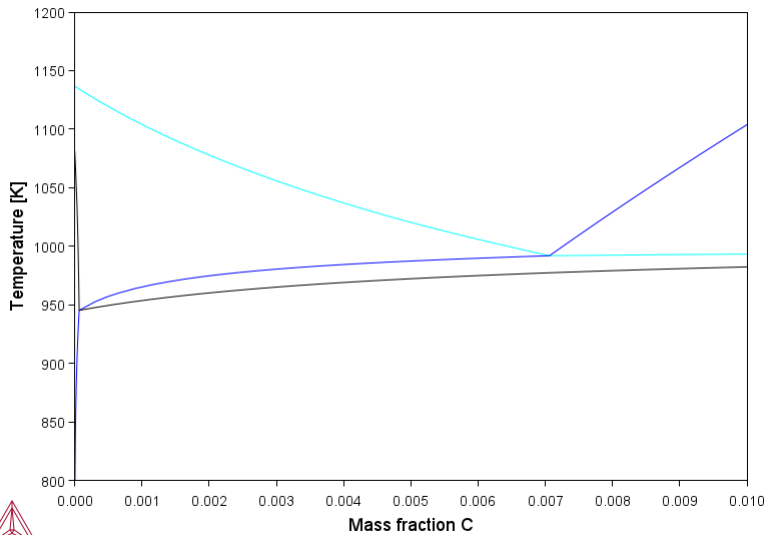
POST:
POST:Hit RETURN to continue
POST: @@ Write the line on a data file
POST: make tcex23b y
      ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: @@ Plot together with a phase diagram
POLY: read tcex23a
      ... the command in full is READ_WORKSPACES
POLY: post
      POLY-3 POSTPROCESSOR VERSION 3.2

      Setting automatic diagram axes

POST:
POST: set-title example 23e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
      ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
      ... the command in full is PLOT_DIAGRAM

```

example 23e

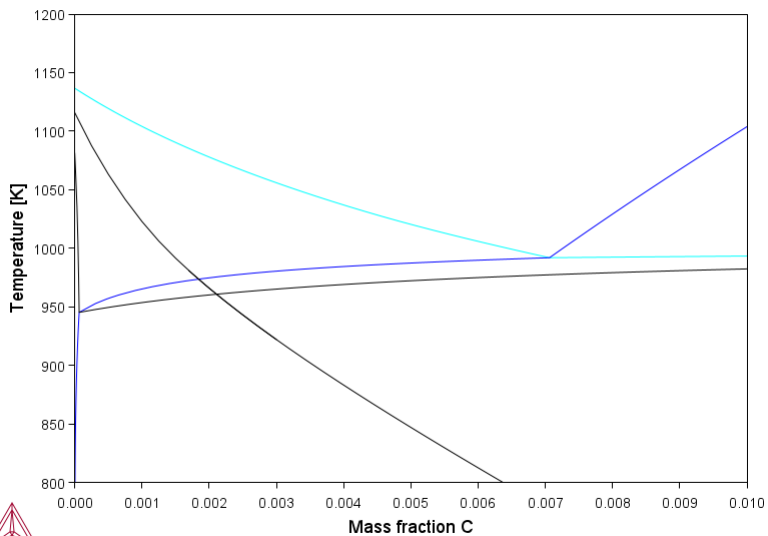


```

POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23b
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23f



```

POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Now calculate the paraequilibrium for the steel.
POLY: @@ At paraequilibrium only C is mobile, the other
POLY: @@ alloying elements have the same compositions in
POLY: @@ both phases
POLY:
POLY: read tcex23a
... the command in full is READ_WORKSPACES
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 31336 grid points in 0.179 s
Found the set of lowest grid points in 0.006 s
Calculated POLY solution 0.084 s, total time 0.269 s
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 973.15 K ( 700.00 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.50671E+01
Total Gibbs energy -4.16101E+04, Enthalpy 2.36448E+04, Volume 7.22672E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               1.3754E-02  3.0000E-03  2.3005E-01 -1.1890E+04 SER
FE              9.6533E-01  9.7900E-01  6.6052E-03 -4.0617E+04 SER
MN              1.5035E-02  1.5000E-02  6.3288E-05 -7.8225E+04 SER

```

```

SI                5.8822E-03  3.0000E-03  2.0682E-10 -1.8043E+05 SER

BCC_A2                Status ENTERED      Driving force  0.0000E+00
Moles 7.9472E-01, Mass 4.4217E+01, Volume fraction 8.0329E-01 Mass fractions:
FE 9.88037E-01 MN 8.63083E-03 SI 3.22040E-03 C 1.11809E-04

FCC_A1                Status ENTERED      Driving force  0.0000E+00
Moles 1.7204E-01, Mass 9.3596E+00, Volume fraction 1.6904E-01 Mass fractions:
FE 9.58089E-01 MN 3.30180E-02 C 6.45696E-03 SI 2.43634E-03

CEMENTITE D011        Status ENTERED      Driving force  0.0000E+00
Moles 3.3244E-02, Mass 1.4900E+00, Volume fraction 2.7670E-02 Mass fractions:
FE 8.42175E-01 MN 9.08298E-02 C 6.69948E-02 SI 4.69956E-13
POLY: advance para
... the command in full is ADVANCED_OPTIONS

```

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.

```

Name of first phase: fcc_al
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
NP(FCC_A1) = 0.4278 with U-fractions C = 3.17321E-02
NP(BCC_A2) = 0.5722 with U-fractions C = 6.47641E-04
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant

```

```

POLY:
POLY:Hit RETURN to continue
POLY:
POLY:
POLY: @@ Now calculate the paraequilibrium for the steel
POLY: @@ at varying temperatures
POLY:
POLY: s-a-v 1 t 800 1200 20
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex23c y
... the command in full is SAVE_WORKSPACES
POLY: step para
... the command in full is STEP_WITH_OPTIONS

```

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.

```

Name of first phase: fcc_al
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

```

Phase	Region	from	973.150	for:		
BCC_A2						
FCC_A1						
9.731500E+02	0.428	0.572	3.173207E-02	6.476405E-04	-1.294536E+00	
9.531500E+02	0.345	0.655	3.908147E-02	7.295252E-04	-8.709572E-01	
9.331500E+02	0.285	0.715	4.698753E-02	8.034098E-04	-4.581102E-01	
9.131500E+02	0.240	0.760	5.533663E-02	8.670323E-04	-5.291004E-02	
8.931500E+02	0.206	0.794	6.403530E-02	9.189130E-04	3.476369E-01	
8.731500E+02	0.180	0.820	7.300677E-02	9.581551E-04	7.462385E-01	
8.531500E+02	0.160	0.840	8.218895E-02	9.843379E-04	1.145330E+00	
8.331500E+02	0.143	0.857	9.153169E-02	9.974272E-04	1.547112E+00	
8.131500E+02	0.129	0.871	1.009946E-01	9.977113E-04	1.953612E+00	
8.000000E+02	0.122	0.878	1.072659E-01	9.911826E-04	2.224380E+00	

Phase	Region	from	973.150	for:		
BCC_A2						
FCC_A1						
9.731500E+02	0.428	0.572	3.169128E-02	6.466406E-04	-1.296235E+00	
9.931500E+02	0.547	0.453	2.503573E-02	5.600526E-04	-1.733345E+00	
1.013150E+03	0.718	0.282	1.922849E-02	4.734693E-04	-2.184104E+00	
1.033150E+03	0.974	0.026	1.430536E-02	3.893313E-04	-2.652658E+00	
1.053150E+03	1.403	-0.403	1.002992E-02	3.022701E-04	-3.169313E+00	
1.073150E+03	2.250	-1.250	6.316301E-03	2.110002E-04	-3.783482E+00	
1.093150E+03	4.635	-3.635	3.098720E-03	1.147920E-04	-4.638561E+00	
1.113150E+03	45.140	-44.140	3.218793E-04	1.322260E-05	-7.038177E+00	

```

*** Buffer savend on file c:\jenkins\WORKSP-1\DEV_PI-1\GENERA-1\examples\tcex23\tcex23c.POLY3
*** ERROR      3 IN NS01AD: Numerical error

```

```

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

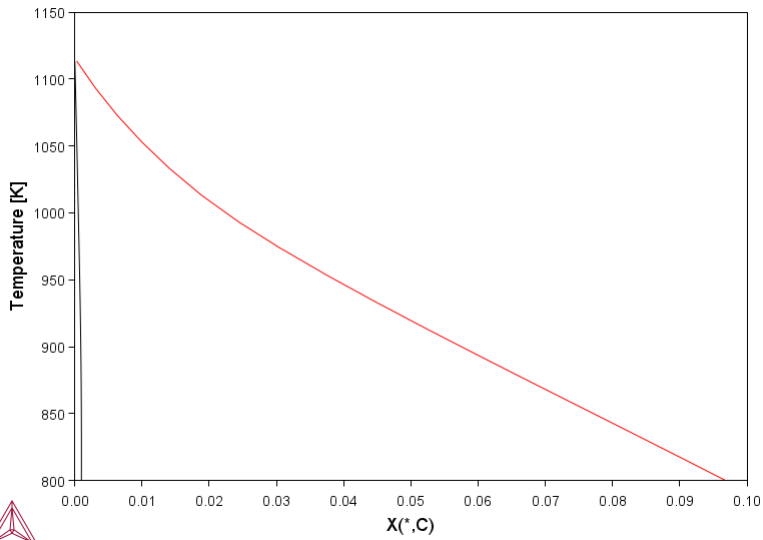
```

```

POST:
POST:
POST: set-title example 23g
POST: s-d-a x x(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

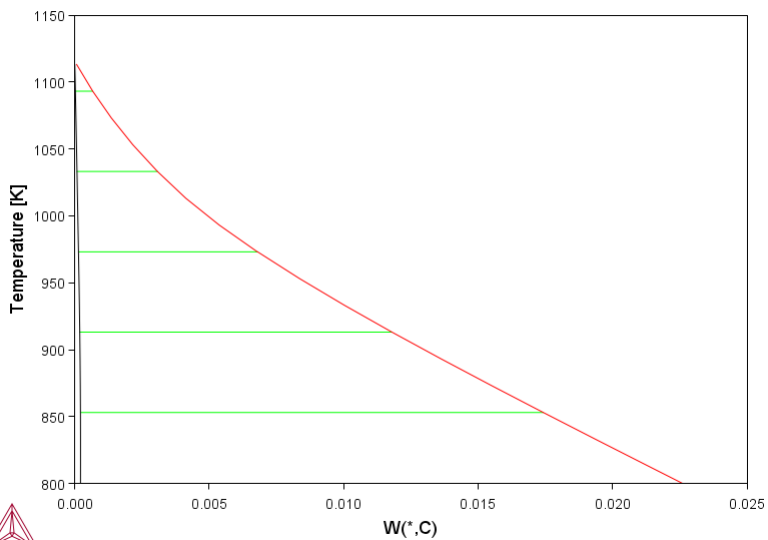
```

example 23g



```
POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-t-s 3
... the command in full is SET_TIELINE_STATUS
POST: set-title example 23h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 23h

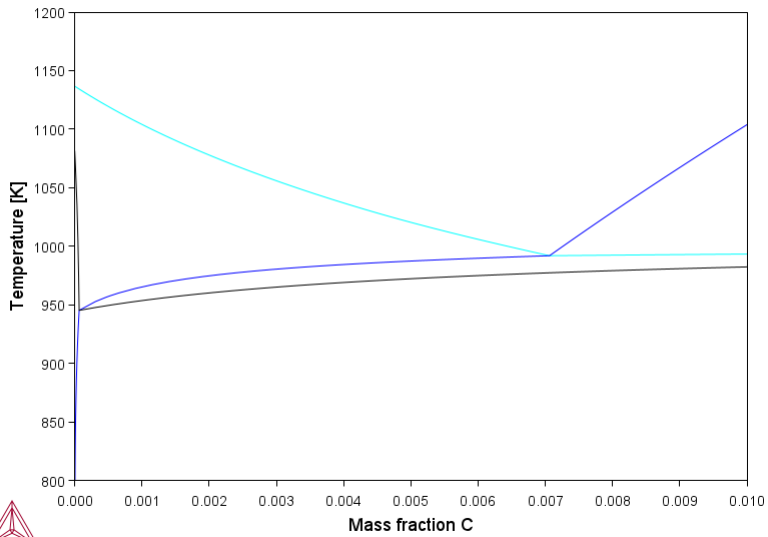


```
POST:
POST:Hit RETURN to continue
POST: make tcex23c y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: read tcex23a
... the command in full is READ_WORKSPACES
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 23i
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```


example 23i

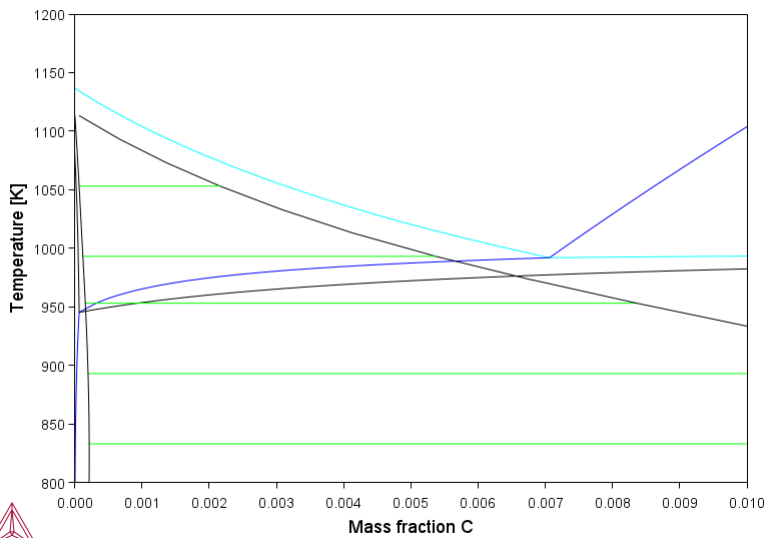


```

POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23c
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23j
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23j

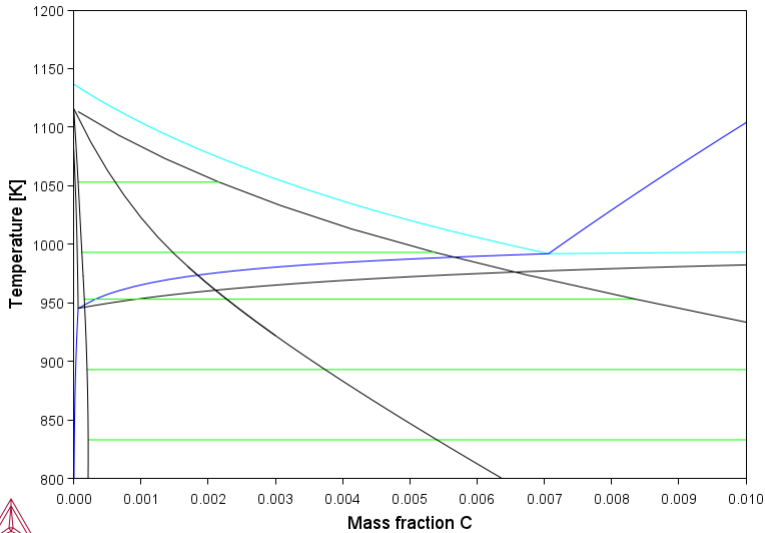


```

POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23b.exp tcex23c.exp 0; 1; 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 23k
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23k



```

POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Now calculate both a normal and paraequilibrium
POLY: @@ for the steel at 1000 K.
POLY:
POLY: @@ Note that a paraequilibrium does not always exist
POLY: @@ for the given conditions. The calculated results
POLY: @@ are the amounts of the two phases. This indicates
POLY: @@ how much of the phases can be transformed at
POLY: @@ paraequilibrium conditions. The carbon content of
POLY: @@ the phases are also listed; the other alloying
POLY: @@ elements have the same fractions in both phases
POLY:
POLY: read tcex23a.POLY3
... the command in full is READ_WORKSPACES
POLY: s-c T=1000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 31336 grid points in 0.167 s
Found the set of lowest grid points in 0.006 s
Calculated POLY solution 0.100 s, total time 0.273 s
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFe11

Conditions:
T=1000, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.50671E+01
Total Gibbs energy -4.34569E+04, Enthalpy 2.63111E+04, Volume 7.20719E-06

Component      Moles      W-Fraction  Activity  Potential Ref.stat
C               1.3754E-02  3.0000E-03  1.6697E-01 -1.4883E+04 SER
FE              9.6533E-01  9.7900E-01  6.1069E-03 -4.2390E+04 SER
MN              1.5035E-02  1.5000E-02  4.0529E-05 -8.4089E+04 SER
SI              5.8822E-03  3.0000E-03  3.3223E-10 -1.8147E+05 SER

FCC_A1          Status ENTERED    Driving force 0.0000E+00
Moles 5.3724E-01, Mass 2.9327E+01, Volume fraction 5.3051E-01 Mass fractions:
FE 9.69681E-01 MN 2.22412E-02 C 5.52941E-03 SI 2.54873E-03

BCC_A2          Status ENTERED    Driving force 0.0000E+00
Moles 4.6276E-01, Mass 2.5740E+01, Volume fraction 4.6949E-01 Mass fractions:
FE 9.89618E-01 MN 6.74998E-03 SI 3.51414E-03 C 1.18192E-04
POLY: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
NP(FCC A1) = 0.5976 with U-fractions C = 2.29802E-02
NP(BCC A2) = 0.4024 with U-fractions C = 5.31092E-04
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant
POLY:
POLY:Hit RETURN to continue
POLY: @@ Now calculate an isothermal phase diagram at 1000 K
POLY: s-a-v 2 w(mn) 0 .1,,,,
... the command in full is SET_AXIS_VARIABLE
POLY:Hit RETURN to continue
POLY: save tcex23d y
... the command in full is SAVE_WORKSPACES
POLY: map
Version 3 mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8

```

Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10

Working hard

Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20

Working hard

Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30

Working hard

Generating start point 31
Generating start point 32

Phase region boundary 1 at: 2.521E-03 2.500E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated. 11 equilibria

Phase region boundary 2 at: 1.815E-04 1.155E-03
BCC_A2
** CEMENTITE_D011
** FCC_A1

Phase region boundary 3 at: 1.815E-04 1.155E-03
BCC_A2
** CEMENTITE_D011
Calculated 10 equilibria

Phase region boundary 4 at: 1.815E-04 1.155E-03
BCC_A2
** FCC_A1
Calculated 31 equilibria

Phase region boundary 5 at: 1.815E-04 1.155E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated.. 41 equilibria
Terminating at axis limit.

Phase region boundary 6 at: 1.815E-04 1.155E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated. 30 equilibria

Phase region boundary 7 at: 7.338E-03 6.999E-03
** BCC_A2
** CEMENTITE_D011
FCC_A1

Phase region boundary 8 at: 7.338E-03 6.999E-03
** CEMENTITE_D011
FCC_A1
Calculated.. 39 equilibria
Terminating at axis limit.

Phase region boundary 9 at: 7.338E-03 6.999E-03
** BCC_A2
FCC_A1
Calculated 42 equilibria

Phase region boundary 10 at: 7.338E-03 6.999E-03
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.. 13 equilibria
Terminating at axis limit.

Phase region boundary 11 at: 2.521E-03 2.500E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated. 21 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 2.500E-04 5.820E-02
** BCC_A2
FCC_A1
Calculated 22 equilibria

Phase region boundary 13 at: 2.500E-04 5.820E-02

```

** BCC_A2
FCC_A1
Calculated. 30 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 3.417E-03 3.130E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated. 14 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 3.417E-03 3.130E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated. 17 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 6.583E-03 6.081E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated. 27 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 6.583E-03 6.081E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 6.969E-03 2.500E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated. 29 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 6.969E-03 2.500E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated.. 14 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 9.750E-03 3.142E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated. 40 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 9.750E-03 3.142E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 4.029E-03 3.417E-02
** BCC_A2
FCC_A1
Calculated. 22 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 4.029E-03 3.417E-02
** BCC_A2
FCC_A1
Calculated 36 equilibria

Phase region boundary 24 at: 7.086E-03 3.417E-02
** CEMENTITE_D011
FCC_A1
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 7.086E-03 3.417E-02
** CEMENTITE_D011
FCC_A1
Calculated.. 28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 26 at: 6.838E-03 6.583E-02
** CEMENTITE_D011
FCC_A1
Calculated. 25 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 6.838E-03 6.583E-02
** CEMENTITE_D011
FCC_A1
Calculated.. 15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at: 6.838E-03 6.583E-02
** CEMENTITE_D011
FCC_A1
Calculated. 25 equilibria
Terminating at known equilibrium

Phase region boundary 29 at: 6.838E-03 6.583E-02
** CEMENTITE_D011
FCC_A1
Calculated.. 15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 30 at: 6.634E-03 9.750E-02
** CEMENTITE_D011
FCC_A1

```

```

Calculated.                38 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 6.634E-03 9.750E-02
** CEMENTITE_D011
FCC_A1
Calculated..                3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 32 at: 2.500E-04 5.820E-02
** BCC_A2
FCC_A1
Calculated                4 equilibria

Phase region boundary 33 at: 2.500E-04 5.820E-02
** BCC_A2
FCC_A1
Calculated.                30 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 3.417E-03 3.851E-02
** BCC_A2
FCC_A1
Calculated                26 equilibria

Phase region boundary 35 at: 3.417E-03 3.851E-02
** BCC_A2
FCC_A1
Calculated.                17 equilibria
Terminating at known equilibrium

Phase region boundary 36 at: 6.583E-03 1.378E-02
** BCC_A2
FCC_A1
Calculated                38 equilibria

Phase region boundary 37 at: 6.583E-03 1.378E-02
** BCC_A2
FCC_A1
Calculated.                5 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 6.634E-03 9.750E-02
** CEMENTITE_D011
FCC_A1
Calculated.                38 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.634E-03 9.750E-02
** CEMENTITE_D011
FCC_A1
Calculated..                3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 40 at: 9.750E-03 7.763E-03
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.                11 equilibria
Terminating at known equilibrium

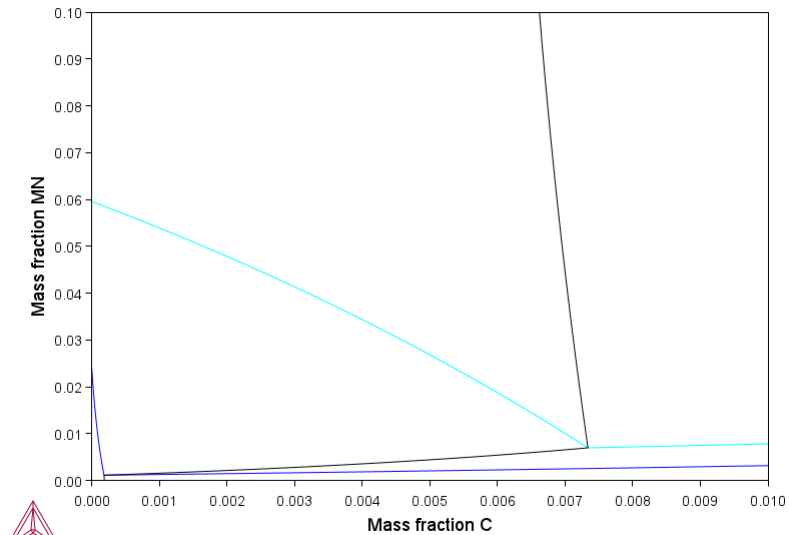
Phase region boundary 41 at: 9.750E-03 7.763E-03
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated..                3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex23\tcex23d.POLY3
CPU time for mapping                12 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 231
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

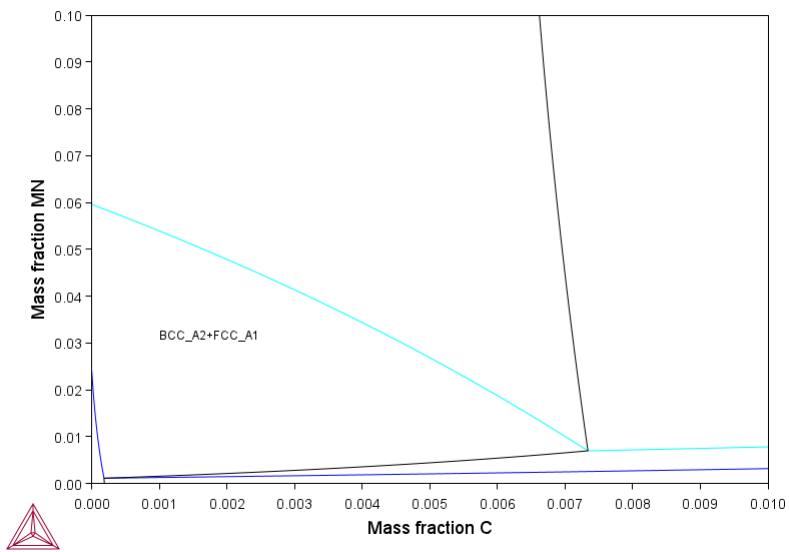
```

example 23l



POST:
 POST:Hit RETURN to continue
 POST: add .001 .03,,,,
 ... the command in full is ADD_LABEL_TEXT
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in 0.010 s
 Calculated POLY solution 0.088 s, total time 0.098 s
 Stable phases are: BCC_A2+FCC_A1
 POST: set-title example_23m
 POST:
 POST:
 POST:
 POST: SET_EXP_FILE_FORMAT 5
 POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 POST: SET_EXP_FILE_FORMAT 10
 POST:
 POST: plot
 ... the command in full is PLOT_DIAGRAM

example 23m



POST:
 POST:Hit RETURN to continue
 POST: back
 POLY: @@ Calculate the corresponding paraequilibrium diagram
 POLY: @@ where fcc and bcc have the same alloy composition.
 POLY:
 POLY: read tcex23d
 ... the command in full is READ_WORKSPACES
 POLY: @@ Only one axis is set, the interstitial
 POLY: @@ composition must not be an axis
 POLY:
 POLY: s-a-v 1 w(mn) 0 .1,,,,
 ... the command in full is SET_AXIS_VARIABLE
 POLY: s-a-v 2 none
 ... the command in full is SET_AXIS_VARIABLE
 POLY: save tcex23e y
 ... the command in full is SAVE_WORKSPACES
 POLY: step
 ... the command in full is STEP_WITH_OPTIONS
 Option? /NORMAL/: ?
 The following options are available:
 NORMAL Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE Specified variables evaluated after each step
 SEPARATE_PHASES Each phase calculated separately
 T-ZERO T0 line calculation
 PARAEQUILIBRIUM Paraequilibrium diagram
 MIXED_SCHEIL Scheil with fast diffusing elements

ONE_PHASE_AT_TIME One phase at a time
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.

Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:

Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

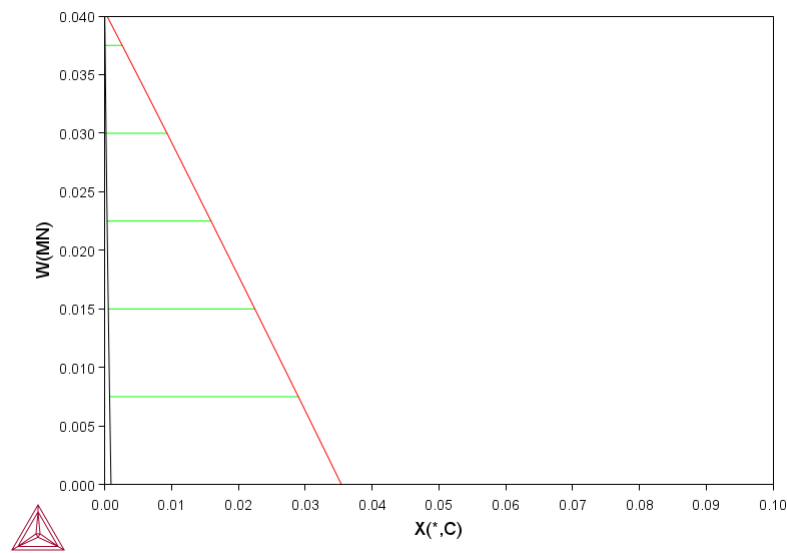
Phase Region from 0.150000E-01 for:
BCC_A2
FCC_A1
1.500000E-02 0.598 0.402 2.298022E-02 5.310923E-04 -1.884317E+00
1.250000E-02 0.541 0.459 2.526500E-02 5.938109E-04 -1.755858E+00
1.000000E-02 0.494 0.506 2.755370E-02 6.585896E-04 -1.635468E+00
7.500000E-03 0.454 0.546 2.984541E-02 7.254514E-04 -1.521908E+00
5.000000E-03 0.420 0.580 3.213933E-02 7.944190E-04 -1.414210E+00
2.500000E-03 0.390 0.610 3.443471E-02 8.655154E-04 -1.311599E+00
2.500000E-09 0.363 0.637 3.673089E-02 9.387636E-04 -1.213448E+00

Phase Region from 0.150000E-01 for:
BCC_A2
FCC_A1
1.500000E-02 0.597 0.403 2.298398E-02 5.312222E-04 -1.883912E+00
1.750000E-02 0.666 0.334 2.070420E-02 4.705375E-04 -2.022034E+00
2.000000E-02 0.751 0.249 1.843022E-02 4.118621E-04 -2.172021E+00
2.250000E-02 0.860 0.140 1.616367E-02 3.551844E-04 -2.336856E+00
2.500000E-02 1.003 -0.003 1.390572E-02 3.004774E-04 -2.520888E+00
2.750000E-02 1.201 -0.201 1.165535E-02 2.476621E-04 -2.730954E+00
3.000000E-02 1.493 -0.493 9.402954E-03 1.964659E-04 -2.979282E+00
3.250000E-02 1.971 -0.971 7.146299E-03 1.468099E-04 -3.287374E+00
3.500000E-02 2.894 -1.894 4.884077E-03 9.864281E-05 -3.701739E+00
3.750000E-02 5.421 -4.421 2.614914E-03 5.191598E-05 -4.360340E+00
4.000000E-02 42.141 -41.141 3.373635E-04 6.583378E-06 -6.442132E+00
*** Buffer savend on file c:\jenkins\WORKSP~1\DEV_PI~1\GENERA~1\examples\tcex23\tcex23e.POLY3
*** ERROR 3 IN NS01AD: Numerical error

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

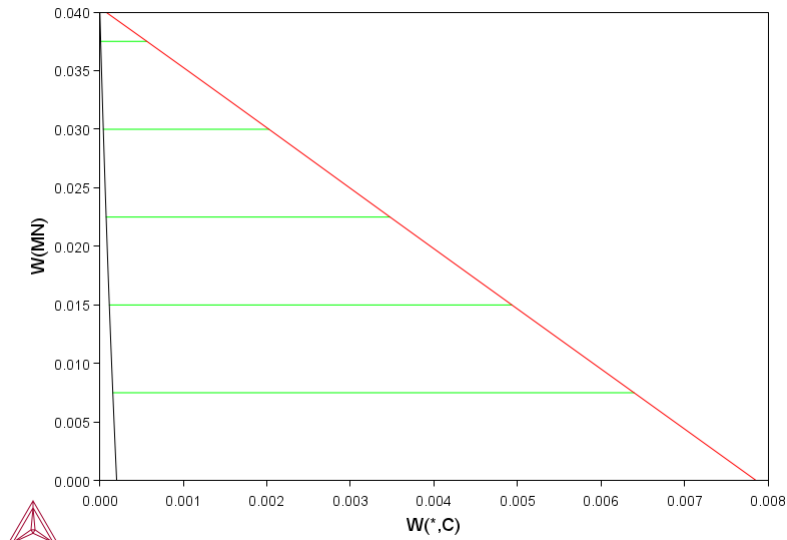
Setting automatic diagram axes

POST:
POST:
POST: s-t-s 3
... the command in full is SET_TIELINE_STATUS
POST: set-title example 23n
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 23n



POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-title example 23o
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

example 23o



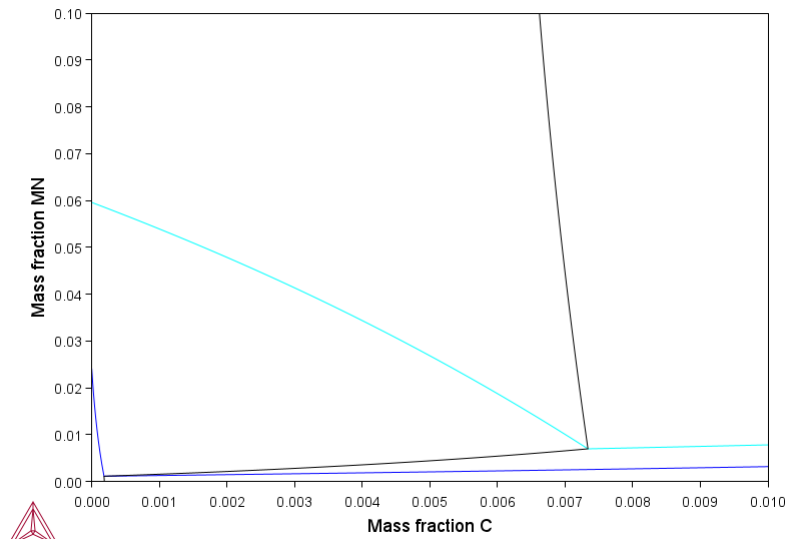
```

POST:
POST: make tcex23e y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST: back
POLY: @@ Now overlay the two diagrams
POLY: read tcex23d
... the command in full is READ_WORKSPACES
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 23p
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
  
```

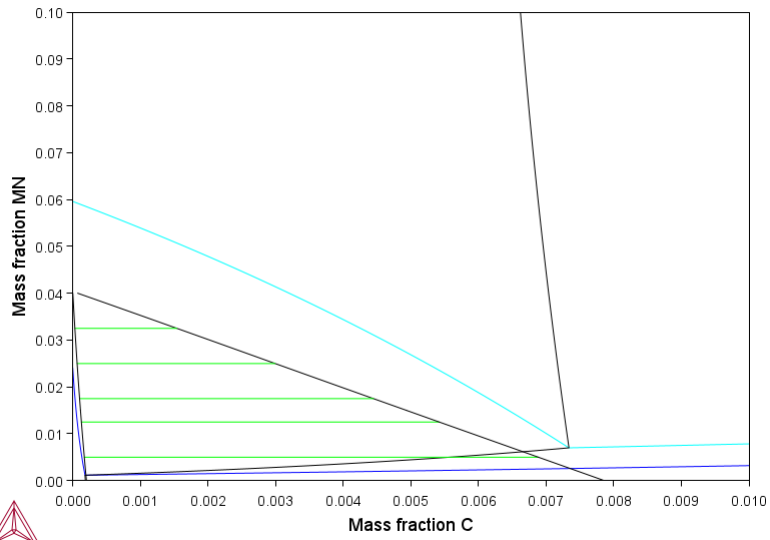
example 23p



```

POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23e
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23q
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
  
```


example 23q



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex24\tcex24.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Simulation of the silicon arc furnace using the REACTOR module

SYS:

SYS: @@ This is a simple reactor model with output of gases at the top

SYS: @@ and output of condensed phases at the bottom. The gas phase

SYS: @@ from one segment flows to higher segments, 80% reacts in the

SYS: @@ first above, 15% in the second above and 5 % in the third

SYS: @@ above. The condensed phases flow downwards and all of it goes

SYS: @@ to the next lowest segment.

SYS:

SYS: @@ Heat can be added at any module. The only way to specify the

SYS: @@ initial state of the reactants added to the reactor is to

SYS: @@ specify the heat content.

SYS:

SYS: @@ Note that a SSUB database license is required to run

SYS: @@ the example.

SYS:

SYS: @@ First fetch data

SYS: GO DAT

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: SW SSUB6

Current database: SGTE Substances v6.0

VA DEFINED

TDB_SSUB6:

TDB_SSUB6: @@ Define-species means that data for just these species is

TDB_SSUB6: @@ retrieved. Define-system means that data for all

TDB_SSUB6: @@ combinations of the elements would be retrieved and this

TDB_SSUB6: @@ is not necessary.

TDB_SSUB6:

TDB_SSUB6: DEF-SPECIES C C101 C102 C1SI1 C2 C3 N101 N2 N4SI3

C

C1SI1

N101

DEFINED

TDB_SSUB6: DEF-SP O O2 SI O1SI1 O2SI1

O

O1SI1

O2SI1

DEFINED

TDB_SSUB6: GET

09:10:25,000 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_SSUB6: GO G

GIBBS ENERGY SYSTEM

GES6: CH-ST EL Y VA

ELEMENT VA

SPECIES VA

GES6: L-ST

GAS CONSTANT IN USER ENERGY UNITS:

1 BAR IN USER PRESSURE UNITS:

CURRENT VALUE OF TEMPERATURE (KELVIN):

CURRENT VALUE OF PRESSURE (PASCAL):

CURRENT NUMBER OF ELEMENT

ELEMENT

STABLE

ELEMENT

REFERENCE

MASS

H298-H0

S298

-1 /- ELECTRON_GAS

0 VA VACUUM

1 C GRAPHITE

2 N 1/2_MOLE_N2(GAS)

3 O 1/2_MOLE_O2(GAS)

4 SI DIAMOND_A4

CURRENT NUMBER OF PHASE

PHASE

STATUS

SUBLATTICES

1 GAS

2 BETA_QUARTZ

3 C1SI1_ALPHA

4 C1SI1_BETA

5 CRISTOBALITE

6 C_L

7 C_S

8 DIAMOND

9 N4SI3_S

10 O2SI1_L

11 O2SI1_QUARTZ

12 O2SI1_QUARTZ_S2

13 SI_L

14 SI_S

15 TRIDYMITE

```

16 TRIDYMITE_S2      82200000      1
17 TRIDYMITE_S3      82200000      1

CURRENT NUMBER OF SPECIES      15

SPECIES                                STOICHIOMETRY
1 C                                80800000 C
2 C1O1                            00000000 C1O1
3 C1O2                            00000000 C1O2
4 C1SI1                           00000000 C1SI1
5 C2                              00000000 C2
6 C3                              00000000 C3
7 N                               80800000 N
8 N1O1                           00000000 N1O1
9 N2                             00000000 N2
10 N4SI3                         00000000 N4SI3
11 O                             80800000 O
12 O1SI1                        00000000 O1SI1
13 O2                           00000000 O2
14 O2SI1                        00000000 O2SI1
15 SI                           80800000 SI
16 VA                           D1800000 VA

```

GES6: GO R

```

Thermo-Calc REACTOR version 1.0
REACTOR: ?
AMEND_INPUT          CREATE_STAGE_BOXES      LIST_RECORDS
AMEND_RECORD         EQUILIBRATE             MACRO-FILE-OPEN
BACK                 EXECUTE_POLY3_COMMAND    READ_WORKSPACE
CHANGE_SURROUNDINGS  EXIT                   SAVE_WORKSPACE
CONTINUE_SIMULATION  GOTO_MODULE             SET_INTERACTIVE
CREATE_DIVIDERS       HELP                   SHOW_PROBE
CREATE_PIPES          INFORMATION            START_SIMULATION
CREATE_PROBE          LIST_DESIGN

REACTOR: @@ Create a reactor with 4 segments which is heat controlled.
REACTOR: @@ At the top segment 1 mole of quartz (SiO2) and 1.8 mole of
REACTOR: @@ graphite (C) is added. A small amount of N is also added to
REACTOR: @@ simplify calculations. The reactants have room temperature.
REACTOR: @@ In the other three segments only heat is added.
REACTOR:
REACTOR: @@ A guess of the initial temperature in each segment must be
REACTOR: @@ provided.
REACTOR:
REACTOR: CREATE_STAGE
NUMBER OF STAGE BOXES /4/: 4
YOU MUST FIRST DEFINE FEED FROM SURROUNDINGS!
GIVE FEED TO SYSTEM: N(C)=1.8
Input temperature /298.15/:
GIVE FEED TO SYSTEM: N(O2SI1)=1
Input temperature /298.15/:
GIVE FEED TO SYSTEM: H=876000
GIVE FEED TO SYSTEM: N(N2)=4e-4
Input temperature /298.15/:
GIVE FEED TO SYSTEM:

GIVE FOR STAGE BOX      1
NAME: /SEGMENT_1/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1750
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

GIVE FOR STAGE BOX      2
NAME: /SEGMENT_2/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1900
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

GIVE FOR STAGE BOX      3
NAME: /SEGMENT_3/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2050
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

GIVE FOR STAGE BOX      4
NAME: /SEGMENT_4/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2200
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST
REACTOR: l-r

Number:  0 name: SURROUNDINGS          stage box at:    23,
Feed of C                                with 1.8000E+00 mol to record:   -1
Feed of O2SI1                          with 1.0000E+00 mol to record:   -1
Feed of heat 8.7600E+05 J to record:    -1
Feed of N2                             with 4.0000E-04 mol to record:   -1

Number:  1 name: SEGMENT_1              stage box at:    72, H controlled
Output for phase GAS                    to record:    -1
Output for phase REST                   to record:    -1

Number:  2 name: SEGMENT_2              stage box at:   114, H controlled
Output for phase GAS                    to record:    -1
Output for phase REST                   to record:    -1

Number:  3 name: SEGMENT_3              stage box at:   156, H controlled
Output for phase GAS                    to record:    -1

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Output for phase REST                                to record:  -1

Number:  4 name: SEGMENT_4                          stage box at:  198, H controlled
Output for phase GAS                                to record:  -1
Output for phase REST                                to record:  -1
REACTOR: @@ Create dividers, one for distributing the gas from segment
REACTOR: @@ 2 to 4, one for splitting the heat feed, and one for splitting
REACTOR: @@ the feed on N2
REACTOR:
REACTOR: create-div
Number of dividers /4/: 5
Number of outputs for divider 1: /3/: 2
Percent of input to output 1: /100/: 80
Number of outputs for divider 2: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 3: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 4: /3/: 3
Percent of input to output 1: /100/: 85 10
Number of outputs for divider 5: /3/: 4
Percent of input to output 1: /100/: 25 25 25
REACTOR: l-r

Number:  0 name: SURROUNDINGS                        stage box at:   23,
Feed of C                                           with 1.8000E+00 mol to record:  -1
Feed of O2SI1                                       with 1.0000E+00 mol to record:  -1
Feed of heat 8.7600E+05 J to record:  -1
Feed of N2                                           with 4.0000E-04 mol to record:  -1

Number:  1 name: SEGMENT_1                          stage box at:   72, H controlled
Output for phase GAS                                to record:  -1
Output for phase REST                                to record:  -1

Number:  2 name: SEGMENT_2                          stage box at:  114, H controlled
Output for phase GAS                                to record:  -1
Output for phase REST                                to record:  -1

Number:  3 name: SEGMENT_3                          stage box at:  156, H controlled
Output for phase GAS                                to record:  -1
Output for phase REST                                to record:  -1

Number:  4 name: SEGMENT_4                          stage box at:  198, H controlled
Output for phase GAS                                to record:  -1
Output for phase REST                                to record:  -1

Number:   5 name: DIVIDER_5                          divider at:   240
 80 % of input to record:  -1
 20 % of input to record:  -1

Number:   6 name: DIVIDER_6                          divider at:   268
 80 % of input to record:  -1
 15 % of input to record:  -1
  5 % of input to record:  -1

Number:   7 name: DIVIDER_7                          divider at:   301
 80 % of input to record:  -1
 15 % of input to record:  -1
  5 % of input to record:  -1

Number:   8 name: DIVIDER_8                          divider at:   334
 85 % of input to record:  -1
 10 % of input to record:  -1
  5 % of input to record:  -1

Number:   9 name: DIVIDER_9                          divider at:   367
 25 % of input to record:  -1
 25 % of input to record:  -1
 25 % of input to record:  -1
 25 % of input to record:  -1
REACTOR: @@ Finally create the pipes between the segments first for the feed
REACTOR: c-pipe 0 1 1 8 9
Feed of C
Feed of O2SI1
Feed of heat
Input set to this divider
Feed of N2
Input set to this divider
NO MORE OUTPUT RECORDS
REACTOR: @@ All solid phases are assumed to go down one segment
REACTOR: @@ The gas phase is assumed to go up, 80% to the next segment,
REACTOR: @@ 15% to the second next and 5% to the third segment above.
REACTOR: @@ Output from stage boxes
REACTOR:
REACTOR: c-pipe 1 0 2
Output record for phase GAS
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 2 5 3
Output record for phase GAS
Input set to this divider
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 3 6 4
Output record for phase GAS
Input set to this divider
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 4 7 0
Output record for phase GAS
Input set to this divider
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: @@ Output from dividers
REACTOR: c-pipe 5 1 0
Output record for 80 % of input
Output record for 20 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 6 2 1 0
Output record for 80 % of input
Output record for 15 % of input
Output record for  5 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 7 3 2 1
Output record for 80 % of input

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Output record for 15 % of input
Output record for 5 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 8 4 3 2
Output record for 85 % of input
Output record for 10 % of input
Output record for 5 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 9 1 2 3 4
Output record for 25 % of input
Output record for 25 % of input
Output record for 25 % of input
Output record for 25 % of input
NO MORE OUTPUT RECORDS
REACTOR: 1-r

Number: 0 name: SURROUNDINGS          stage box at: 23,
Feed of C                            with 1.8000E+00 mol to record: 1
Feed of O2Si1                        with 1.0000E+00 mol to record: 1
Feed of heat 8.7600E+05 J to record: 8
Feed of N2                            with 4.0000E-04 mol to record: 9

Number: 1 name: SEGMENT_1              stage box at: 72, H controlled
Output for phase GAS                  to record: 0
Output for phase REST                 to record: 2

Number: 2 name: SEGMENT_2              stage box at: 114, H controlled
Output for phase GAS                  to record: 5
Output for phase REST                 to record: 3

Number: 3 name: SEGMENT_3              stage box at: 156, H controlled
Output for phase GAS                  to record: 6
Output for phase REST                 to record: 4

Number: 4 name: SEGMENT_4              stage box at: 198, H controlled
Output for phase GAS                  to record: 7
Output for phase REST                 to record: 0

Number: 5 name: DIVIDER_5              divider at: 240
80 % of input to record: 1
20 % of input to record: 0

Number: 6 name: DIVIDER_6              divider at: 268
80 % of input to record: 2
15 % of input to record: 1
5 % of input to record: 0

Number: 7 name: DIVIDER_7              divider at: 301
80 % of input to record: 3
15 % of input to record: 2
5 % of input to record: 1

Number: 8 name: DIVIDER_8              divider at: 334
85 % of input to record: 4
10 % of input to record: 3
5 % of input to record: 2

Number: 9 name: DIVIDER_9              divider at: 367
25 % of input to record: 1
25 % of input to record: 2
25 % of input to record: 3
25 % of input to record: 4
REACTOR: save tcex24 y
REACTOR: @@ Now start the process
REACTOR: read tcex24
REACTOR:
REACTOR: @@ The output for each iteration consists of the conditions set in
REACTOR: @@ each segment, and you can also select some state variables,
REACTOR: @@ in this case NP($$) meaning moles of stable phases.
REACTOR: @@ After each loop the temperatures in all segments are listed
REACTOR:
REACTOR: @@ We want to achieve a reactor where only Si<L> leaves at the bottom.
REACTOR: START
Max number of loops: /10/: 50
OUTPUT TO SCREEN OR FILE /SCREEN/:
Output conditions? /Y/:
Output variables: /T BP($$)/: T BP($$)
>>> DATA AT ITERATION 1 FROM STAGE 1
T=1750, P=100000, N(C)=1.8, N(N)=2E-4, N(O)=2, N(SI)=1
DEGREES OF FREEDOM 0
T= 1.750000E+03
BP(GAS)=8.3899239E-3, BP(C1Si1_BETA)=3.9560636E-3,
BP(CRISTOBALITE)=60.077021, BP(C_S)=21.616235
>>> DATA AT ITERATION 1 FROM STAGE 2
T=1900, P=100000, N(C)=1.799801831, N(N)=2E-4, N(O)=1.999800965,
N(SI)=0.9999991472
DEGREES OF FREEDOM 0
T= 1.900000E+03
BP(GAS)=35.781375, BP(C1Si1_BETA)=23.515817, BP(CRISTOBALITE)=22.402821
>>> DATA AT ITERATION 1 FROM STAGE 3
T=2050, P=100000, N(C)=0.5864878616, N(N)=2E-4, N(O)=0.7457290951,
N(SI)=0.9593524091
DEGREES OF FREEDOM 0
T= 2.050000E+03
BP(GAS)=1.1001909E-2, BP(C1Si1_BETA)=23.51327, BP(O2Si1_L)=22.396537,
BP(Si_L)=6.3106228E-4
>>> DATA AT ITERATION 1 FROM STAGE 4
T=2200, P=100000, N(C)=0.5864243231, N(N)=2E-4, N(O)=0.74551992,
N(SI)=0.9592067528
DEGREES OF FREEDOM 0
T= 2.200000E+03
BP(GAS)=27.369406, BP(C1Si1_BETA)=9.7781171, BP(Si_L)=8.7657159
=====
>>> DATA AT ITERATION 2 FROM STAGE 1
H=-969231.6342, P=100000, N(C)=2.78778854, N(N)=4E-4, N(O)=3.040564868,
N(SI)=1.052700505
DEGREES OF FREEDOM 0
T= 1.098651E+03
BP(GAS)=25.395955, BP(BETA_QUARTZ)=63.249404, BP(C_S)=23.055463
>>> DATA AT ITERATION 2 FROM STAGE 2
H=-837416.4877, P=100000, N(C)=1.970963345, N(N)=3.9E-4, N(O)=2.217396337,
N(SI)=1.113300827
DEGREES OF FREEDOM 0
T= 1.764644E+03
BP(GAS)=2.5771879E-2, BP(C1Si1_BETA)=0.19891753, BP(CRISTOBALITE)=66.592185,

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BP(C_S)=23.605007
>>> DATA AT ITERATION      2 FROM STAGE      3
H=-772456.8489, P=100000, N(C)=2.24428875, N(N)=3.6E-4, N(O)=2.813089043,
N(SI)=1.435877836
DEGREES OF FREEDOM 0
T= 1.785830E+03
BP(GAS)=28.121362, BP(C1Si1_BETA)=21.054185, BP(CRISTOBALITE)=54.435284,
BP(C_S)=8.6836041
>>> DATA AT ITERATION      2 FROM STAGE      4
H=33660.30349, P=100000, N(C)=1.248065358, N(N)=2E-4, N(O)=1.812002861,
N(SI)=1.431095835
DEGREES OF FREEDOM 0
T= 2.447572E+03
BP(GAS)=60.210326, BP(C1Si1_BETA)=0.55847707, BP(SI_L)=23.407071
=====
>>> DATA AT ITERATION      3 FROM STAGE      1
H=-922751.4701, P=100000, N(C)=2.011716301, N(N)=5.76E-4, N(O)=2.241341655,
N(SI)=1.029906422
DEGREES OF FREEDOM 0
T= 8.124883E+02
BP(GAS)=4.0693569, BP(C_S)=23.005715, BP(O2Si1_QUARTZ)=61.879868
>>> DATA AT ITERATION      3 FROM STAGE      2
H=-903970.2067, P=100000, N(C)=2.89748639, N(N)=5.18E-4, N(O)=3.13248222,
N(SI)=1.12129161
DEGREES OF FREEDOM 0
T= 1.746338E+03
BP(GAS)=25.042951, BP(CRISTOBALITE)=67.278274, BP(C_S)=24.095798
>>> DATA AT ITERATION      3 FROM STAGE      3
H=-804917.287, P=100000, N(C)=2.993453661, N(N)=3.6E-4, N(O)=3.689113428,
N(SI)=1.586740032
DEGREES OF FREEDOM 0
T= 1.785838E+03
BP(GAS)=55.589668, BP(C1Si1_BETA)=28.960504, BP(CRISTOBALITE)=51.37138,
BP(C_S)=3.6235824
>>> DATA AT ITERATION      3 FROM STAGE      4
H=61307.14323, P=100000, N(C)=1.023967769, N(N)=2E-4, N(O)=1.7100138,
N(SI)=1.57728602
DEGREES OF FREEDOM 0
T= 2.594647E+03
BP(GAS)=59.391022, BP(SI_L)=24.567245
=====
>>> DATA AT ITERATION      4 FROM STAGE      1
H=-975672.9943, P=100000, N(C)=2.859695045, N(N)=6.784E-4, N(O)=3.096742498,
N(SI)=1.037773929
DEGREES OF FREEDOM 0
T= 1.067994E+03
BP(GAS)=27.303365, BP(BETA_QUARTZ)=62.352571, BP(C_S)=23.392027
>>> DATA AT ITERATION      4 FROM STAGE      2
H=-926156.1401, P=100000, N(C)=3.676734224, N(N)=5.18E-4, N(O)=3.915329631,
N(SI)=1.150718124
DEGREES OF FREEDOM 0
T= 1.785833E+03
BP(GAS)=48.987037, BP(C1Si1_BETA)=2.2730167, BP(CRISTOBALITE)=65.232008,
BP(C_S)=22.635726
>>> DATA AT ITERATION      4 FROM STAGE      3
H=-759974.2114, P=100000, N(C)=2.760446561, N(N)=3.6E-4, N(O)=3.53940754,
N(SI)=1.704419532
DEGREES OF FREEDOM 0
T= 1.856422E+03
BP(GAS)=54.420155, BP(C1Si1_BETA)=34.739066, BP(CRISTOBALITE)=48.497149
>>> DATA AT ITERATION      4 FROM STAGE      4
H=97718.13178, P=100000, N(C)=0.8663972889, N(N)=2E-4, N(O)=1.614338479,
N(SI)=1.673566528
DEGREES OF FREEDOM 0
T= 2.773504E+03
BP(GAS)=58.669424, BP(SI_L)=24.569593
=====
>>> DATA AT ITERATION      5 FROM STAGE      1
H=-1013577.447, P=100000, N(C)=3.515796758, N(N)=6.784E-4, N(O)=3.764623788,
N(SI)=1.0512292
DEGREES OF FREEDOM 0
T= 1.163508E+03
BP(GAS)=45.980219, BP(C_S)=22.850503, BP(TRIDYMITE_S3)=63.161004
>>> DATA AT ITERATION      5 FROM STAGE      2
H=-913270.225, P=100000, N(C)=3.54766363, N(N)=5.18E-4, N(O)=3.884664421,
N(SI)=1.195722123
DEGREES OF FREEDOM 0
T= 1.785833E+03
BP(GAS)=49.603255, BP(C1Si1_BETA)=5.1279345, BP(CRISTOBALITE)=63.651652,
BP(C_S)=19.968004
>>> DATA AT ITERATION      5 FROM STAGE      3
H=-720022.7646, P=100000, N(C)=2.483485629, N(N)=3.6E-4, N(O)=3.410261538,
N(SI)=1.826276239
DEGREES OF FREEDOM 0
T= 1.974923E+03
BP(GAS)=54.11176, BP(C1Si1_BETA)=33.932787, BP(CRISTOBALITE)=47.641383
>>> DATA AT ITERATION      5 FROM STAGE      4
H=121546.0246, P=100000, N(C)=0.8462885911, N(N)=2E-4, N(O)=1.585852345,
N(SI)=1.639214763
DEGREES OF FREEDOM 0
T= 2.880121E+03
BP(GAS)=58.994116, BP(SI_L)=22.582856
=====
>>> DATA AT ITERATION      6 FROM STAGE      1
H=-1010753.26, P=100000, N(C)=3.493730651, N(N)=6.784E-4, N(O)=3.765652929,
N(SI)=1.076563738
DEGREES OF FREEDOM 0
T= 1.245814E+03
BP(GAS)=44.984991, BP(C_S)=22.786504, BP(TRIDYMITE_S3)=64.683179
>>> DATA AT ITERATION      6 FROM STAGE      2
H=-907819.0229, P=100000, N(C)=3.333837247, N(N)=5.18E-4, N(O)=3.850532682,
N(SI)=1.351481692
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=49.986925, BP(C1Si1_BETA)=12.328795, BP(CRISTOBALITE)=62.215898,
BP(C_S)=15.079393
>>> DATA AT ITERATION      6 FROM STAGE      3
H=-689981.5847, P=100000, N(C)=2.239978012, N(N)=3.6E-4, N(O)=3.339680256,
N(SI)=2.011081244
DEGREES OF FREEDOM 0
T= 2.024859E+03
BP(GAS)=55.901308, BP(C1Si1_BETA)=33.947222, BP(O2Si1_L)=46.973649
>>> DATA AT ITERATION      6 FROM STAGE      4
H=142731.8649, P=100000, N(C)=0.8466486045, N(N)=2E-4, N(O)=1.563625285,
N(SI)=1.628461247
DEGREES OF FREEDOM 0
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T= 2.939413E+03
BP(GAS)=59.078725, BP(SI_L)=21.844948
=====
>>> DATA AT ITERATION    7 FROM STAGE    1
H=-1008944.095, P=100000, N(C)=3.468043928, N(N)=6.784E-4, N(O)=3.768216951,
  N(SI)=1.106725752
DEGREES OF FREEDOM 0
T= 1.360090E+03
BP(GAS)=43.509997, BP(C_S)=23.028873, BP(TRIDYMITE_S3)=66.495403
>>> DATA AT ITERATION    7 FROM STAGE    2
H=-908459.8575, P=100000, N(C)=3.15897605, N(N)=5.179999999E-4,
  N(O)=3.868839264, N(SI)=1.540418611
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=51.714963, BP(C1SI1_BETA)=20.759109, BP(CRISTOBALITE)=60.91749,
  BP(C_S)=9.7183714
>>> DATA AT ITERATION    7 FROM STAGE    3
H=-668400.8309, P=100000, N(C)=2.00417664, N(N)=3.6E-4, N(O)=3.278678122,
  N(SI)=2.212140734
DEGREES OF FREEDOM 0
T= 2.054719E+03
BP(GAS)=58.391064, BP(C1SI1_BETA)=34.178134, BP(O2SI1_L)=46.091554
>>> DATA AT ITERATION    7 FROM STAGE    4
H=157520.1356, P=100000, N(C)=0.8524075704, N(N)=2E-4, N(O)=1.53426275,
  N(SI)=1.619538945
DEGREES OF FREEDOM 0
T= 2.970399E+03
BP(GAS)=58.350805, BP(SI_L)=21.921685
=====
>>> DATA AT ITERATION    8 FROM STAGE    1
H=-1010260.226, P=100000, N(C)=3.481080374, N(N)=6.784E-4, N(O)=3.811224539,
  N(SI)=1.137875423
DEGREES OF FREEDOM 0
T= 1.482989E+03
BP(GAS)=43.00392, BP(C_S)=23.382924, BP(TRIDYMITE_S3)=68.366927
>>> DATA AT ITERATION    8 FROM STAGE    2
H=-910878.3294, P=100000, N(C)=2.996068864, N(N)=5.18E-4, N(O)=3.901421156,
  N(SI)=1.737804825
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=53.791867, BP(C1SI1_BETA)=29.488661, BP(CRISTOBALITE)=59.674774,
  BP(C_S)=4.2628222
>>> DATA AT ITERATION    8 FROM STAGE    3
H=-655233.1078, P=100000, N(C)=1.772287341, N(N)=3.6E-4, N(O)=3.213821477,
  N(SI)=2.39984998
DEGREES OF FREEDOM 0
T= 2.072919E+03
BP(GAS)=59.871551, BP(C1SI1_BETA)=34.480045, BP(O2SI1_L)=45.758107
>>> DATA AT ITERATION    8 FROM STAGE    4
H=163921.0654, P=100000, N(C)=0.859937269, N(N)=2E-4, N(O)=1.523163185,
  N(SI)=1.621518862
DEGREES OF FREEDOM 0
T= 2.980408E+03
BP(GAS)=57.971021, BP(SI_L)=22.269932
=====
>>> DATA AT ITERATION    9 FROM STAGE    1
H=-1012646.88, P=100000, N(C)=3.504415438, N(N)=6.784E-4, N(O)=3.861764807,
  N(SI)=1.165496436
DEGREES OF FREEDOM 0
T= 1.587698E+03
BP(GAS)=42.882392, BP(C_S)=23.711015, BP(TRIDYMITE_S3)=70.024972
>>> DATA AT ITERATION    9 FROM STAGE    2
H=-913275.5572, P=100000, N(C)=2.83297897, N(N)=5.18E-4, N(O)=3.911942365,
  N(SI)=1.91242122
DEGREES OF FREEDOM 0
T= 1.813659E+03
BP(GAS)=54.528551, BP(C1SI1_BETA)=36.500133, BP(CRISTOBALITE)=59.302998
>>> DATA AT ITERATION    9 FROM STAGE    3
H=-654500.8518, P=100000, N(C)=1.598268366, N(N)=3.6E-4, N(O)=3.1925664,
  N(SI)=2.560193535
DEGREES OF FREEDOM 0
T= 2.082775E+03
BP(GAS)=61.270688, BP(C1SI1_BETA)=34.761698, BP(O2SI1_L)=46.150363
>>> DATA AT ITERATION    9 FROM STAGE    4
H=160038.1017, P=100000, N(C)=0.8669617393, N(N)=2E-4, N(O)=1.536220324,
  N(SI)=1.635071901
DEGREES OF FREEDOM 0
T= 2.968716E+03
BP(GAS)=58.16585, BP(SI_L)=22.749012
=====
>>> DATA AT ITERATION   10 FROM STAGE    1
H=-1011746.004, P=100000, N(C)=3.491172416, N(N)=6.784E-4, N(O)=3.875588138,
  N(SI)=1.192089346
DEGREES OF FREEDOM 0
T= 1.688378E+03
BP(GAS)=41.819001, BP(C_S)=24.015589, BP(TRIDYMITE_S3)=71.592748
>>> DATA AT ITERATION   10 FROM STAGE    2
H=-917570.6537, P=100000, N(C)=2.714555789, N(N)=5.18E-4, N(O)=3.938638187,
  N(SI)=2.055421364
DEGREES OF FREEDOM 0
T= 1.931654E+03
BP(GAS)=54.443862, BP(C1SI1_BETA)=37.245342, BP(CRISTOBALITE)=61.663362
>>> DATA AT ITERATION   10 FROM STAGE    3
H=-675805.5217, P=100000, N(C)=1.622473584, N(N)=3.6E-4, N(O)=3.28158221,
  N(SI)=2.615260062
DEGREES OF FREEDOM 0
T= 2.082796E+03
BP(GAS)=62.678066, BP(C1SI1_BETA)=35.07906, BP(O2SI1_L)=47.687059
>>> DATA AT ITERATION   10 FROM STAGE    4
H=140324.593, P=100000, N(C)=0.8748767964, N(N)=2E-4, N(O)=1.587372774,
  N(SI)=1.668563184
DEGREES OF FREEDOM 0
T= 2.917962E+03
BP(GAS)=59.278419, BP(SI_L)=23.490502
=====
>>> DATA AT ITERATION   11 FROM STAGE    1
H=-1003110.741, P=100000, N(C)=3.384404635, N(N)=6.784E-4, N(O)=3.842325843,
  N(SI)=1.263783677
DEGREES OF FREEDOM 0
T= 1.785825E+03
BP(GAS)=40.181408, BP(C1SI1_BETA)=2.0429771, BP(CRISTOBALITE)=72.460052,
  BP(C_S)=22.941885
>>> DATA AT ITERATION   11 FROM STAGE    2
H=-922616.7773, P=100000, N(C)=2.690333937, N(N)=5.18E-4, N(O)=4.005471932,
  N(SI)=2.139132245
DEGREES OF FREEDOM 0
```

T= 1.964263E+03
BP(GAS)=56.690326, BP(C1Si1_BETA)=37.355783, BP(CRISTOBALITE)=62.435823
>>> DATA AT ITERATION 11 FROM STAGE 3
H=-699253.1697, P=100000, N(C)=1.631560023, N(N)=3.6E-4, N(O)=3.348217302,
N(SI)=2.636542748
DEGREES OF FREEDOM 0
T= 2.082357E+03
BP(GAS)=62.812323, BP(C1Si1_BETA)=34.943937, BP(O2Si1_L)=49.460881
>>> DATA AT ITERATION 11 FROM STAGE 4
H=117365.2447, P=100000, N(C)=0.8715068211, N(N)=2E-4, N(O)=1.646418502,
N(SI)=1.694716072
DEGREES OF FREEDOM 0
T= 2.855981E+03
BP(GAS)=60.986548, BP(SI_L)=23.421073
=====

>>> DATA AT ITERATION 12 FROM STAGE 1
H=-1003449.781, P=100000, N(C)=3.364523602, N(N)=6.784E-4, N(O)=3.879313025,
N(SI)=1.318964335
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.745844, BP(C1Si1_BETA)=4.6200258, BP(CRISTOBALITE)=71.897831,
BP(C_S)=21.265337
>>> DATA AT ITERATION 12 FROM STAGE 2
H=-923111.7485, P=100000, N(C)=2.624481148, N(N)=5.18E-4, N(O)=4.001685486,
N(SI)=2.194444401
DEGREES OF FREEDOM 0
T= 1.981583E+03
BP(GAS)=56.956866, BP(C1Si1_BETA)=37.363041, BP(CRISTOBALITE)=62.863929
>>> DATA AT ITERATION 12 FROM STAGE 3
H=-719678.5635, P=100000, N(C)=1.629045072, N(N)=3.6E-4, N(O)=3.409704375,
N(SI)=2.666749027
DEGREES OF FREEDOM 0
T= 2.082497E+03
BP(GAS)=63.21919, BP(C1Si1_BETA)=34.784905, BP(O2Si1_L)=51.014914
>>> DATA AT ITERATION 12 FROM STAGE 4
H=97299.1725, P=100000, N(C)=0.8675405344, N(N)=2E-4, N(O)=1.698148023,
N(SI)=1.716614546
DEGREES OF FREEDOM 0
T= 2.791245E+03
BP(GAS)=62.594967, BP(SI_L)=23.207654
=====

>>> DATA AT ITERATION 13 FROM STAGE 1
H=-1002049.949, P=100000, N(C)=3.311715933, N(N)=6.784E-4, N(O)=3.868933584,
N(SI)=1.360090086
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.782601, BP(C1Si1_BETA)=6.5030779, BP(CRISTOBALITE)=71.546701,
BP(C_S)=20.051341
>>> DATA AT ITERATION 13 FROM STAGE 2
H=-924576.1057, P=100000, N(C)=2.57093722, N(N)=5.18E-4, N(O)=4.005562773,
N(SI)=2.246634771
DEGREES OF FREEDOM 0
T= 1.994519E+03
BP(GAS)=57.417427, BP(C1Si1_BETA)=37.390387, BP(CRISTOBALITE)=63.260705
>>> DATA AT ITERATION 13 FROM STAGE 3
H=-737399.7005, P=100000, N(C)=1.626554057, N(N)=3.6E-4, N(O)=3.464295589,
N(SI)=2.697632851
DEGREES OF FREEDOM 0
T= 2.082731E+03
BP(GAS)=63.654311, BP(C1Si1_BETA)=34.710227, BP(O2Si1_L)=52.365328
>>> DATA AT ITERATION 13 FROM STAGE 4
H=79895.15705, P=100000, N(C)=0.8656780544, N(N)=2E-4, N(O)=1.743099657,
N(SI)=1.737227883
DEGREES OF FREEDOM 0
T= 2.721648E+03
BP(GAS)=64.038962, BP(SI_L)=23.039395
=====

>>> DATA AT ITERATION 14 FROM STAGE 1
H=-1001186.959, P=100000, N(C)=3.268147776, N(N)=6.784E-4, N(O)=3.865162855,
N(SI)=1.398884525
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.977201, BP(C1Si1_BETA)=8.2717563, BP(CRISTOBALITE)=71.225272,
BP(C_S)=18.915409
>>> DATA AT ITERATION 14 FROM STAGE 2
H=-925814.1596, P=100000, N(C)=2.519691747, N(N)=5.18E-4, N(O)=4.00931768,
N(SI)=2.297603161
DEGREES OF FREEDOM 0
T= 2.001975E+03
BP(GAS)=56.899726, BP(C1Si1_BETA)=37.678344, BP(O2Si1_L)=64.366461
>>> DATA AT ITERATION 14 FROM STAGE 3
H=-753439.8049, P=100000, N(C)=1.632245752, N(N)=3.6E-4, N(O)=3.537064525,
N(SI)=2.744501863
DEGREES OF FREEDOM 0
T= 2.083146E+03
BP(GAS)=65.078534, BP(C1Si1_BETA)=34.687761, BP(O2Si1_L)=53.512482
>>> DATA AT ITERATION 14 FROM STAGE 4
H=65149.88177, P=100000, N(C)=0.8651177304, N(N)=2E-4, N(O)=1.781285276,
N(SI)=1.755760368
DEGREES OF FREEDOM 0
T= 2.649675E+03
BP(GAS)=65.32767, BP(SI_L)=22.875374
=====

>>> DATA AT ITERATION 15 FROM STAGE 1
H=-999862.6594, P=100000, N(C)=3.222315841, N(N)=6.784E-4, N(O)=3.845817455,
N(SI)=1.424659953
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.607103, BP(C1Si1_BETA)=9.4314277, BP(CRISTOBALITE)=71.039976,
BP(C_S)=18.17504
>>> DATA AT ITERATION 15 FROM STAGE 2
H=-928208.0514, P=100000, N(C)=2.491890778, N(N)=5.18E-4, N(O)=4.036544188,
N(SI)=2.349766657
DEGREES OF FREEDOM 0
T= 2.011374E+03
BP(GAS)=58.095636, BP(C1Si1_BETA)=37.727938, BP(O2Si1_L)=64.687648
>>> DATA AT ITERATION 15 FROM STAGE 3
H=-766271.329, P=100000, N(C)=1.633034383, N(N)=3.6E-4, N(O)=3.57830447,
N(SI)=2.770582598
DEGREES OF FREEDOM 0
T= 2.083324E+03
BP(GAS)=65.468306, BP(C1Si1_BETA)=34.724896, BP(O2Si1_L)=54.487322
>>> DATA AT ITERATION 15 FROM STAGE 4
H=52615.98817, P=100000, N(C)=0.8660438866, N(N)=2E-4, N(O)=1.813735075,
N(SI)=1.772911424
DEGREES OF FREEDOM 0

T= 2.575864E+03
BP(GAS)=66.468905, BP(SI_L)=22.746115
=====

>>> DATA AT ITERATION 16 FROM STAGE 1
H=-1000065.826, P=100000, N(C)=3.199111232, N(N)=6.784E-4, N(O)=3.861986514,
N(SI)=1.463551784
DEGREES OF FREEDOM 0

T= 1.785826E+03
BP(GAS)=42.375409, BP(C1SI1_BETA)=11.209864, BP(CRISTOBALITE)=70.703914,
BP(C_S)=17.036615
>>> DATA AT ITERATION 16 FROM STAGE 2
H=-928526.6617, P=100000, N(C)=2.441492291, N(N)=5.18E-4, N(O)=4.037257166,
N(SI)=2.398934572
DEGREES OF FREEDOM 0

T= 2.020037E+03
BP(GAS)=58.591617, BP(C1SI1_BETA)=37.771358, BP(O2SI1_L)=64.9352
>>> DATA AT ITERATION 16 FROM STAGE 3
H=-776567.9245, P=100000, N(C)=1.634858192, N(N)=3.6E-4, N(O)=3.612504638,
N(SI)=2.793188429
DEGREES OF FREEDOM 0

T= 2.083472E+03
BP(GAS)=65.828605, BP(C1SI1_BETA)=34.789072, BP(O2SI1_L)=55.266805
>>> DATA AT ITERATION 16 FROM STAGE 4
H=42605.34375, P=100000, N(C)=0.8676444654, N(N)=2E-4, N(O)=1.839681949,
N(SI)=1.78748544
DEGREES OF FREEDOM 0

T= 2.507706E+03
BP(GAS)=67.422079, BP(SI_L)=22.6366
=====

>>> DATA AT ITERATION 17 FROM STAGE 1
H=-999180.6623, P=100000, N(C)=3.158039649, N(N)=6.784E-4, N(O)=3.858499971,
N(SI)=1.500852121
DEGREES OF FREEDOM 0

T= 1.785826E+03
BP(GAS)=42.570551, BP(C1SI1_BETA)=12.913321, BP(CRISTOBALITE)=70.390442,
BP(C_S)=15.949975
>>> DATA AT ITERATION 17 FROM STAGE 2
H=-928656.1645, P=100000, N(C)=2.393925051, N(N)=5.18E-4, N(O)=4.037317209,
N(SI)=2.445398182
DEGREES OF FREEDOM 0

T= 2.027376E+03
BP(GAS)=59.074263, BP(C1SI1_BETA)=37.816728, BP(O2SI1_L)=65.141744
>>> DATA AT ITERATION 17 FROM STAGE 3
H=-784668.4856, P=100000, N(C)=1.637270201, N(N)=3.6E-4, N(O)=3.64013743,
N(SI)=2.812536347
DEGREES OF FREEDOM 0

T= 2.083598E+03
BP(GAS)=66.144586, BP(C1SI1_BETA)=34.875519, BP(O2SI1_L)=55.878832
>>> DATA AT ITERATION 17 FROM STAGE 4
H=34757.5077, P=100000, N(C)=0.8698004529, N(N)=2E-4, N(O)=1.860054666,
N(SI)=1.799827786
DEGREES OF FREEDOM 0

T= 2.447965E+03
BP(GAS)=68.189742, BP(SI_L)=22.56741
=====

>>> DATA AT ITERATION 18 FROM STAGE 1
H=-998330.5261, P=100000, N(C)=3.119226823, N(N)=6.784E-4, N(O)=3.855155418,
N(SI)=1.536158786
DEGREES OF FREEDOM 0

T= 1.785827E+03
BP(GAS)=42.754619, BP(C1SI1_BETA)=14.526163, BP(CRISTOBALITE)=70.093081,
BP(C_S)=14.922323
>>> DATA AT ITERATION 18 FROM STAGE 2
H=-928546.6456, P=100000, N(C)=2.349118506, N(N)=5.18E-4, N(O)=4.036282852,
N(SI)=2.488498887
DEGREES OF FREEDOM 0

T= 2.033605E+03
BP(GAS)=59.522044, BP(C1SI1_BETA)=37.858508, BP(O2SI1_L)=65.307947
>>> DATA AT ITERATION 18 FROM STAGE 3
H=-790950.0036, P=100000, N(C)=1.640037002, N(N)=3.6E-4, N(O)=3.661968022,
N(SI)=2.82818931
DEGREES OF FREEDOM 0

T= 2.083688E+03
BP(GAS)=66.403735, BP(C1SI1_BETA)=34.965078, BP(O2SI1_L)=56.352237
>>> DATA AT ITERATION 18 FROM STAGE 4
H=28693.23597, P=100000, N(C)=0.8720340597, N(N)=2E-4, N(O)=1.875813041,
N(SI)=1.80994058
DEGREES OF FREEDOM 0

T= 2.398231E+03
BP(GAS)=68.793577, BP(SI_L)=22.526539
=====

>>> DATA AT ITERATION 19 FROM STAGE 1
H=-997507.3643, P=100000, N(C)=3.082739638, N(N)=6.784E-4, N(O)=3.85160075,
N(SI)=1.569002202
DEGREES OF FREEDOM 0

T= 1.785827E+03
BP(GAS)=42.913712, BP(C1SI1_BETA)=16.026794, BP(CRISTOBALITE)=69.816123,
BP(C_S)=13.966846
>>> DATA AT ITERATION 19 FROM STAGE 2
H=-928272.7054, P=100000, N(C)=2.307755915, N(N)=5.18E-4, N(O)=4.034285195,
N(SI)=2.527482587
DEGREES OF FREEDOM 0

T= 2.038832E+03
BP(GAS)=59.919121, BP(C1SI1_BETA)=37.89491, BP(O2SI1_L)=65.440558
>>> DATA AT ITERATION 19 FROM STAGE 3
H=-795775.5069, P=100000, N(C)=1.642731742, N(N)=3.6E-4, N(O)=3.678989003,
N(SI)=2.840558755
DEGREES OF FREEDOM 0

T= 2.083751E+03
BP(GAS)=66.611155, BP(C1SI1_BETA)=35.0469, BP(O2SI1_L)=56.715076
>>> DATA AT ITERATION 19 FROM STAGE 4
H=24048.61575, P=100000, N(C)=0.874074715, N(N)=2E-4, N(O)=1.887890951,
N(SI)=1.818020191
DEGREES OF FREEDOM 0

T= 2.358284E+03
BP(GAS)=69.261145, BP(SI_L)=22.503632
=====

>>> DATA AT ITERATION 20 FROM STAGE 1
H=-996726.5575, P=100000, N(C)=3.049123427, N(N)=6.784E-4, N(O)=3.847816555,
N(SI)=1.598785404
DEGREES OF FREEDOM 0

T= 1.785827E+03
BP(GAS)=43.042146, BP(C1SI1_BETA)=17.387648, BP(CRISTOBALITE)=69.565063,
BP(C_S)=13.100771
>>> DATA AT ITERATION 20 FROM STAGE 2
H=-927908.7559, P=100000, N(C)=2.270418378, N(N)=5.18E-4, N(O)=4.031694238,

```
N(SI)=2.562010096
DEGREES OF FREEDOM 0
T= 2.043175E+03
BP(GAS)=60.262859, BP(C1SI1_BETA)=37.925514, BP(O2SI1_L)=65.546007
>>> DATA AT ITERATION 20 FROM STAGE 3
H=-799465.3769, P=100000, N(C)=1.645127539, N(N)=3.6E-4, N(O)=3.692161448,
N(SI)=2.850193272
DEGREES OF FREEDOM 0
T= 2.083795E+03
BP(GAS)=66.774913, BP(C1SI1_BETA)=35.116375, BP(O2SI1_L)=56.99195
>>> DATA AT ITERATION 20 FROM STAGE 4
H=20506.06526, P=100000, N(C)=0.875807435, N(N)=2E-4, N(O)=1.897107338,
N(SI)=1.824361104
DEGREES OF FREEDOM 0
T= 2.326901E+03
BP(GAS)=69.620225, BP(SI_L)=22.490901
=====
>>> DATA AT ITERATION 21 FROM STAGE 1
H=-996006.4834, P=100000, N(C)=3.018828876, N(N)=6.784E-4, N(O)=3.843989924,
N(SI)=1.625226498
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.142842, BP(C1SI1_BETA)=18.595738, BP(CRISTOBALITE)=69.342397,
BP(C_S)=12.332159
>>> DATA AT ITERATION 21 FROM STAGE 2
H=-927507.941, P=100000, N(C)=2.237346302, N(N)=5.18E-4, N(O)=4.028829598,
N(SI)=2.59208808
DEGREES OF FREEDOM 0
T= 2.046761E+03
BP(GAS)=60.555654, BP(C1SI1_BETA)=37.950682, BP(O2SI1_L)=65.629725
>>> DATA AT ITERATION 21 FROM STAGE 3
H=-802280.7389, P=100000, N(C)=1.647141399, N(N)=3.6E-4, N(O)=3.702321276,
N(SI)=2.857649697
DEGREES OF FREEDOM 0
T= 2.083827E+03
BP(GAS)=66.903688, BP(C1SI1_BETA)=35.172897, BP(O2SI1_L)=57.202803
>>> DATA AT ITERATION 21 FROM STAGE 4
H=17809.09594, P=100000, N(C)=0.8772171086, N(N)=2E-4, N(O)=1.904126048,
N(SI)=1.829280133
DEGREES OF FREEDOM 0
T= 2.302568E+03
BP(GAS)=69.894828, BP(SI_L)=22.483673
=====
>>> DATA AT ITERATION 22 FROM STAGE 1
H=-995357.8297, P=100000, N(C)=2.992030179, N(N)=6.784E-4, N(O)=3.840290941,
N(SI)=1.648311479
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.220494, BP(C1SI1_BETA)=19.65041, BP(CRISTOBALITE)=69.148216,
BP(C_S)=11.6613
>>> DATA AT ITERATION 22 FROM STAGE 2
H=-927105.1562, P=100000, N(C)=2.208491049, N(N)=5.18E-4, N(O)=4.02593153,
N(SI)=2.617966229
DEGREES OF FREEDOM 0
T= 2.049708E+03
BP(GAS)=60.802619, BP(C1SI1_BETA)=37.971115, BP(O2SI1_L)=65.696167
>>> DATA AT ITERATION 22 FROM STAGE 3
H=-804426.7663, P=100000, N(C)=1.648778757, N(N)=3.6E-4, N(O)=3.710147941,
N(SI)=2.863406275
DEGREES OF FREEDOM 0
T= 2.083850E+03
BP(GAS)=67.004967, BP(C1SI1_BETA)=35.217746, BP(O2SI1_L)=57.363233
>>> DATA AT ITERATION 22 FROM STAGE 4
H=15757.52444, P=100000, N(C)=0.8783356412, N(N)=2E-4, N(O)=1.90946634,
N(SI)=1.833068811
DEGREES OF FREEDOM 0
T= 2.283843E+03
BP(GAS)=70.104358, BP(SI_L)=22.479422
=====
>>> DATA AT ITERATION 23 FROM STAGE 1
H=-994784.2939, P=100000, N(C)=2.968672033, N(N)=6.784E-4, N(O)=3.836843099,
N(SI)=1.668213811
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.280012, BP(C1SI1_BETA)=20.559615, BP(CRISTOBALITE)=68.980975,
BP(C_S)=11.083057
>>> DATA AT ITERATION 23 FROM STAGE 2
H=-926721.2024, P=100000, N(C)=2.183606873, N(N)=5.18E-4, N(O)=4.023154666,
N(SI)=2.640023764
DEGREES OF FREEDOM 0
T= 2.052127E+03
BP(GAS)=61.009567, BP(C1SI1_BETA)=37.987587, BP(O2SI1_L)=65.748922
>>> DATA AT ITERATION 23 FROM STAGE 3
H=-806061.969, P=100000, N(C)=1.650084396, N(N)=3.6E-4, N(O)=3.716176236,
N(SI)=2.867847152
DEGREES OF FREEDOM 0
T= 2.083867E+03
BP(GAS)=67.084742, BP(C1SI1_BETA)=35.252805, BP(O2SI1_L)=57.48525
>>> DATA AT ITERATION 23 FROM STAGE 4
H=14197.44278, P=100000, N(C)=0.8792100206, N(N)=2E-4, N(O)=1.913527955,
N(SI)=1.835973998
DEGREES OF FREEDOM 0
T= 2.269499E+03
BP(GAS)=70.264035, BP(SI_L)=22.476822
=====
>>> DATA AT ITERATION 24 FROM STAGE 1
H=-994284.2942, P=100000, N(C)=2.948544449, N(N)=6.784E-4, N(O)=3.833714842,
N(SI)=1.685209007
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.325563, BP(C1SI1_BETA)=21.335974, BP(CRISTOBALITE)=68.838274,
BP(C_S)=10.589356
>>> DATA AT ITERATION 24 FROM STAGE 2
H=-926367.3584, P=100000, N(C)=2.162341468, N(N)=5.18E-4, N(O)=4.020587131,
N(SI)=2.658689431
DEGREES OF FREEDOM 0
T= 2.054109E+03
BP(GAS)=61.182139, BP(C1SI1_BETA)=38.000817, BP(O2SI1_L)=65.790849
>>> DATA AT ITERATION 24 FROM STAGE 3
H=-807307.8891, P=100000, N(C)=1.651113845, N(N)=3.6E-4, N(O)=3.720821166,
N(SI)=2.871273146
DEGREES OF FREEDOM 0
T= 2.083880E+03
BP(GAS)=67.147684, BP(C1SI1_BETA)=35.279965, BP(O2SI1_L)=57.578046
>>> DATA AT ITERATION 24 FROM STAGE 4
H=13011.13493, P=100000, N(C)=0.879887402, N(N)=2E-4, N(O)=1.916616877,
```

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      N(SI)=1.838195841
DEGREES OF FREEDOM 0
T= 2.258539E+03
BP(GAS)=70.385643, BP(SI_L)=22.475169
=====
>>> DATA AT ITERATION 25 FROM STAGE 1
H=-993853.078, P=100000, N(C)=2.931354848, N(N)=6.784E-4, N(O)=3.83093215,
  N(SI)=1.699613986
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.360425, BP(C1SI1_BETA)=21.993991, BP(CRISTOBALITE)=68.717388,
  BP(C_S)=10.170943
>>> DATA AT ITERATION 25 FROM STAGE 2
H=-926048.8089, P=100000, N(C)=2.144299891, N(N)=5.18E-4, N(O)=4.018271317,
  N(SI)=2.674393903
DEGREES OF FREEDOM 0
T= 2.055734E+03
BP(GAS)=61.32549, BP(C1SI1_BETA)=38.011422, BP(O2SI1_L)=65.824206
>>> DATA AT ITERATION 25 FROM STAGE 3
H=-808257.3351, P=100000, N(C)=1.651920239, N(N)=3.6E-4, N(O)=3.724402657,
  N(SI)=2.87391735
DEGREES OF FREEDOM 0
T= 2.083891E+03
BP(GAS)=67.197436, BP(C1SI1_BETA)=35.300887, BP(O2SI1_L)=57.648621
>>> DATA AT ITERATION 25 FROM STAGE 4
H=12109.00357, P=100000, N(C)=0.8804091855, N(N)=2E-4, N(O)=1.918966121,
  N(SI)=1.839892246
DEGREES OF FREEDOM 0
T= 2.250176E+03
BP(GAS)=70.478226, BP(SI_L)=22.474083
=====
>>> DATA AT ITERATION 26 FROM STAGE 1
H=-993484.313, P=100000, N(C)=2.916778776, N(N)=6.784E-4, N(O)=3.828493516,
  N(SI)=1.711750755
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.387123, BP(C1SI1_BETA)=22.548392, BP(CRISTOBALITE)=68.615571,
  BP(C_S)=9.8184336
>>> DATA AT ITERATION 26 FROM STAGE 2
H=-925766.9054, P=100000, N(C)=2.129083817, N(N)=5.18E-4, N(O)=4.01622029,
  N(SI)=2.687544634
DEGREES OF FREEDOM 0
T= 2.057064E+03
BP(GAS)=61.44419, BP(C1SI1_BETA)=38.019916, BP(O2SI1_L)=65.850775
>>> DATA AT ITERATION 26 FROM STAGE 3
H=-808981.006, P=100000, N(C)=1.652549523, N(N)=3.6E-4, N(O)=3.72716646,
  N(SI)=2.875959479
DEGREES OF FREEDOM 0
T= 2.083898E+03
BP(GAS)=67.236829, BP(C1SI1_BETA)=35.316943, BP(O2SI1_L)=57.702301
>>> DATA AT ITERATION 26 FROM STAGE 4
H=11422.903, P=100000, N(C)=0.8808096399, N(N)=2E-4, N(O)=1.920752976,
  N(SI)=1.841186128
DEGREES OF FREEDOM 0
T= 2.243802E+03
BP(GAS)=70.548698, BP(SI_L)=22.473348
=====
>>> DATA AT ITERATION 27 FROM STAGE 1
H=-993171.0972, P=100000, N(C)=2.904490778, N(N)=6.784E-4, N(O)=3.826381053,
  N(SI)=1.721926331
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.407588, BP(C1SI1_BETA)=23.013211, BP(CRISTOBALITE)=68.53022,
  BP(C_S)=9.522894
>>> DATA AT ITERATION 27 FROM STAGE 2
H=-925520.6734, P=100000, N(C)=2.116313849, N(N)=5.18E-4, N(O)=4.014428773,
  N(SI)=2.698513336
DEGREES OF FREEDOM 0
T= 2.058154E+03
BP(GAS)=61.542213, BP(C1SI1_BETA)=38.02672, BP(O2SI1_L)=65.871962
>>> DATA AT ITERATION 27 FROM STAGE 3
H=-809532.7294, P=100000, N(C)=1.653039565, N(N)=3.6E-4, N(O)=3.729301201,
  N(SI)=2.877537839
DEGREES OF FREEDOM 0
T= 2.083905E+03
BP(GAS)=67.26807, BP(C1SI1_BETA)=35.329236, BP(O2SI1_L)=57.743135
>>> DATA AT ITERATION 27 FROM STAGE 4
H=10901.03517, P=100000, N(C)=0.8811162334, N(N)=2E-4, N(O)=1.922112232,
  N(SI)=1.84217235
DEGREES OF FREEDOM 0
T= 2.238946E+03
BP(GAS)=70.602335, BP(SI_L)=22.472838
=====
>>> DATA AT ITERATION 28 FROM STAGE 1
H=-992906.5531, P=100000, N(C)=2.894181908, N(N)=6.784E-4, N(O)=3.824567919,
  N(SI)=1.730422487
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.423289, BP(C1SI1_BETA)=23.401323, BP(CRISTOBALITE)=68.458956,
  BP(C_S)=9.2761306
>>> DATA AT ITERATION 28 FROM STAGE 2
H=-925307.808, P=100000, N(C)=2.105641395, N(N)=5.18E-4, N(O)=4.012880868,
  N(SI)=2.70763119
DEGREES OF FREEDOM 0
T= 2.059046E+03
BP(GAS)=61.622969, BP(C1SI1_BETA)=38.032171, BP(O2SI1_L)=65.888878
>>> DATA AT ITERATION 28 FROM STAGE 3
H=-809953.5031, P=100000, N(C)=1.653420784, N(N)=3.6E-4, N(O)=3.730951698,
  N(SI)=2.878758837
DEGREES OF FREEDOM 0
T= 2.083910E+03
BP(GAS)=67.292879, BP(C1SI1_BETA)=35.338634, BP(O2SI1_L)=57.774205
>>> DATA AT ITERATION 28 FROM STAGE 4
H=10503.98754, P=100000, N(C)=0.8813506141, N(N)=2E-4, N(O)=1.923146472,
  N(SI)=1.84292385
DEGREES OF FREEDOM 0
T= 2.235248E+03
BP(GAS)=70.643164, BP(SI_L)=22.472477
=====
>>> DATA AT ITERATION 29 FROM STAGE 1
H=-992684.171, P=100000, N(C)=2.885568934, N(N)=6.784E-4, N(O)=3.823023273,
  N(SI)=1.73749142
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.435345, BP(C1SI1_BETA)=23.724249, BP(CRISTOBALITE)=68.399657,
  BP(C_S)=9.0708148

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>>> DATA AT ITERATION   29 FROM STAGE    2
H=-925125.3288, P=100000, N(C)=2.096753877, N(N)=5.18E-4, N(O)=4.011555106,
  N(SI)=2.715188322
DEGREES OF FREEDOM 0
T= 2.059777E+03
BP(GAS)=61.68937, BP(C1SI1_BETA)=38.036538, BP(O2SI1_L)=65.902393
>>> DATA AT ITERATION   29 FROM STAGE    3
H=-810274.4652, P=100000, N(C)=1.653717209, N(N)=3.6E-4, N(O)=3.732228968,
  N(SI)=2.879704176
DEGREES OF FREEDOM 0
T= 2.083913E+03
BP(GAS)=67.312613, BP(C1SI1_BETA)=35.345808, BP(O2SI1_L)=57.797842
>>> DATA AT ITERATION   29 FROM STAGE    4
H=10201.9537, P=100000, N(C)=0.8815295324, N(N)=2E-4, N(O)=1.923933285,
  N(SI)=1.843496175
DEGREES OF FREEDOM 0
T= 2.232432E+03
BP(GAS)=70.674234, BP(SI_L)=22.472217
=====
>>> DATA AT ITERATION   30 FROM STAGE    1
H=-992497.9898, P=100000, N(C)=2.878398355, N(N)=6.784E-4, N(O)=3.821715669,
  N(SI)=1.743355069
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.444616, BP(C1SI1_BETA)=23.992127, BP(CRISTOBALITE)=68.350459,
  BP(C_S)=8.9004991
>>> DATA AT ITERATION   30 FROM STAGE    2
H=-924969.9618, P=100000, N(C)=2.08937566, N(N)=5.18E-4, N(O)=4.010427806,
  N(SI)=2.721436042
DEGREES OF FREEDOM 0
T= 2.060375E+03
BP(GAS)=61.743863, BP(C1SI1_BETA)=38.040041, BP(O2SI1_L)=65.913208
>>> DATA AT ITERATION   30 FROM STAGE    3
H=-810519.3972, P=100000, N(C)=1.653947718, N(N)=3.6E-4, N(O)=3.733218433,
  N(SI)=2.880436815
DEGREES OF FREEDOM 0
T= 2.083916E+03
BP(GAS)=67.328322, BP(C1SI1_BETA)=35.351283, BP(O2SI1_L)=57.815834
>>> DATA AT ITERATION   30 FROM STAGE    4
H=9972.074742, P=100000, N(C)=0.8816660729, N(N)=2E-4, N(O)=1.924532182,
  N(SI)=1.843932164
DEGREES OF FREEDOM 0
T= 2.230287E+03
BP(GAS)=70.69789, BP(SI_L)=22.472028
=====
>>> DATA AT ITERATION   31 FROM STAGE    1
H=-992342.658, P=100000, N(C)=2.872446805, N(N)=6.784E-4, N(O)=3.820614348,
  N(SI)=1.748205973
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.451746, BP(C1SI1_BETA)=24.21375, BP(CRISTOBALITE)=68.309747,
  BP(C_S)=8.7595923
>>> DATA AT ITERATION   31 FROM STAGE    2
H=-924838.4596, P=100000, N(C)=2.083267123, N(N)=5.18E-4, N(O)=4.009474898,
  N(SI)=2.72658946
DEGREES OF FREEDOM 0
T= 2.060864E+03
BP(GAS)=61.788521, BP(C1SI1_BETA)=38.04285, BP(O2SI1_L)=65.92186
>>> DATA AT ITERATION   31 FROM STAGE    3
H=-810706.2979, P=100000, N(C)=1.654126991, N(N)=3.6E-4, N(O)=3.733985558,
  N(SI)=2.881005032
DEGREES OF FREEDOM 0
T= 2.083919E+03
BP(GAS)=67.340847, BP(C1SI1_BETA)=35.355456, BP(O2SI1_L)=57.829521
>>> DATA AT ITERATION   31 FROM STAGE    4
H=9797.207162, P=100000, N(C)=0.8817701392, N(N)=2E-4, N(O)=1.924987799,
  N(SI)=1.844264039
DEGREES OF FREEDOM 0
T= 2.228655E+03
BP(GAS)=70.715889, BP(SI_L)=22.471889
=====
>>> DATA AT ITERATION   32 FROM STAGE    1
H=-992213.4673, P=100000, N(C)=2.867520427, N(N)=6.784E-4, N(O)=3.819691122,
  N(SI)=1.752209764
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.457242, BP(C1SI1_BETA)=24.39668, BP(CRISTOBALITE)=68.276133,
  BP(C_S)=8.6432845
>>> DATA AT ITERATION   32 FROM STAGE    2
H=-924727.6862, P=100000, N(C)=2.078221778, N(N)=5.18E-4, N(O)=4.008673528,
  N(SI)=2.730831915
DEGREES OF FREEDOM 0
T= 2.061265E+03
BP(GAS)=61.825058, BP(C1SI1_BETA)=38.045105, BP(O2SI1_L)=65.928797
>>> DATA AT ITERATION   32 FROM STAGE    3
H=-810848.9985, P=100000, N(C)=1.654266499, N(N)=3.6E-4, N(O)=3.734580946,
  N(SI)=2.8814462
DEGREES OF FREEDOM 0
T= 2.083921E+03
BP(GAS)=67.350836, BP(C1SI1_BETA)=35.358637, BP(O2SI1_L)=57.839941
>>> DATA AT ITERATION   32 FROM STAGE    4
H=9664.091239, P=100000, N(C)=0.8818494838, N(N)=2E-4, N(O)=1.925334663,
  N(SI)=1.844516815
DEGREES OF FREEDOM 0
T= 2.227412E+03
BP(GAS)=70.729594, BP(SI_L)=22.471786
=====
>>> DATA AT ITERATION   33 FROM STAGE    1
H=-992106.302, P=100000, N(C)=2.863452139, N(N)=6.784E-4, N(O)=3.818919933,
  N(SI)=1.755507448
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.461476, BP(C1SI1_BETA)=24.547358, BP(CRISTOBALITE)=68.248437,
  BP(C_S)=8.5474823
>>> DATA AT ITERATION   33 FROM STAGE    2
H=-924634.7873, P=100000, N(C)=2.074063526, N(N)=5.18E-4, N(O)=4.008002459,
  N(SI)=2.734318059
DEGREES OF FREEDOM 0
T= 2.061592E+03
BP(GAS)=61.854914, BP(C1SI1_BETA)=38.046916, BP(O2SI1_L)=65.934357
>>> DATA AT ITERATION   33 FROM STAGE    3
H=-810957.9826, P=100000, N(C)=1.65437514, N(N)=3.6E-4, N(O)=3.735043514,
  N(SI)=2.881789059
DEGREES OF FREEDOM 0
T= 2.083922E+03
BP(GAS)=67.358815, BP(C1SI1_BETA)=35.361061, BP(O2SI1_L)=57.847873
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>>> DATA AT ITERATION   33 FROM STAGE    4
H=9562.774404, P=100000, N(C)=0.8819099437, N(N)=2E-4, N(O)=1.925598692,
  N(SI)=1.84470929
DEGREES OF FREEDOM 0
T= 2.226466E+03
BP(GAS)=70.740027, BP(SI_L)=22.471709
=====
>>> DATA AT ITERATION   34 FROM STAGE    1
H=-992017.6263, P=100000, N(C)=2.860099655, N(N)=6.784E-4, N(O)=3.818277998,
  N(SI)=1.758218518
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.464741, BP(C1SI1_BETA)=24.671239, BP(CRISTOBALITE)=68.225659,
  BP(C_S)=8.4687163
>>> DATA AT ITERATION   34 FROM STAGE    2
H=-924557.1655, P=100000, N(C)=2.070642938, N(N)=5.18E-4, N(O)=4.007442677,
  N(SI)=2.737178163
DEGREES OF FREEDOM 0
T= 2.061859E+03
BP(GAS)=61.87929, BP(C1SI1_BETA)=38.048369, BP(O2SI1_L)=65.938812
>>> DATA AT ITERATION   34 FROM STAGE    3
H=-811041.1735, P=100000, N(C)=1.654459753, N(N)=3.6E-4, N(O)=3.73540305,
  N(SI)=2.882055631
DEGREES OF FREEDOM 0
T= 2.083924E+03
BP(GAS)=67.365192, BP(C1SI1_BETA)=35.362906, BP(O2SI1_L)=57.853906
>>> DATA AT ITERATION   34 FROM STAGE    4
H=9485.720096, P=100000, N(C)=0.8819559639, N(N)=2E-4, N(O)=1.925799513,
  N(SI)=1.844855721
DEGREES OF FREEDOM 0
T= 2.225747E+03
BP(GAS)=70.747963, BP(SI_L)=22.471651
=====
>>> DATA AT ITERATION   35 FROM STAGE    1
H=-991944.4124, P=100000, N(C)=2.857342278, N(N)=6.784E-4, N(O)=3.81774537,
  N(SI)=1.760443726
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.467268, BP(C1SI1_BETA)=24.772926, BP(CRISTOBALITE)=68.206955,
  BP(C_S)=8.4040612
>>> DATA AT ITERATION   35 FROM STAGE    2
H=-924492.5038, P=100000, N(C)=2.067833804, N(N)=5.18E-4, N(O)=4.006977172,
  N(SI)=2.739521327
DEGREES OF FREEDOM 0
T= 2.062077E+03
BP(GAS)=61.899162, BP(C1SI1_BETA)=38.049538, BP(O2SI1_L)=65.942391
>>> DATA AT ITERATION   35 FROM STAGE    3
H=-811104.7322, P=100000, N(C)=1.654525724, N(N)=3.6E-4, N(O)=3.73568284,
  N(SI)=2.882263143
DEGREES OF FREEDOM 0
T= 2.083924E+03
BP(GAS)=67.37029, BP(C1SI1_BETA)=35.364312, BP(O2SI1_L)=57.858499
>>> DATA AT ITERATION   35 FROM STAGE    4
H=9427.063386, P=100000, N(C)=0.8819910243, N(N)=2E-4, N(O)=1.925952402,
  N(SI)=1.844967225
DEGREES OF FREEDOM 0
T= 2.225199E+03
BP(GAS)=70.754005, BP(SI_L)=22.471608
=====
>>> DATA AT ITERATION   36 FROM STAGE    1
H=-991884.0731, P=100000, N(C)=2.855078037, N(N)=6.784E-4, N(O)=3.81730434,
  N(SI)=1.762267333
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.469218, BP(C1SI1_BETA)=24.856265, BP(CRISTOBALITE)=68.191621,
  BP(C_S)=8.3510709
>>> DATA AT ITERATION   36 FROM STAGE    2
H=-924438.8067, P=100000, N(C)=2.065530474, N(N)=5.18E-4, N(O)=4.006591184,
  N(SI)=2.741438367
DEGREES OF FREEDOM 0
T= 2.062255E+03
BP(GAS)=61.91535, BP(C1SI1_BETA)=38.050478, BP(O2SI1_L)=65.945263
>>> DATA AT ITERATION   36 FROM STAGE    3
H=-811153.2902, P=100000, N(C)=1.654577197, N(N)=3.6E-4, N(O)=3.735900752,
  N(SI)=2.882424806
DEGREES OF FREEDOM 0
T= 2.083925E+03
BP(GAS)=67.374369, BP(C1SI1_BETA)=35.365382, BP(O2SI1_L)=57.861994
>>> DATA AT ITERATION   36 FROM STAGE    4
H=9382.42917, P=100000, N(C)=0.8820177177, N(N)=2E-4, N(O)=1.926068754,
  N(SI)=1.845052094
DEGREES OF FREEDOM 0
T= 2.224782E+03
BP(GAS)=70.758603, BP(SI_L)=22.471575
=====
>>> DATA AT ITERATION   37 FROM STAGE    1
H=-991834.4377, P=100000, N(C)=2.853221685, N(N)=6.784E-4, N(O)=3.81694012,
  N(SI)=1.763759806
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.470726, BP(C1SI1_BETA)=24.924476, BP(CRISTOBALITE)=68.179065,
  BP(C_S)=8.3076994
>>> DATA AT ITERATION   37 FROM STAGE    2
H=-924394.3259, P=100000, N(C)=2.0636445, N(N)=5.18E-4, N(O)=4.006271953,
  N(SI)=2.743004922
DEGREES OF FREEDOM 0
T= 2.062401E+03
BP(GAS)=61.928527, BP(C1SI1_BETA)=38.051232, BP(O2SI1_L)=65.947568
>>> DATA AT ITERATION   37 FROM STAGE    3
H=-811190.3803, P=100000, N(C)=1.654617376, N(N)=3.6E-4, N(O)=3.736070571,
  N(SI)=2.882550827
DEGREES OF FREEDOM 0
T= 2.083926E+03
BP(GAS)=67.377635, BP(C1SI1_BETA)=35.366197, BP(O2SI1_L)=57.864653
>>> DATA AT ITERATION   37 FROM STAGE    4
H=9348.481196, P=100000, N(C)=0.8820380289, N(N)=2E-4, N(O)=1.926157259,
  N(SI)=1.845116658
DEGREES OF FREEDOM 0
T= 2.224465E+03
BP(GAS)=70.762101, BP(SI_L)=22.47155
=====
>>> DATA AT ITERATION   38 FROM STAGE    1
H=-991793.6729, P=100000, N(C)=2.851701842, N(N)=6.784E-4, N(O)=3.816639968,
  N(SI)=1.764979787
DEGREES OF FREEDOM 0
T= 1.785827E+03

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BP(GAS)=43.471895, BP(C1SI1_BETA)=24.980236, BP(CRISTOBALITE)=68.168798,
  BP(C_S)=8.2722438
>>> DATA AT ITERATION    38 FROM STAGE    2
H=-924357.5604, P=100000, N(C)=2.06210218, N(N)=5.18E-4, N(O)=4.006008508,
  N(SI)=2.744283687
DEGREES OF FREEDOM 0
T= 2.062519E+03
BP(GAS)=61.939242, BP(C1SI1_BETA)=38.05184, BP(O2SI1_L)=65.949421
>>> DATA AT ITERATION    38 FROM STAGE    3
H=-811218.7258, P=100000, N(C)=1.654648768, N(N)=3.6E-4, N(O)=3.736203041,
  N(SI)=2.88264916
DEGREES OF FREEDOM 0
T= 2.083926E+03
BP(GAS)=67.38025, BP(C1SI1_BETA)=35.366817, BP(O2SI1_L)=57.866676
>>> DATA AT ITERATION    38 FROM STAGE    4
H=9322.652527, P=100000, N(C)=0.882053489, N(N)=2E-4, N(O)=1.926224604,
  N(SI)=1.845165791
DEGREES OF FREEDOM 0
T= 2.224223E+03
BP(GAS)=70.764763, BP(SI_L)=22.471532
=====
>>> DATA AT ITERATION    39 FROM STAGE    1
H=-991760.24, P=100000, N(C)=2.850459034, N(N)=6.784E-4, N(O)=3.816393015,
  N(SI)=1.765975887
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.4728, BP(C1SI1_BETA)=25.025766, BP(CRISTOBALITE)=68.160411,
  BP(C_S)=8.2432925
>>> DATA AT ITERATION    39 FROM STAGE    2
H=-924327.2378, P=100000, N(C)=2.06084238, N(N)=5.18E-4, N(O)=4.005791543,
  N(SI)=2.745326463
DEGREES OF FREEDOM 0
T= 2.062616E+03
BP(GAS)=61.947948, BP(C1SI1_BETA)=38.052328, BP(O2SI1_L)=65.95091
>>> DATA AT ITERATION    39 FROM STAGE    3
H=-811240.4012, P=100000, N(C)=1.654673322, N(N)=3.6E-4, N(O)=3.736306488,
  N(SI)=2.88272597
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.382345, BP(C1SI1_BETA)=35.367289, BP(O2SI1_L)=57.868216
>>> DATA AT ITERATION    39 FROM STAGE    4
H=9302.99418, P=100000, N(C)=0.8820652601, N(N)=2E-4, N(O)=1.926275868,
  N(SI)=1.845203194
DEGREES OF FREEDOM 0
T= 2.224040E+03
BP(GAS)=70.766789, BP(SI_L)=22.471517
=====
>>> DATA AT ITERATION    40 FROM STAGE    1
H=-991732.8581, P=100000, N(C)=2.849443952, N(N)=6.784E-4, N(O)=3.816190178,
  N(SI)=1.766788338
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.473501, BP(C1SI1_BETA)=25.062904, BP(CRISTOBALITE)=68.153568,
  BP(C_S)=8.2196773
>>> DATA AT ITERATION    40 FROM STAGE    2
H=-924302.2778, P=100000, N(C)=2.059814461, N(N)=5.18E-4, N(O)=4.005613193,
  N(SI)=2.746176007
DEGREES OF FREEDOM 0
T= 2.062694E+03
BP(GAS)=61.955019, BP(C1SI1_BETA)=38.052721, BP(O2SI1_L)=65.952106
>>> DATA AT ITERATION    40 FROM STAGE    3
H=-811256.962, P=100000, N(C)=1.65469253, N(N)=3.6E-4, N(O)=3.736387293,
  N(SI)=2.882785985
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.384024, BP(C1SI1_BETA)=35.367648, BP(O2SI1_L)=57.869387
>>> DATA AT ITERATION    40 FROM STAGE    4
H=9288.050447, P=100000, N(C)=0.8820742099, N(N)=2E-4, N(O)=1.926314843,
  N(SI)=1.845231631
DEGREES OF FREEDOM 0
T= 2.223900E+03
BP(GAS)=70.76833, BP(SI_L)=22.471507
=====
>>> DATA AT ITERATION    41 FROM STAGE    1
H=-991710.4614, P=100000, N(C)=2.84861577, N(N)=6.784E-4, N(O)=3.816023885,
  N(SI)=1.7674504
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474046, BP(C1SI1_BETA)=25.09317, BP(CRISTOBALITE)=68.14799,
  BP(C_S)=8.2004319
>>> DATA AT ITERATION    41 FROM STAGE    2
H=-924281.7623, P=100000, N(C)=2.05897652, N(N)=5.18E-4, N(O)=4.005466808,
  N(SI)=2.746867562
DEGREES OF FREEDOM 0
T= 2.062758E+03
BP(GAS)=61.960757, BP(C1SI1_BETA)=38.053037, BP(O2SI1_L)=65.953067
>>> DATA AT ITERATION    41 FROM STAGE    3
H=-811269.6297, P=100000, N(C)=1.654707575, N(N)=3.6E-4, N(O)=3.736450489,
  N(SI)=2.882832935
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.38537, BP(C1SI1_BETA)=35.367921, BP(O2SI1_L)=57.870278
>>> DATA AT ITERATION    41 FROM STAGE    4
H=9276.679365, P=100000, N(C)=0.8820810225, N(N)=2E-4, N(O)=1.926344504,
  N(SI)=1.845253274
DEGREES OF FREEDOM 0
T= 2.223794E+03
BP(GAS)=70.769502, BP(SI_L)=22.471498
=====
>>> DATA AT ITERATION    42 FROM STAGE    1
H=-991692.1606, P=100000, N(C)=2.847940684, N(N)=6.784E-4, N(O)=3.815887677,
  N(SI)=1.767989422
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474468, BP(C1SI1_BETA)=25.117811, BP(CRISTOBALITE)=68.143446,
  BP(C_S)=8.1847622
>>> DATA AT ITERATION    42 FROM STAGE    2
H=-924264.9293, P=100000, N(C)=2.058294082, N(N)=5.18E-4, N(O)=4.005346844,
  N(SI)=2.747430048
DEGREES OF FREEDOM 0
T= 2.062810E+03
BP(GAS)=61.965412, BP(C1SI1_BETA)=38.053291, BP(O2SI1_L)=65.95384
>>> DATA AT ITERATION    42 FROM STAGE    3
H=-811279.3087, P=100000, N(C)=1.654719361, N(N)=3.6E-4, N(O)=3.736499924,
  N(SI)=2.882869671
DEGREES OF FREEDOM 0
```

T= 2.083928E+03
BP(GAS)=67.38645, BP(C1Si1_BETA)=35.368128, BP(O2Si1_L)=57.870955
>>> DATA AT ITERATION 42 FROM STAGE 4
H=9268.040365, P=100000, N(C)=0.8820861988, N(N)=2E-4, N(O)=1.926367042,
N(SI)=1.84526972
DEGREES OF FREEDOM 0
T= 2.223713E+03
BP(GAS)=70.770393, BP(SI_L)=22.471492
=====

>>> DATA AT ITERATION 43 FROM STAGE 1
H=-991677.2241, P=100000, N(C)=2.847390915, N(N)=6.784E-4, N(O)=3.815776303,
N(SI)=1.768427937
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474797, BP(C1Si1_BETA)=25.137859, BP(CRISTOBALITE)=68.139749,
BP(C_S)=8.1720134
>>> DATA AT ITERATION 43 FROM STAGE 2
H=-924251.1341, P=100000, N(C)=2.057738722, N(N)=5.18E-4, N(O)=4.005248656,
N(SI)=2.747887239
DEGREES OF FREEDOM 0
T= 2.062852E+03
BP(GAS)=61.969185, BP(C1Si1_BETA)=38.053496, BP(O2Si1_L)=65.954461
>>> DATA AT ITERATION 43 FROM STAGE 3
H=-811286.7148, P=100000, N(C)=1.654728606, N(N)=3.6E-4, N(O)=3.736538644,
N(SI)=2.882898453
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.387316, BP(C1Si1_BETA)=35.368286, BP(O2Si1_L)=57.871471
>>> DATA AT ITERATION 43 FROM STAGE 4
H=9261.468452, P=100000, N(C)=0.8820901381, N(N)=2E-4, N(O)=1.92638419,
N(SI)=1.845282233
DEGREES OF FREEDOM 0
T= 2.223652E+03
BP(GAS)=70.771071, BP(SI_L)=22.471487
=====

>>> DATA AT ITERATION 44 FROM STAGE 1
H=-991665.0434, P=100000, N(C)=2.846943538, N(N)=6.784E-4, N(O)=3.815685294,
N(SI)=1.768784406
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475052, BP(C1Si1_BETA)=25.154157, BP(CRISTOBALITE)=68.136742,
BP(C_S)=8.1616493
>>> DATA AT ITERATION 44 FROM STAGE 2
H=-924239.8455, P=100000, N(C)=2.057287143, N(N)=5.18E-4, N(O)=4.005168396,
N(SI)=2.748258581
DEGREES OF FREEDOM 0
T= 2.062886E+03
BP(GAS)=61.972242, BP(C1Si1_BETA)=38.05366, BP(O2Si1_L)=65.954961
>>> DATA AT ITERATION 44 FROM STAGE 3
H=-811292.378, P=100000, N(C)=1.654735861, N(N)=3.6E-4, N(O)=3.736568985,
N(SI)=2.882921012
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.38801, BP(C1Si1_BETA)=35.368406, BP(O2Si1_L)=57.871862
>>> DATA AT ITERATION 44 FROM STAGE 4
H=9256.47465, P=100000, N(C)=0.8820931318, N(N)=2E-4, N(O)=1.926397222,
N(SI)=1.845291743
DEGREES OF FREEDOM 0
T= 2.223605E+03
BP(GAS)=70.771586, BP(SI_L)=22.471484
=====

>>> DATA AT ITERATION 45 FROM STAGE 1
H=-991655.1203, P=100000, N(C)=2.84657978, N(N)=6.784E-4, N(O)=3.815611036,
N(SI)=1.769073987
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475251, BP(C1Si1_BETA)=25.167398, BP(CRISTOBALITE)=68.134298,
BP(C_S)=8.1532294
>>> DATA AT ITERATION 45 FROM STAGE 2
H=-924230.6177, P=100000, N(C)=2.0569202, N(N)=5.18E-4, N(O)=4.005102862,
N(SI)=2.748560014
DEGREES OF FREEDOM 0
T= 2.062914E+03
BP(GAS)=61.974718, BP(C1Si1_BETA)=38.053792, BP(O2Si1_L)=65.955362
>>> DATA AT ITERATION 45 FROM STAGE 3
H=-811296.7085, P=100000, N(C)=1.654741557, N(N)=3.6E-4, N(O)=3.736592775,
N(SI)=2.882938706
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.388568, BP(C1Si1_BETA)=35.368497, BP(O2Si1_L)=57.87216
>>> DATA AT ITERATION 45 FROM STAGE 4
H=9252.681311, P=100000, N(C)=0.8820954063, N(N)=2E-4, N(O)=1.926407124,
N(SI)=1.845298968
DEGREES OF FREEDOM 0
T= 2.223570E+03
BP(GAS)=70.771977, BP(SI_L)=22.471481
=====

>>> DATA AT ITERATION 46 FROM STAGE 1
H=-991647.0425, P=100000, N(C)=2.846284212, N(N)=6.784E-4, N(O)=3.815550496,
N(SI)=1.769309083
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475406, BP(C1Si1_BETA)=25.178147, BP(CRISTOBALITE)=68.132314,
BP(C_S)=8.1463933
>>> DATA AT ITERATION 46 FROM STAGE 2
H=-924223.0827, P=100000, N(C)=2.056622224, N(N)=5.18E-4, N(O)=4.005049404,
N(SI)=2.748804557
DEGREES OF FREEDOM 0
T= 2.062937E+03
BP(GAS)=61.976723, BP(C1Si1_BETA)=38.053899, BP(O2Si1_L)=65.955685
>>> DATA AT ITERATION 46 FROM STAGE 3
H=-811300.0162, P=100000, N(C)=1.65474603, N(N)=3.6E-4, N(O)=3.73661143,
N(SI)=2.882952585
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389015, BP(C1Si1_BETA)=35.368567, BP(O2Si1_L)=57.872385
>>> DATA AT ITERATION 46 FROM STAGE 4
H=9249.804768, P=100000, N(C)=0.8820971313, N(N)=2E-4, N(O)=1.926414634,
N(SI)=1.845304448
DEGREES OF FREEDOM 0
T= 2.223543E+03
BP(GAS)=70.772274, BP(SI_L)=22.471479
=====

>>> DATA AT ITERATION 47 FROM STAGE 1
H=-991640.472, P=100000, N(C)=2.846044206, N(N)=6.784E-4, N(O)=3.815501189,
N(SI)=1.769499838

```

DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475527, BP(C1SI1_BETA)=25.18687, BP(CRISTOBALITE)=68.130703,
  BP(C_S)=8.1408463
>>> DATA AT ITERATION 47 FROM STAGE 2
H=-924216.9351, P=100000, N(C)=2.056380391, N(N)=5.18E-4, N(O)=4.005005835,
  N(SI)=2.749002844
DEGREES OF FREEDOM 0
T= 2.062955E+03
BP(GAS)=61.978345, BP(C1SI1_BETA)=38.053985, BP(O2SI1_L)=65.955944
>>> DATA AT ITERATION 47 FROM STAGE 3
H=-811302.5458, P=100000, N(C)=1.654749547, N(N)=3.6E-4, N(O)=3.736626076,
  N(SI)=2.882963484
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389374, BP(C1SI1_BETA)=35.368619, BP(O2SI1_L)=57.872557
>>> DATA AT ITERATION 47 FROM STAGE 4
H=9247.621149, P=100000, N(C)=0.8820984412, N(N)=2E-4, N(O)=1.926420336,
  N(SI)=1.845308609
DEGREES OF FREEDOM 0
T= 2.223522E+03
BP(GAS)=70.7725, BP(SI_L)=22.471477
=====
>>> DATA AT ITERATION 48 FROM STAGE 1
H=-991635.1308, P=100000, N(C)=2.845849427, N(N)=6.784E-4, N(O)=3.81546105,
  N(SI)=1.769654524
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475621, BP(C1SI1_BETA)=25.193943, BP(CRISTOBALITE)=68.129397,
  BP(C_S)=8.1363478
>>> DATA AT ITERATION 48 FROM STAGE 2
H=-924211.925, P=100000, N(C)=2.056184242, N(N)=5.18E-4, N(O)=4.004970358,
  N(SI)=2.749163537
DEGREES OF FREEDOM 0
T= 2.062970E+03
BP(GAS)=61.979657, BP(C1SI1_BETA)=38.054054, BP(O2SI1_L)=65.956153
>>> DATA AT ITERATION 48 FROM STAGE 3
H=-811304.4807, P=100000, N(C)=1.654752314, N(N)=3.6E-4, N(O)=3.736637583,
  N(SI)=2.882972049
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389662, BP(C1SI1_BETA)=35.368659, BP(O2SI1_L)=57.872687
>>> DATA AT ITERATION 48 FROM STAGE 4
H=9245.964088, P=100000, N(C)=0.8820994355, N(N)=2E-4, N(O)=1.926424664,
  N(SI)=1.845311767
DEGREES OF FREEDOM 0
T= 2.223507E+03
BP(GAS)=70.772671, BP(SI_L)=22.471476
=====
>>> DATA AT ITERATION 49 FROM STAGE 1
H=-991630.7921, P=100000, N(C)=2.845691448, N(N)=6.784E-4, N(O)=3.815428406,
  N(SI)=1.769779897
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475694, BP(C1SI1_BETA)=25.199676, BP(CRISTOBALITE)=68.128338,
  BP(C_S)=8.1327017
>>> DATA AT ITERATION 49 FROM STAGE 2
H=-924207.8454, P=100000, N(C)=2.056025232, N(N)=5.18E-4, N(O)=4.004941495,
  N(SI)=2.749293703
DEGREES OF FREEDOM 0
T= 2.062982E+03
BP(GAS)=61.980718, BP(C1SI1_BETA)=38.054109, BP(O2SI1_L)=65.956321
>>> DATA AT ITERATION 49 FROM STAGE 3
H=-811305.9606, P=100000, N(C)=1.654754493, N(N)=3.6E-4, N(O)=3.73664663,
  N(SI)=2.882978785
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389893, BP(C1SI1_BETA)=35.368689, BP(O2SI1_L)=57.872785
>>> DATA AT ITERATION 49 FROM STAGE 4
H=9244.707136, P=100000, N(C)=0.8821001899, N(N)=2E-4, N(O)=1.926427948,
  N(SI)=1.845314164
DEGREES OF FREEDOM 0
T= 2.223495E+03
BP(GAS)=70.7728, BP(SI_L)=22.471475
=====
>>> DATA AT ITERATION 50 FROM STAGE 1
H=-991627.27, P=100000, N(C)=2.845563385, N(N)=6.784E-4, N(O)=3.815401877,
  N(SI)=1.769881461
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475751, BP(C1SI1_BETA)=25.204321, BP(CRISTOBALITE)=68.12748,
  BP(C_S)=8.1297479
>>> DATA AT ITERATION 50 FROM STAGE 2
H=-924204.5262, P=100000, N(C)=2.055896392, N(N)=5.18E-4, N(O)=4.004918031,
  N(SI)=2.749399094
DEGREES OF FREEDOM 0
T= 2.062992E+03
BP(GAS)=61.981575, BP(C1SI1_BETA)=38.054154, BP(O2SI1_L)=65.956456
>>> DATA AT ITERATION 50 FROM STAGE 3
H=-811307.0956, P=100000, N(C)=1.654756211, N(N)=3.6E-4, N(O)=3.736653755,
  N(SI)=2.882984092
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.390079, BP(C1SI1_BETA)=35.368712, BP(O2SI1_L)=57.87286
>>> DATA AT ITERATION 50 FROM STAGE 4
H=9243.751136, P=100000, N(C)=0.8821007639, N(N)=2E-4, N(O)=1.926430446,
  N(SI)=1.845315987
DEGREES OF FREEDOM 0
T= 2.223486E+03
BP(GAS)=70.772899, BP(SI_L)=22.471475
=====
REACTOR: @@ Use POLY-3 to list the constitution in each segment
REACTOR: GO P-3
POLY: L-E
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1004, label A0 , database: SSUB6

Conditions:
H=9243.751136, P=100000, N(C)=0.8821007639, N(N)=2E-4, N(O)=1.926430446,
  N(SI)=1.845315987
DEGREES OF FREEDOM 0

Temperature 2223.49 K ( 1950.34 C), Pressure 1.000000E+05
Number of moles of components 4.65405E+00, Mass in grams 9.32444E+01
Total Gibbs energy -1.35902E+06, Enthalpy 9.24375E+03, Volume 3.56321E-01

```


Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	8.8210E-01	1.1363E-01	5.0908E-03	-9.7618E+04	SER
N	2.0000E-04	3.0044E-05	8.4815E-09	-3.4359E+05	SER
O	1.9264E+00	3.3054E-01	1.4658E-13	-5.4632E+05	SER
SI	1.8453E+00	5.5581E-01	1.5639E-03	-1.1944E+05	SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 3.8539E+00, Mass 7.0773E+01, Volume fraction 1.0000E+00 Mass fractions:
O 4.35491E-01 SI 4.14766E-01 C 1.49703E-01 N 3.95829E-05

Constitution:

O1SI1	5.41812E-01	C1O2	2.03423E-05	C	2.35264E-10	O2	9.78900E-14
C1O1	4.57645E-01	O2SI1	1.70445E-06	N1O1	7.37248E-11		
SI	4.69580E-04	C1SI1	3.44146E-09	C3	4.10890E-12		
N2	5.18835E-05	O	9.79789E-10	C2	3.46788E-12		

SI_L Status ENTERED Driving force 0.0000E+00
Moles 8.0012E-01, Mass 2.2471E+01, Volume fraction 0.0000E+00 Mass fractions:
SI 1.00000E+00 C 0.00000E+00 O 0.00000E+00 N 0.00000E+00

POLY: @@ This equilibrium is valid for the fourth segment. Note it is
POLY: @@ identified with number 1004. The other have numbers 1001,
POLY: @@ 1002 and 1003.
POLY:
POLY: go sys
SYS: set-inter
SYS:

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_PG35: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Set conditions at the As rich side of the system. We want

POLY: @@ to calculate the metastable system without gas phase but

POLY: @@ then plot the gas constitution. Set gas to be dormant.

POLY:

POLY: s-c t=1200 p=1e5 n=1 x(ga)=.3

... the command in full is SET_CONDITION

POLY: c-s p gas=dor

... the command in full is CHANGE_STATUS

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 212 grid points in 0.041 s

Found the set of lowest grid points in 0.000 s

Calculated POLY solution 0.089 s, total time 0.130 s

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:-

Options /VWCS/: x

Output from POLY-3, equilibrium = 1, label A0 , database: PG35

Conditions:

T=1200, P=100000, N=1, X(GA)=0.3

DEGREES OF FREEDOM 0

Temperature 1200.00 K (926.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 7.33623E+01

Total Gibbs energy -8.75968E+04, Enthalpy 1.20850E+04, Volume 0.00000E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
AS	7.0000E-01	7.0000E-01	1.2211E-03	-6.6929E+01	SER
GA	3.0000E-01	3.0000E-01	1.2244E-06	-1.3582E+05	SER

GAS Status DORMANT Driving force 8.1507E-01

Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:

AS 1.00000E+00 GA 9.09718E-11

Constitution:

AS4 9.80210E-01 AS3 2.00768E-03 GA1 3.55191E-10 GA2 1.87160E-17

AS2 1.77817E-02 AS1 2.30505E-07 AS1GA1 5.27773E-12

LIQUID Status ENTERED Driving force 0.0000E+00

Moles 5.0575E-01, Mass 3.7617E+01, Volume fraction 0.0000E+00 Mole fractions:

AS 8.95449E-01 GA 1.04551E-01

FCC_B3 Status ENTERED Driving force 0.0000E+00

Moles 4.9425E-01, Mass 3.5745E+01, Volume fraction 0.0000E+00 Mole fractions:

AS 5.00000E-01 GA 5.00000E-01

POLY:Hit RETURN to continue

POLY: @@ Note that the gas would like to be stable (driving force

POLY: @@ positive) but it is not allowed to form as it is dormant.

POLY:

POLY: l-st ph

... the command in full is LIST_STATUS

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES

FCC_B3	ENTERED	0.000000E+00	4.942461E-01

LIQUID	ENTERED	0.000000E+00	5.057539E-01

RHOMBO_A7	ENTERED	-4.059045E-01	0.000000E+00

ORTHO	ENTERED	-6.644230E+00	0.000000E+00

GAS	DORMANT	8.150658E-01	

POLY: @@ The phase diagram is calculated with the composition and

POLY: @@ temperature on the axis as usual

POLY: s-a-v 1 x(ga)

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 0

Max value /1/: 1

Increment /.025/: .025

POLY: s-a-v 2 t

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 300

Max value /1/: 2000

Increment /42.5/: 25

POLY: @@ For an explanation of these symbols see below

POLY: ent fun pas1=0.4343*lnacr(as1,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pas2=0.4343*lnacr(as2,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pas3=0.4343*lnacr(as3,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pas4=0.4343*lnacr(as4,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pasga=0.4343*lnacr(as1ga1,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pgal=0.4343*lnacr(ga1,gas);

... the command in full is ENTER_SYMBOL

POLY: ent tab pp

... the command in full is ENTER_SYMBOL

Variable(s): pas1 pas2 pas3 pas4 pasga pgal;

POLY:

POLY: l-sym

... the command in full is LIST_SYMBOLS

DEFINED FUNCTIONS AND VARIABLES%

PAS1=.4343*LNACR(AS1,GAS)

PAS2=.4343*LNACR(AS2,GAS)

PAS3=.4343*LNACR(AS3,GAS)

PAS4=.4343*LNACR(AS4,GAS)

PASGA=.4343*LNACR(AS1GA1,GAS)

PGAL=.4343*LNACR(GA1,GAS)

DEFINED TABLES

PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1

POLY:Hit RETURN to continue

POLY: ent fun dd=0.4343*dgf(gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun qas1=log10(y(gas,as1))+dd;

... the command in full is ENTER_SYMBOL

POLY: ent fun qas2=log10(y(gas,as2))+dd;

```

... the command in full is ENTER_SYMBOL
POLY: ent fun qas3=log10(y(gas,as3))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qas4=log10(y(gas,as4))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qasga=log10(y(gas,as1gal))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qgal=log10(y(gas,gal))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent tab qq
... the command in full is ENTER_SYMBOL
Variable(s): qas1 qas2 qas3 qas4 qasga qgal;
POLY:
POLY: ent fun it=1000/T;
... the command in full is ENTER_SYMBOL
POLY: save tcex26 y
... the command in full is SAVE_WORKSPACES
POLY: l-sym
... the command in full is LIST_SYMBOLS
DEFINED FUNCTIONS AND VARIABLES%
PAS1=.4343*LNACR(AS1,GAS)
PAS2=.4343*LNACR(AS2,GAS)
PAS3=.4343*LNACR(AS3,GAS)
PAS4=.4343*LNACR(AS4,GAS)
PASGA=.4343*LNACR(AS1GA1,GAS)
PGA1=.4343*LNACR(GA1,GAS)
DD=.4343*DGF(GAS)
QAS1= LOG10(Y(GAS,AS1) )+DD
QAS2= LOG10(Y(GAS,AS2) )+DD
QAS3= LOG10(Y(GAS,AS3) )+DD
QAS4= LOG10(Y(GAS,AS4) )+DD
QASGA= LOG10(Y(GAS,AS1GA1) )+DD
QGA1= LOG10(Y(GAS,GA1) )+DD
IT=1000/T
DEFINED TABLES
PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POLY:Hit RETURN to continue
POLY: @@ Map follows all lines in the phase diagram
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 2.500E-01 3.100E+02
** FCC_B3
RHOMBO_A7
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 2.500E-01 3.000E+02
** FCC_B3
RHOMBO_A7
Calculated.. 32 equilibria

Phase region boundary 3 at: 2.500E-01 1.067E+03
** LIQUID
** FCC_B3
RHOMBO_A7

Phase region boundary 4 at: 2.345E-02 1.067E+03
** LIQUID
RHOMBO_A7
Calculated 10 equilibria

Phase region boundary 5 at: 2.734E-01 1.067E+03
** LIQUID
FCC_B3
Calculated.. 101 equilibria

```

Phase region boundary 6 at: 7.500E-01 3.029E+02
 ** LIQUID
 FCC_B3
 ** ORTHO

Phase region boundary 7 at: 7.500E-01 3.029E+02
 FCC_B3
 ** ORTHO
 Calculated.. 2 equilibria
 Terminating at axis limit.

Phase region boundary 8 at: 1.000E+00 3.029E+02
 LIQUID
 ** ORTHO
 Calculated 12 equilibria

Phase region boundary 9 at: 2.500E-01 3.100E+02
 ** FCC_B3
 RHOMBO_A7
 Calculated.. 32 equilibria
 Terminating at known equilibrium

Phase region boundary 10 at: 2.500E-01 3.100E+02
 ** FCC_B3
 RHOMBO_A7
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 11 at: 2.500E-01 3.100E+02
 ** FCC_B3
 RHOMBO_A7
 Calculated.. 32 equilibria
 Terminating at known equilibrium

Phase region boundary 12 at: 2.500E-01 3.100E+02
 ** FCC_B3
 RHOMBO_A7
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 13 at: 2.500E-01 3.100E+02
 ** FCC_B3
 RHOMBO_A7
 Calculated.. 32 equilibria
 Terminating at known equilibrium

Phase region boundary 14 at: 7.500E-01 3.100E+02
 LIQUID
 ** FCC_B3
 Calculated.. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 7.500E-01 3.100E+02
 LIQUID
 ** FCC_B3
 Calculated.. 100 equilibria
 Terminating at known equilibrium

Phase region boundary 16 at: 7.500E-01 3.100E+02
 LIQUID
 ** FCC_B3
 Calculated.. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.500E-01 3.100E+02
 LIQUID
 ** FCC_B3
 Calculated.. 100 equilibria
 Terminating at known equilibrium

Phase region boundary 18 at: 7.500E-01 3.100E+02
 LIQUID
 ** FCC_B3
 Calculated.. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.500E-01 3.100E+02
 LIQUID
 ** FCC_B3
 Calculated.. 100 equilibria
 Terminating at known equilibrium

Phase region boundary 20 at: 2.500E-01 8.700E+02
 ** FCC_B3
 RHOMBO_A7
 Calculated.. 24 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 21 at: 2.500E-01 8.700E+02
 ** FCC_B3
 RHOMBO_A7
 Calculated.. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 22 at: 7.492E-01 8.700E+02
 LIQUID
 ** FCC_B3
 Calculated.. 24 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.492E-01 8.700E+02
 LIQUID
 ** FCC_B3
 Calculated.. 81 equilibria
 Terminating at known equilibrium

Phase region boundary 24 at: 3.939E-01 1.430E+03
 LIQUID
 ** FCC_B3
 Calculated.. 18 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.939E-01 1.430E+03

```

    LIQUID
    ** FCC_B3
    Calculated.                87  equilibria
    Terminating at known equilibrium

Phase region boundary 26 at:  6.143E-01  1.430E+03
    LIQUID
    ** FCC_B3
    Calculated.                50  equilibria
    Terminating at known equilibrium

Phase region boundary 27 at:  6.143E-01  1.430E+03
    LIQUID
    ** FCC_B3
    Calculated.                55  equilibria
    Terminating at known equilibrium

Phase region boundary 28 at:  5.000E-03  1.086E+03
    LIQUID
    ** RHOMBO_A7
    Calculated.                15  equilibria

Phase region boundary 29 at:  5.000E-03  1.086E+03
    LIQUID
    ** RHOMBO_A7
    Calculated.                 3  equilibria
    Terminating at known equilibrium

Phase region boundary 30 at:  4.183E-01  1.463E+03
    LIQUID
    ** FCC_B3
    Calculated.                21  equilibria
    Terminating at known equilibrium

Phase region boundary 31 at:  4.183E-01  1.463E+03
    LIQUID
    ** FCC_B3
    Calculated.                67  equilibria
    Terminating at known equilibrium

Phase region boundary 32 at:  5.817E-01  1.468E+03
    LIQUID
    ** FCC_B3
    Calculated.                34  equilibria
    Terminating at known equilibrium

Phase region boundary 33 at:  5.817E-01  1.468E+03
    LIQUID
    ** FCC_B3
    Calculated.                54  equilibria
    Terminating at known equilibrium

Phase region boundary 34 at:  7.450E-01  9.995E+02
    LIQUID
    ** FCC_B3
    Calculated.                74  equilibria
    Terminating at known equilibrium

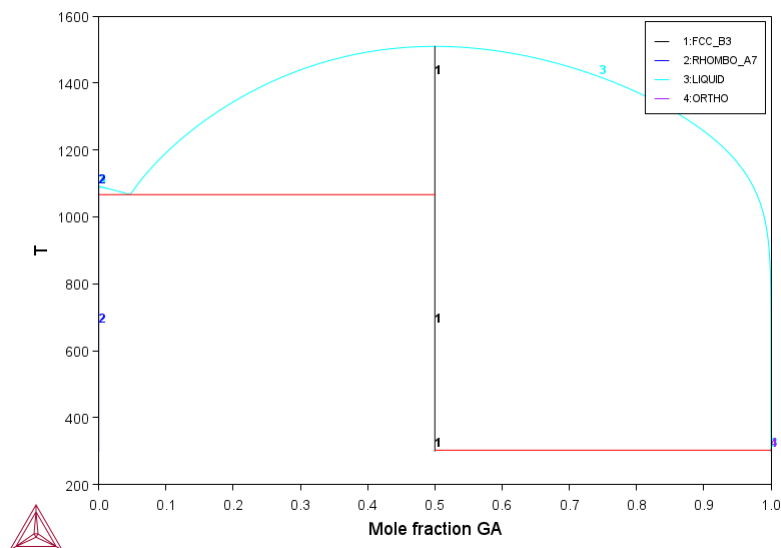
Phase region boundary 35 at:  7.450E-01  9.995E+02
    LIQUID
    ** FCC_B3
    Calculated.                29  equilibria
    Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex26\tcex26.POLY3
CPU time for mapping          8  seconds
POLY: @@ Now we plot this in the post processor
POLY: post
    POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x m-f ga
    ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
    ... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
    ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 26a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
    ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
    ... the command in full is PLOT_DIAGRAM

```

example 26a

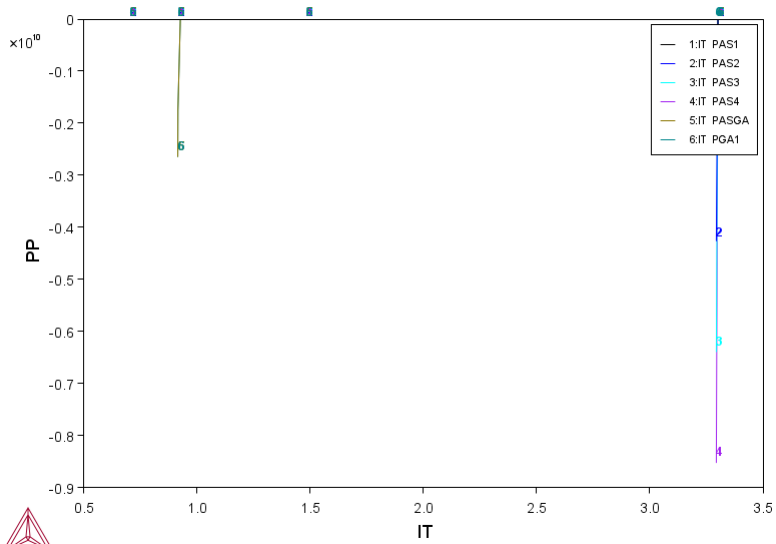


```

POST:
POST:Hit RETURN to continue
POST: @@ This is the traditional phase diagram.
POST:
POST: @@ Now those who work with this system is interesting to
POST: @@ know the partial pressures of the different gas species
POST: @@ along the solubility lines. As Thermo-Calc saves the
POST: @@ complete description of all tie-lines calculated in a
POST: @@ MAP or STEP command, even for dormant phases, we can
POST: @@ now plot these.
POST:
POST: @@ The partial pressures of a species in the gas is equal
POST: @@ to the fraction of that species if the gas is stable
POST: @@ (Dalton's law). If the gas is not stable then add the
POST: @@ driving force per formula unit of the gas (the formula
POST: @@ unit depends on the species).
POST:
POST: @@ We can directly get the activity of a gas species using
POST: @@ the state variable acr(species,gas) which has as
POST: @@ reference state a pure gas of the species itself. The
POST: @@ state variable lnacr(species,gas) is the natural logarithm
POST: @@ of this quantity. To make it into log10, multiply by 0.4343
POST:
POST: s-d-a y pp
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: @@ Plot against the inverse of temperature
POST: s-d-a x it
... the command in full is SET_DIAGRAM_AXIS
POST: l-sy
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
PAS1=.4343*LNACR(AS1,GAS)
PAS2=.4343*LNACR(AS2,GAS)
PAS3=.4343*LNACR(AS3,GAS)
PAS4=.4343*LNACR(AS4,GAS)
PASGA=.4343*LNACR(AS1GA1,GAS)
PGA1=.4343*LNACR(GA1,GAS)
DD=.4343*DGF(GAS)
QAS1= LOG10(Y(GAS,AS1) )+DD
QAS2= LOG10(Y(GAS,AS2) )+DD
QAS3= LOG10(Y(GAS,AS3) )+DD
QAS4= LOG10(Y(GAS,AS4) )+DD
QASGA= LOG10(Y(GAS,AS1GA1) )+DD
QGA1= LOG10(Y(GAS,GA1) )+DD
IT=1000/T
TEMP_C=T-273.15
DEFINED TABLES
PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POST: set-title example 26b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 26b

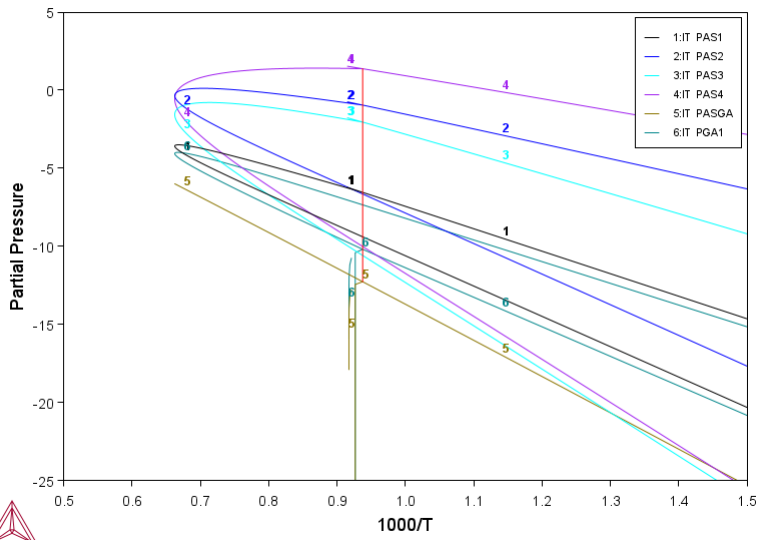


```

POST:
POST:Hit RETURN to continue
POST: @@ Now make the plot readable by adding axis text and labels
POST: s-s x n 0.5 1.5
... the command in full is SET_SCALING_STATUS
POST: s-s y n -25 5
... the command in full is SET_SCALING_STATUS
POST: s-a-text x n 1000/T
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-text y n Partial Pressure
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 26c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 26c



```

POST:
POST: set-interactive
... the command in full is SET_INTERACTIVE_MODE
POST:

```


tcex27

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex27\tcex27.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating chemical vapor depositions (CVD)

SYS:

SYS: @@ Note that a SSUB database license is required

SYS: @@ to run the example.

SYS:

SYS: @@ Get data from the database

SYS: set-log ex27,,,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw ssub6

... the command in full is SWITCH_DATABASE
Current database: SGTE Substances V6.0

VA DEFINED

TDB_SSUB6:

TDB_SSUB6: d-sys h cl ar w si

... the command in full is DEFINE_SYSTEM

H CL AR

W SI DEFINED

TDB_SSUB6: get

... the command in full is GET_DATA

09:12:33,599 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_SSUB6:

TDB_SSUB6: @@ Calculations are made in POLY-3 module

TDB_SSUB6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: @@ Very many stoichiometric phases can make equilibrium calculations

POLY: @@ difficult. Setting a very high maximum number of grid points can

POLY: @@ avoid this.

POLY: adv g y 10000000

... the command in full is ADVANCED_OPTIONS

Settings for global minimization:

POLY:

POLY: @@ In POLY-3 you define new components

POLY: def-com ar cl4w1 cl2h2si1 h2 cl1h1

... the command in full is DEFINE_COMPONENTS

POLY: l-st c

... the command in full is LIST_STATUS

*** STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
AR	ENTERED	SER		
CL4W1	ENTERED	SER		
CL2H2SI1	ENTERED	SER		
H2	ENTERED	SER		
CL1H1	ENTERED	SER		

POLY:Hit RETURN to continue

POLY:

POLY: @@ Set conditions for input of gases. The best way is

POLY: @@ to set amounts equal to moles/minutes, for example.

POLY: @@ In this case we had initial partial pressures of

POLY: @@ argon 0.9 atm, WCL4 1e-5..0.1 SiH2Cl2 1e-5..0.1 unknown

POLY: @@ pressure of H2. Should be no addition of HCl nor Cl but

POLY: @@ added a small addition of Cl1H1 to get equilibrium to

POLY: @@ converge.

POLY: s-c n=1 x(ar)=.9 x(cl2h2si)=1e-3 x(cl4w)=.001 x(cl1h1)=1e-12

... the command in full is SET_CONDITION

POLY:

POLY: @@ At the reaction zone T=1000 and total pressure is 1 atm

POLY: s-c t=1000 p=101325

... the command in full is SET_CONDITION

POLY: l-c

... the command in full is LIST_CONDITIONS

N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
P=101325

DEGREES OF FREEDOM 0

POLY:

POLY: @@ Save the file, then calculate and list the results

POLY: save tcex27 y

... the command in full is SAVE_WORKSPACES

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

```

Calculated      8347817 grid points in      48.122 s
Found the set of lowest grid points in      1.557 s
Calculated POLY solution      0.234 s, total time  49.913 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: SSUB6

Conditions:
N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
P=101325
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 3.65774E+01
Total Gibbs energy -1.67561E+05, Enthalpy 1.45855E+04, Volume 8.21892E-02

Component      Moles      W-Fraction Activity Potential Ref.stat
AR              9.0000E-01  9.8293E-01 2.0867E-09 -1.6619E+05 SER
CL4W1           1.0000E-03  8.9034E-03 8.9672E-57 -1.0730E+06 SER
CL2H2SI1        1.0000E-03  2.7615E-03 1.5207E-40 -7.6231E+05 SER
H2              9.8000E-02  5.4008E-03 2.4479E-09 -1.6486E+05 SER
CL1H1           1.0022E-12  9.9898E-13 1.9600E-18 -3.3901E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.0016E+00, Mass 3.6377E+01, Volume fraction 1.0000E+00 Mass fractions:
AR              9.88357E-01 CL1H1      5.21203E-03 CL4W1      1.31332E-10
H2              5.31980E-03 CL2H2SI1  1.11068E-03
Constitution:
AR              8.98562E-01 CL          3.03070E-11 H1SI1      1.54528E-17
H2              9.65533E-02 CL1H1SI1  2.25619E-11 SI        2.70199E-19
CL1H1           4.48535E-03 CL2W1      1.46463E-11 H6SI2      1.36833E-22
CL4SI1          3.16220E-04 H4SI1      6.03281E-12 CL5W1      4.37795E-24
CL3H1SI1        7.81990E-05 CL1SI1     1.41372E-12 SI2       1.26468E-26
CL1H3SI1        4.29796E-06 CL2        6.15724E-15 CL1W1      1.35601E-30
CL2H2SI1        3.50040E-07 H3SI1      4.22110E-16 SI3       1.15600E-30
CL2SI1          2.90182E-07 H2SI1      3.80095E-16 W          1.00000E-30
CL3SI1          3.29494E-09 CL4W1      1.12601E-16 CL10W2     1.00000E-30
H               7.01220E-10 CL3W1      1.62069E-17 CL6W1      1.00000E-30

SI3W5_S         Status ENTERED      Driving force 0.0000E+00
Moles-1.6000E-03, Mass 2.0070E-01, Volume fraction 0.0000E+00 Mass fractions:
CL4W1           1.62262E+00 H2         2.00876E-02 CL1H1      -9.44672E-01
CL2H2SI1        3.01962E-01 AR          0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Now set axis to vary along the input amounts of WC14
POLY: @@ and SiH2Cl2. Use a logarithmic step as the magnitudes
POLY: @@ vary. Note that a limit equal to zero should not be
POLY: @@ used with log.axis
POLY:
POLY: s-a-v 1 x(cl2h2si)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.9999975E-04/: 2.0*
Logarithmic step set
POLY: s-a-v 2 x(cl4w)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.9999975E-04/: 2.0*
Logarithmic step set
POLY: @@ Add with both direction and continuation ">" to be
POLY: @@ sure to get all lines
POLY: add
... the command in full is ADD_INITIAL_EQUILIBRIUM
Direction /Default/: 2>
POLY: add -2>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: l-ax
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: X(CL2H2SI1)      Min: 1E-8      Max: 2E-2      Inc: 2*
Axis No 2: X(CL4W1)         Min: 1E-8      Max: 2E-2      Inc: 2*
POLY: li-in
... the command in full is LIST_INITIAL_EQUILIBRIA
No 1 +2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
X(CL1H1)=1.002279E-12, T=1000, P=101325
No 2 -2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
X(CL1H1)=1.0022374E-12, T=1000, P=101325
POLY:Hit RETURN to continue
POLY: @@
POLY: @@ Save again with the start point before mapping
POLY: save tcex27 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18

Phase region boundary 1 at: 1.435E-02 1.970E-03

```

```

      GAS
      SI2W1_S
** SI_S
Calculated                      78  equilibria

Phase region boundary  2 at:   1.435E-02  1.970E-03
      GAS
      SI2W1_S
** SI_S
Calculated..                  2  equilibria
Terminating at axis limit.

Phase region boundary  3 at:   2.000E-02  2.810E-03
      GAS
      SI2W1_S
** SI_S
Calculated                      77  equilibria

Phase region boundary  4 at:   9.344E-03  1.970E-03
      GAS
      SI2W1_S
** SI3W5_S
Calculated                      88  equilibria

Phase region boundary  5 at:   9.344E-03  1.970E-03
      GAS
      SI2W1_S
** SI3W5_S
Calculated..                  3  equilibria
Terminating at axis limit.

Phase region boundary  6 at:   2.000E-02  3.793E-03
      GAS
      SI2W1_S
** SI3W5_S
Calculated                      80  equilibria

Phase region boundary  7 at:   4.095E-03  1.970E-03
      GAS
      SI2W1_S
      SI3W5_S
Calculated                      65  equilibria

Phase region boundary  8 at:   4.095E-03  1.970E-03
      GAS
      SI2W1_S
      SI3W5_S
Calculated..                  4  equilibria
Terminating at axis limit.

Phase region boundary  9 at:   2.000E-02  7.114E-03
      GAS
      SI2W1_S
      SI3W5_S
Calculated                      86  equilibria

Phase region boundary 10 at:   2.938E-03  1.970E-03
      GAS
      SI3W5_S
** W_S
Calculated                      80  equilibria

Phase region boundary 11 at:   2.938E-03  1.970E-03
      GAS
      SI3W5_S
** W_S
Calculated..                  4  equilibria
Terminating at axis limit.

Phase region boundary 12 at:   2.000E-02  7.879E-03
      GAS
      SI3W5_S
** W_S
Calculated                      83  equilibria

Phase region boundary 13 at:   1.000E-03  1.970E-03
      GAS
      SI3W5_S
      W_S
Calculated                      90  equilibria

Phase region boundary 14 at:   1.000E-03  1.970E-03
      GAS
      SI3W5_S
      W_S
Calculated..                  6  equilibria
Terminating at axis limit.

Phase region boundary 15 at:   2.000E-02  1.266E-02
      GAS
      SI3W5_S
      W_S
Calculated                      97  equilibria

Phase region boundary 16 at:   1.000E-03  1.970E-03
      GAS
      SI3W5_S
      W_S
Calculated                      36  equilibria

Phase region boundary 17 at:   1.000E-03  1.970E-03
      GAS
      SI3W5_S
      W_S
Calculated..                  7  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:   1.000E-03  1.037E-03
      GAS
      SI3W5_S
** W_S
Calculated                      35  equilibria

Phase region boundary 19 at:   1.000E-03  1.037E-03
      GAS

```

```

    SI3W5_S
** W_S
Calculated..                6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  1.000E-03  3.753E-04
    GAS
    SI2W1_S
** SI3W5_S
Calculated                33 equilibria

Phase region boundary 21 at:  1.000E-03  3.753E-04
    GAS
    SI2W1_S
** SI3W5_S
Calculated..                6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  1.000E-03  7.855E-04
    GAS
    SI2W1_S
    SI3W5_S
Calculated                33 equilibria

Phase region boundary 23 at:  1.000E-03  7.855E-04
    GAS
    SI2W1_S
    SI3W5_S
Calculated..                6 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex27\tcex27.POLY3
CPU time for mapping          20 seconds
POLY: @@
POLY: @@ Plot the diagram in the Post module
POLY: post
    POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

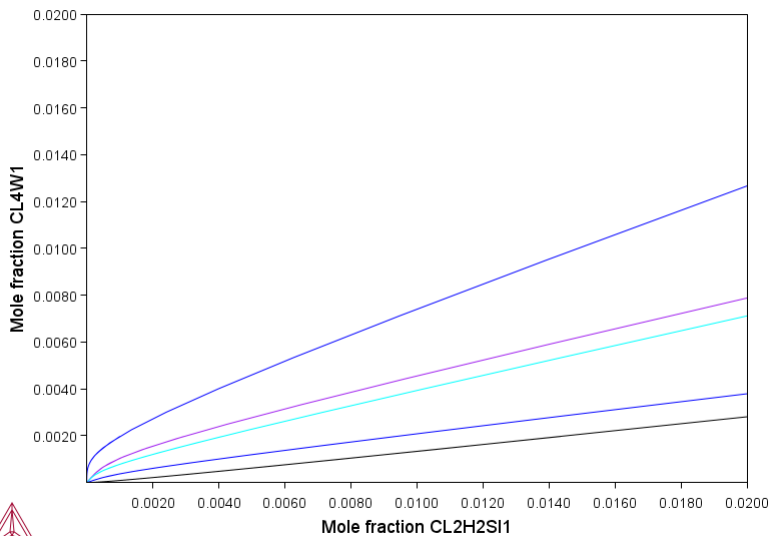
```

```

POST:
POST: set-title example 27a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 27a



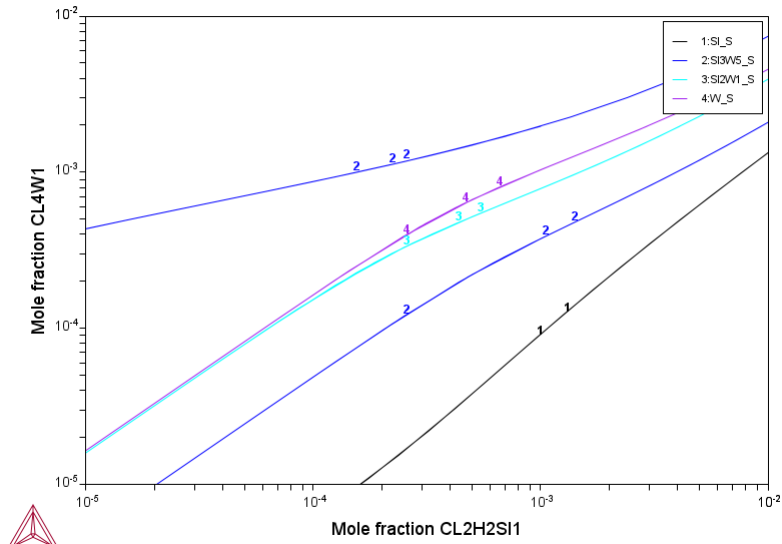


```

POST:
POST:Hit RETURN to continue
POST: @@ Better with logarithmic axis
POST: s-a-ty x log
... the command in full is SET_AXIS_TYPE
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-s x n 1e-5 .01
... the command in full is SET_SCALING_STATUS
POST: s-s y n 1e-5 .01
... the command in full is SET_SCALING_STATUS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: @@
POST: set-title example 27b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 27b

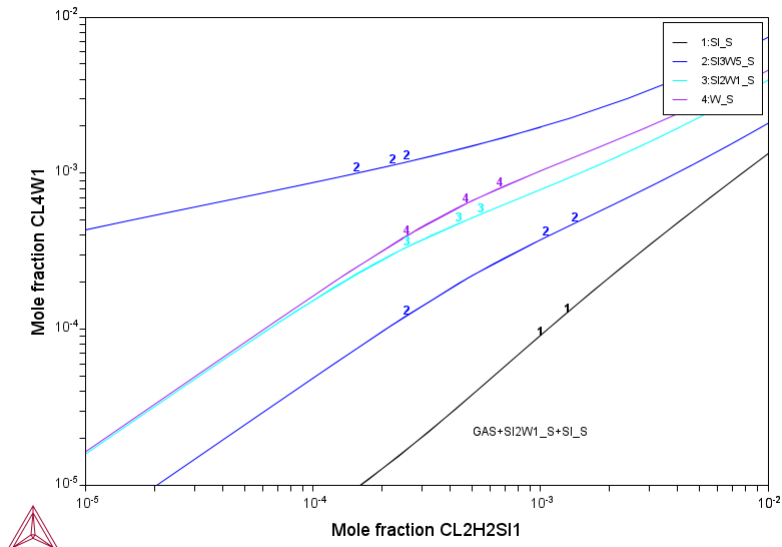


```

POST:
POST:Hit RETURN to continue
POST: @@Identify one of the phase regions
POST: add .0005 2e-5
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0.910 s
Calculated POLY solution      0.227 s, total time      1.137 s
Stable phases are: GAS+SI2W1_S+SI_S
Text size: /.36/:
POST: set-title example 27c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 27c



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex28

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex28\tcex28.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Pitting Resistance Equivalence (PRE)

SYS: @@ for a duplex stainless steel.

SYS:

SYS: @@ Note that a TCFE database license is required

SYS: @@ to run the example.

SYS:

SYS: set-log ex28,,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Set the nominal composition

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfell

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/:

1st alloying element: cr 25 ni 7 mo 4 c .002 n .27 si .3 mn .3

Next alloying element:

Temperature (C) /1000/: 1050

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

... the command in full is DEFINE_ELEMENTS

NI DEFINED

... the command in full is DEFINE_ELEMENTS

MO DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

N DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	MC_ETA	MC_SHP
KSI_CARBIIDE	Z_PHASE	FE4N_LP1
PI_A13	SIGMA_D8B	HIGH_SIGMA
MU_D85	P_PHASE	R_PHASE
CHI_A12	C14_LAVES	C15_LAVES
M3SI	MN9SI2	MN11SI19
MN6SI	G_PHASE	ETA_M5SIN
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	MOSI2_C11B	MO5SI3_D8M
NB5SI3_D8L	MSI2_C40	M11SI8
M6SI5	AL4C3_D71	FE8SI2C
SIC_B3	MN5SIC	CRZN17
CUZN_EPSILON	NI2N_B2	NI2N_L10
NI2ZN11_D82	AL5FE4	SI3N4
MN3N2	MN6N5	MNP_B31
M2P_C22	M4SI1_G3	NI31SI12
CO2SI_C37	M2SI_TETA	NISI_B31
NI3SI2	CR5SI3_D8M	

Reject phase(s) /NONE/: *

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	MC_ETA	MC_SHP
KSI_CARBIIDE	Z_PHASE	FE4N_LP1
PI_A13	SIGMA_D8B	HIGH_SIGMA
MU_D85	P_PHASE	R_PHASE
CHI_A12	C14_LAVES	C15_LAVES
M3SI	MN9SI2	MN11SI19
MN6SI	G_PHASE	ETA_M5SIN
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	MOSI2_C11B	MO5SI3_D8M
NB5SI3_D8L	MSI2_C40	M11SI8
M6SI5	AL4C3_D71	FE8SI2C
SIC_B3	MN5SIC	CRZN17

```

CUZN_EPSILON          NIZN_B2          NIZN_L10
NI2ZN11_D82           AL5FE4           SI3N4
MN3N2                 MN6N5           MNP_B31
M2P_C22               M4SI1_G3          NI31SI12
CO2SI_C37             M2SI_TETA         NISI_B31
NI3SI2               CR5SI3_D8M   REJECTED
Restore phase(s):: fcc_a1 bcc_a2 hcp_a3 m23 sigma
FCC_A1                BCC_A2          HCP_A3
M23C6_D84             SIGMA_D8B   RESTORED
Restore phase(s): /NONE/

```

```

.....

The following phases are retained in this system:

BCC_A2                FCC_A1          HCP_A3
M23C6_D84             SIGMA_D8B

.....

```

```

OK? /Y/:
09:14:47,511 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
PARAMETERS ...
FUNCTIONS ....

```

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

```

Using global minimization procedure
Calculated      7296 grid points in      0.583 s
Found the set of lowest grid points in      0.006 s
Calculated POLY solution      0.479 s, total time      1.068 s

```

```

POLY:
POLY: save tcex28 y
... the command in full is SAVE_WORKSPACES
POLY: l-e
... the command in full is LIST_EQUILIBRIUM

```

OUTPUT TO SCREEN OR FILE /SCREEN/:

```

Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE11

```

```

Conditions:
T=1323.15, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

```

```

Temperature 1323.15 K ( 1050.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.53180E+01
Total Gibbs energy -7.36566E+04, Enthalpy 3.92934E+04, Volume 7.43528E-06

```

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	9.2112E-05	2.0000E-05	3.4290E-05	-1.1310E+05	SER
CR	2.6597E-01	2.5000E-01	2.5349E-03	-6.5761E+04	SER
FE	6.2530E-01	6.3128E-01	1.6027E-03	-7.0806E+04	SER
MN	3.0208E-03	3.0000E-03	2.8578E-06	-1.4044E+05	SER
MO	2.3064E-02	4.0000E-02	6.4306E-04	-8.0852E+04	SER
N	1.0663E-02	2.7000E-03	4.3489E-07	-1.6115E+05	SER
NI	6.5978E-02	7.0000E-02	1.1328E-04	-9.9955E+04	SER
SI	5.9090E-03	3.0000E-03	2.8769E-09	-2.1636E+05	SER

```

FCC_A1#1                Status ENTERED      Driving force 0.0000E+00
Moles 5.6930E-01, Mass 3.1283E+01, Volume fraction 5.6483E-01 Mass fractions:
FE 6.3811E-01 NI 8.5250E-02 N 4.38243E-03 SI 3.16161E-03
CR 2.34121E-01 MO 3.1700E-02 MN 3.24360E-03 C 2.81314E-05

```

```

BCC_A2                Status ENTERED      Driving force 0.0000E+00
Moles 4.3070E-01, Mass 2.4035E+01, Volume fraction 4.3517E-01 Mass fractions:
FE 6.22389E-01 MO 5.08020E-02 SI 2.78966E-03 N 5.10240E-04
CR 2.70667E-01 NI 5.01505E-02 MN 2.68295E-03 C 9.41666E-06

```

```

POLY:
POLY:Hit RETURN to continue
POLY: @@ Calculate the temperature for an equal amount
POLY: c-s p bcc_a2=fix .5
... the command in full is CHANGE_STATUS
POLY: s-c t=none
... the command in full is SET_CONDITION

```

```

POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      7296 grid points in      0.077 s
12 ITS, CPU TIME USED 2 SECONDS

```

```

POLY: sh t
... the command in full is SHOW_VALUE
T=1382.2188
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE11

```

```

Conditions:
W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3, W(SI)=3E-3,
W(MN)=3E-3, P=100000, N=1
FIXED PHASES
BCC_A2=.5
DEGREES OF FREEDOM 0

```

```

Temperature 1382.22 K ( 1109.07 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.53180E+01
Total Gibbs energy -7.87487E+04, Enthalpy 4.15704E+04, Volume 7.46475E-06

```

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	9.2112E-05	2.0000E-05	3.2717E-05	-1.1869E+05	SER
CR	2.6597E-01	2.5000E-01	2.1012E-03	-7.0854E+04	SER
FE	6.2530E-01	6.3128E-01	1.3662E-03	-7.5802E+04	SER
MN	3.0208E-03	3.0000E-03	2.5263E-06	-1.4812E+05	SER
MO	2.3064E-02	4.0000E-02	4.8253E-04	-8.7762E+04	SER

```

N          1.0663E-02  2.7000E-03  6.2930E-07 -1.6410E+05 SER
NI         6.5978E-02  7.0000E-02  1.0285E-04 -1.0553E+05 SER
SI         5.9090E-03  3.0000E-03  4.1845E-09 -2.2171E+05 SER

BCC_A2          Status FIXED          Driving force  0.0000E+00
Moles 5.0146E-01, Mass 2.7959E+01, Volume fraction 5.0593E-01 Mass fractions:
FE  6.25815E-01 NI  5.42157E-02 SI  2.86526E-03 N   7.17191E-04
CR  2.64835E-01 MO  4.88074E-02 MN  2.73452E-03 C   1.01462E-05

FCC_A1#1          Status ENTERED          Driving force  0.0000E+00
Moles 4.9854E-01, Mass 2.7359E+01, Volume fraction 4.9407E-01 Mass fractions:
FE  6.36865E-01 NI  8.61301E-02 N   4.72624E-03 SI  3.13769E-03
CR  2.34840E-01 MO  3.09997E-02 MN  3.27129E-03 C   3.00697E-05
POLY: @@ Enter the PRE functions
POLY: ent fun prefcc
... the command in full is ENTER_SYMBOL
Function: 100*w(fcc_a1,cr)+300*w(fcc_a1,mo)+1600*w(fcc_a1,n);
POLY: ent fun prebcc
... the command in full is ENTER_SYMBOL
Function: 100*w(bcc_a2,cr)+300*w(bcc_a2,mo)+1600*w(bcc_a2,n);
POLY: l-sy
... the command in full is LIST_SYMBOLS
DEFINED FUNCTIONS AND VARIABLES%
  PREFCC=100*W(FCC_A1#1,CR)+300*W(FCC_A1#1,MO)+1600*W(FCC_A1#1,N)
  PREBCC=100*W(BCC_A2,CR)+300*W(BCC_A2,MO)+1600*W(BCC_A2,N)
POLY: eval
... the command in full is EVALUATE_FUNCTIONS
Name(s): *
  PREFCC=40.345889
  PREBCC=42.273231
POLY:Hit RETURN to continue
POLY: @@ Then vary the nitrogen content
POLY: s-a-v 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(n)
Min value /0/: .001
Max value /1/: .005
Increment /1E-04/: 1E-04
POLY: li-ax
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W(N)          Min: 1E-3          Max: 5E-3          Inc: 1E-4
POLY: save tcex28 y
... the command in full is SAVE_WORKSPACES
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value  0.270000E-02
...OK

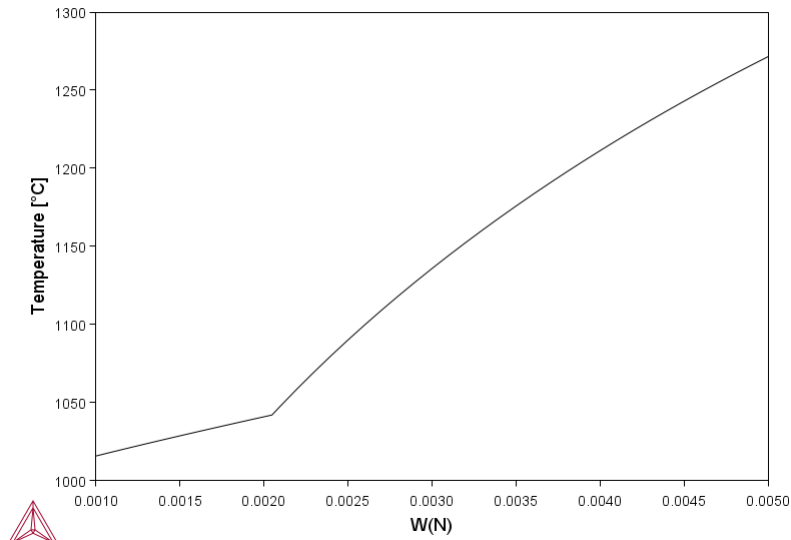
Phase Region from  0.270000E-02 for:
  BCC_A2
  FCC_A1#1
Global Test at  3.50000E-03 .... OK
Global test at  4.50000E-03 .... OK
Terminating at  0.500000E-02
Calculated  26 equilibria

Phase Region from  0.270000E-02 for:
  BCC_A2
  FCC_A1#1
Global Check of adding phase at  2.04865E-03
Calculated  9 equilibria

Phase Region from  0.204865E-02 for:
  BCC_A2
  FCC_A1#1
  SIGMA_D8B
Global test at  1.30000E-03 .... OK
Terminating at  0.100000E-02
Calculated  14 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex28\tcex28.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: @@ First plot how the temperature varies
POST: s-d-a x w(n)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 28a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

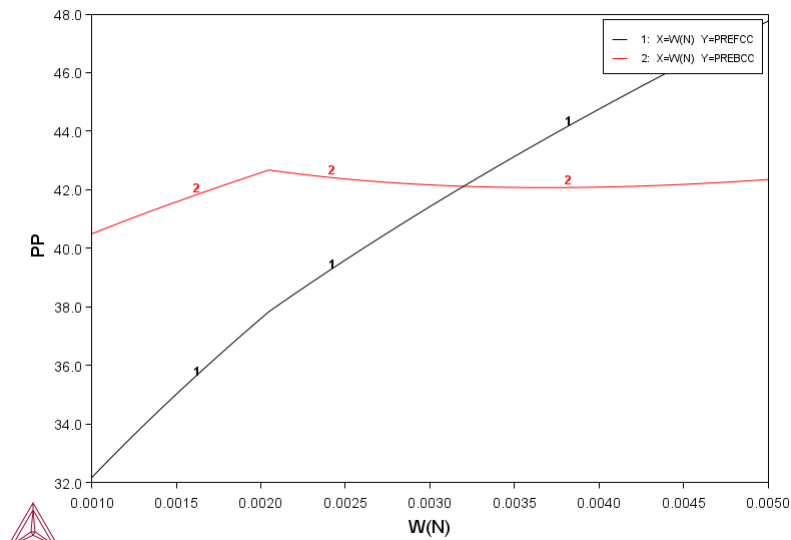

example 28a



```

POST:
POST:Hit RETURN to continue
POST: @@ Then plot the PRE
POST: ent tab pp
... the command in full is ENTER_SYMBOL
Variable(s): prefcc prebcc
&
POST:
POST: s-d-a y pp
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 28b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
  
```

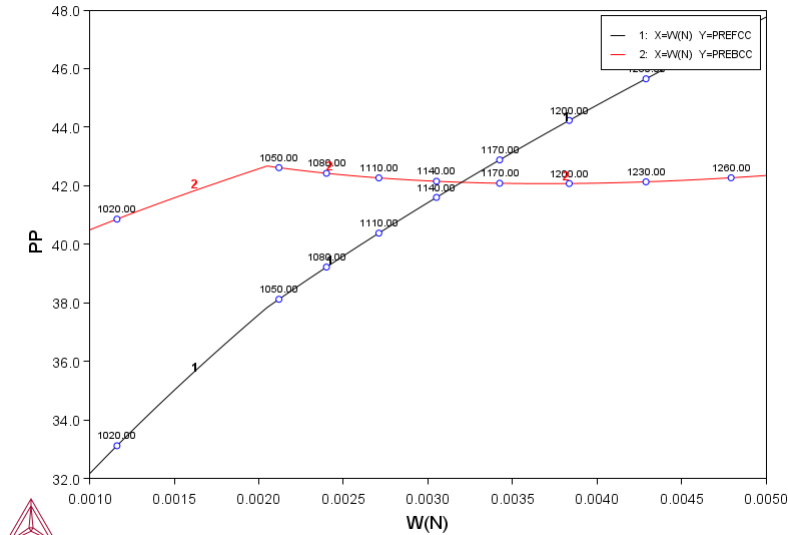
example 28b



```

POST:
POST:Hit RETURN to continue
POST: @@ Add the temperature as tic marks to the plot
POST: s-d-a z t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 800 1300
... the command in full is SET_SCALING_STATUS
POST: set-title example 28c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
  
```

example 28c



```

POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Check how close we are to form Cr2N
POLY: read tcex28
... the command in full is READ_WORKSPACES
POLY:
POLY: @@ Restore BCC as entered
POLY: c-s p bcc_a2=ent 1
... the command in full is CHANGE_STATUS
POLY: s-c t=1323
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 7296 grid points in 0.144 s
Found the set of lowest grid points in 0.010 s
Calculated POLY solution 0.361 s, total time 0.515 s
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=1E-3, W(SI)=3E-3,
W(MN)=3E-3, P=100000, N=1.
DEGREES OF FREEDOM 0

Temperature 1323.00 K ( 1049.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.55977E+01
Total Gibbs energy -7.30381E+04, Enthalpy 4.01860E+04, Volume 7.46615E-06

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
C               9.2578E-05  2.0000E-05  4.8447E-05 -1.0929E+05 SER
CR             2.6732E-01  2.5000E-01  2.5383E-03 -6.5739E+04 SER
FE             6.3015E-01  6.3298E-01  1.6023E-03 -7.0800E+04 SER
MN            3.0360E-03  3.0000E-03  2.9354E-06 -1.4013E+05 SER
MO            2.3180E-02  4.0000E-02  5.8417E-04 -8.1899E+04 SER
N             3.9693E-03  1.0000E-03  2.9950E-07 -1.6523E+05 SER
NI            6.6312E-02  7.0000E-02  1.2334E-04 -9.9007E+04 SER
SI            5.9389E-03  3.0000E-03  2.4675E-09 -2.1802E+05 SER

BCC_A2          Status ENTERED      Driving force 0.0000E+00
Moles 6.5584E-01, Mass 3.6561E+01, Volume fraction 6.5960E-01 Mass fractions:
FE 6.24172E-01 NI 5.47570E-02 MN 2.77966E-03 N 3.56006E-04
CR 2.69277E-01 MO 4.60252E-02 SI 2.62000E-03 C 1.26171E-05

FCC_A1#1        Status ENTERED      Driving force 0.0000E+00
Moles 3.4416E-01, Mass 1.9037E+01, Volume fraction 3.4040E-01 Mass fractions:
FE 6.49896E-01 NI 9.92748E-02 SI 3.72981E-03 N 2.23682E-03
CR 2.12977E-01 MO 2.84283E-02 MN 3.42317E-03 C 3.41791E-05
POLY:Hit RETURN to continue
POLY: @@ Find out at which temperature sigma forms
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: sigma
You must release one of these conditions
T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=1E-3, W(SI)=3E-3,
W(MN)=3E-3, P=100000, N=1. DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 7296 grid points in 0.063 s
To form SIGMA the condition is set to T=1306.35398916
POLY:Hit RETURN to continue
POLY: @@ Find the temperature for Cr2N, set the start
POLY: @@ constitution. but first make sure hcp#2 is nitride
POLY: s-s-c hcp_a3#2 *
... the command in full is SET_START_CONSTITUTION
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: hcp_a3#2
You must release one of these conditions
T=1306.353989, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=1E-3,
W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1. DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 7296 grid points in 0.091 s
To form HCP_A3 the condition is set to T=1172.76011565

```

POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=1172.760116, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=1E-3,
W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1.
DEGREES OF FREEDOM 0

Temperature 1172.76 K (899.61 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.55977E+01
Total Gibbs energy -6.05906E+04, Enthalpy 3.35974E+04, Volume 7.31497E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	9.2578E-05	2.0000E-05	7.3259E-05	-9.2843E+04	SER
CR	2.6732E-01	2.5000E-01	3.9510E-03	-5.3960E+04	SER
FE	6.3015E-01	6.3298E-01	2.5785E-03	-5.8121E+04	SER
MN	3.0360E-03	3.0000E-03	4.0650E-06	-1.2104E+05	SER
MO	2.3180E-02	4.0000E-02	7.4864E-04	-7.0180E+04	SER
N	3.9693E-03	1.0000E-03	1.1884E-07	-1.5548E+05	SER
NI	6.6312E-02	7.0000E-02	1.4494E-04	-8.6190E+04	SER
SI	5.9389E-03	3.0000E-03	9.0627E-10	-2.0303E+05	SER

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Moles 6.4668E-01, Mass 3.5670E+01, Volume fraction 6.4588E-01 Mass fractions:
FE 6.85602E-01 NI 8.86229E-02 SI 4.46799E-03 N 1.55865E-03
CR 1.99019E-01 MO 1.72828E-02 MN 3.41574E-03 C 3.11731E-05

SIGMA_D8B Status ENTERED Driving force 0.0000E+00
Moles 3.5332E-01, Mass 1.9927E+01, Volume fraction 3.5412E-01 Mass fractions:
FE 5.38786E-01 MO 8.06643E-02 MN 2.25582E-03 C 0.00000E+00
CR 3.41257E-01 NI 3.66646E-02 SI 3.72270E-04 N 0.00000E+00

HCP_A3#2 Status ENTERED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CR 8.27227E-01 MO 4.56975E-02 MN 1.13224E-03 C 5.84328E-04
N 1.09139E-01 FE 1.54868E-02 NI 7.33072E-04 SI 4.64348E-09

POLY: @@ Rapid cooling is needed to avoid these phases.
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex29\tcex29.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating the speciation of a gas

SYS:

SYS: @@ Note that a SSUB database license is required

SYS: @@ to run the example.

SYS:

SYS: set-log ex29,,,,

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw ssub6

... the command in full is SWITCH_DATABASE

Current database: SGTE Substances v6.0

VA DEFINED

TDB_SSUB6:

TDB_SSUB6: d-sys c o h s

... the command in full is DEFINE_SYSTEM

C O H

S DEFINED

TDB_SSUB6: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT

GAS:G :C ClH1 ClH101 ClH102 ClH2 ClH201 ClH202_CIS ClH202_DIOXIRANE
ClH202_TRANS ClH3 ClH301 CH2OH ClH301_CH3O ClH4 ClH401 ClH4S1 ClO1 ClO1S1
ClO2 ClS1 ClS2 C2 C2H1 C2H2 C2H201 C2H3 C2H4 C2H401 ACETALDEHYDE
C2H401_OXIRANE C2H402 ACETICACID C2H402_DIOXETANE C2H403 123TRIOXOLANE
C2H403 124TRIOXOLANE C2H5 C2H6 C2H601_1 C2H601_2 C2H602 C2O1 C3 C3H1
C3H4 1_C3H4 2 C3H6 1 C3H6 2 C3H601 1 C3H601 2 C3H8 C3O2 C4 C4H1 C4H10 1
C4H10 2 C4H2 1 C4H2 2 C4H4 1 C4H4 2 C4H6 1 C4H6 2 C4H6 3 C4H6 4 C4H6 5
C4H8 1 C4H8 2 C4H8 3 C4H8 4 C4H8 5 C4H8 6 C5 C60 C6H6 C6H601 H H101
H101S1_HSO H101S1_SOH H102 H1S1 H2 H201 H201S1_H2SO H201S1_HSOH H2O2
H2O4S1 H2S1 H2S2 O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8:

C_S :C:

C_L :C:

DIAMOND :C:

ClH202_L :ClH202:

ClH2S3_L :ClH2S3:

ClH4_L :ClH4:

ClH401_L :ClH401:

ClH4S1_L :ClH4S1:

ClS2_L :ClS2:

C2H402_L :C2H402:

C2H6_L :C2H6:

C2H601_L :C2H601:

C2H602_L :C2H602:

C3H6_L :C3H6:

C3H8_L :C3H8:

C4H8_L :C4H8:

C60_S :C60:

C6H6_L :C6H6:

H1008S1_L :H1008S1:

H15010_5S1_L :H15010.5S1:

H201_L :H201:

H202_L :H202:

H204S1_L :H204S1:

H2S1_L :H2S1:

H2S2_L :H2S2:

H405S1_L :H405S1:

H606S1_L :H606S1:

H807S1_L :H807S1:

O3S1_L :O3S1:

S_S :S:

S_S2 :S:

S_L :S:

TDB_SSUB6:Hit RETURN to continue

TDB_SSUB6: get

... the command in full is GET_DATA

09:15:57,354 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_SSUB6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: l-st c

... the command in full is LIST_STATUS

*** STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T (K)	P (Pa)
VA	ENTERED	SER		
C	ENTERED	SER		
H	ENTERED	SER		

```

O                               ENTERED   SER
S                               ENTERED   SER
POLY: s-i-a n(h2)=10
... the command in full is SET_INPUT_AMOUNTS
POLY: l-c
... the command in full is LIST_CONDITIONS
N(H)=20
DEGREES OF FREEDOM 5
POLY: s-i-a n(clo2)=5
... the command in full is SET_INPUT_AMOUNTS
POLY: s-i-a n(o2s1)=0.1
... the command in full is SET_INPUT_AMOUNTS
POLY: l-c
... the command in full is LIST_CONDITIONS
N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1
DEGREES OF FREEDOM 2
POLY: s-c t=1000 p=1e5
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      132 grid points in      0.258 s
Found the set of lowest grid points in      0.005 s
Calculated POLY solution      0.166 s, total time      0.429 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: SSUB6

Conditions:
N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1, T=1000, P=100000
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 3.53000E+01, Mass in grams 2.46609E+02
Total Gibbs energy -4.82824E+06, Enthalpy -1.54921E+06, Volume 1.23971E+00

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
C      5.0000E+00  2.4352E-01  3.4847E-02 -2.7910E+04 SER
H      2.0000E+01  8.1741E-02  1.0525E-04 -7.6154E+04 SER
O      1.0200E+01  6.6173E-01  7.2141E-17 -3.0903E+05 SER
S      1.0000E-01  1.3003E-02  9.1466E-08 -1.3476E+05 SER

GAS      Status ENTERED      Driving force 0.0000E+00
Moles 3.5300E+01, Mass 2.4661E+02, Volume fraction 1.0000E+00 Mass fractions:
O 6.61734E-01 C 2.43523E-01 H 8.17406E-02 S 1.30027E-02
Constitution:
H2      4.42736E-01  H1O1S1_SOH      3.35036E-14  C4H8_6      1.82465E-21
H2O1     2.15350E-01  C2H6O1_1      2.75193E-14  O2      1.79235E-21
ClO1     1.95778E-01  C2H5      2.60816E-14  C2O1     1.66878E-21
ClO2     1.36417E-01  C3H8      1.55219E-14  S5      8.95084E-22
H2S1     6.57218E-03  C1H3O1_CH2OH  7.69302E-15  C2H2O1   5.16353E-22
ClH4     3.01187E-03  H2O1S1_H2SO   2.59570E-15  C4H6_5   3.26857E-22
ClO1S1    1.34465E-04  C2H3      1.30277E-15  C3H6O1_2 9.94895E-23
H1S1     5.08063E-08  C3H4_2      1.28184E-15  C4H8_4   5.15316E-23
ClH2O1    4.89873E-08  C3O2_2      7.11139E-16  H2O4S1   1.59729E-23
ClH2O2_CIS 4.46604E-08  C3H4_1      3.44164E-16  C4H2_1   8.50232E-24
H2S2     3.75745E-08  H1O1S1_HSO   1.08974E-16  C4H2_2   8.48033E-24
ClS2     1.41821E-08  C3H6_1      5.22179E-17  C6H6O1   6.55562E-24
S2       1.10500E-08  C1H3O1_CH3O   1.80849E-17  H1O2     1.72311E-24
ClH2O2_TRANS 6.42811E-09  C2H6O1_2     9.96672E-18  C2H1     3.18714E-25
C2H6     3.64609E-09  C2H4O1_OXIRA  2.11511E-18  S6       2.65463E-26
C2H4     3.02667E-09  C4H6_2      1.29360E-18  C1H1     5.08634E-27
H        1.51148E-09  S4          1.12104E-18  C4H4_1   4.75003E-27
ClH4O1    1.14083E-09  C4H8_5      6.89221E-19  C3H1     9.91558E-28
O2S1     2.26895E-10  C4H8_1      5.18832E-19  ClH2O2_DIOXI 4.40433E-30
ClH3     1.88514E-10  C4H8_2      4.53214E-19  C      1.00000E-30
ClH4S1    1.76437E-10  C4H8_3      3.93010E-19  C2       1.00000E-30
H2O1S1_HSOH 8.67082E-11  C3H6O1_1     2.60648E-19  C2H4O2_DIOXE 1.00000E-30
C2H4O1_ACETA 2.61120E-11  C2H6O2      2.59417E-19  C2H4O3_123TR 1.00000E-30
C2H2     1.43254E-11  C1H2      2.13894E-19  C2H4O3_124TR 1.00000E-30
O1S1     1.05406E-11  C4H10_1     8.31953E-20  C3       1.00000E-30
ClH1O1    9.19785E-12  C4H10_2     4.22679E-20  C4       1.00000E-30
ClS1     5.40802E-12  C6H6      3.95182E-20  C4H1     1.00000E-30
C2H4O2_ACETI 4.53120E-12  H2O2      2.47048E-20  C5       1.00000E-30
H1O1     1.61961E-12  C4H6_4      1.91129E-20  C6O      1.00000E-30
O1S2     9.69426E-13  O3S1      1.73550E-20  O3       1.00000E-30
ClH1O2    9.05180E-13  C4H6_1     1.14077E-20  S7       1.00000E-30
S        7.19264E-13  O         6.65398E-21  S8       1.00000E-30
S3       1.46179E-13  C4H6_3     6.48690E-21
C3H6_2    1.11399E-13  C4H4_2     3.35580E-21

POLY:Hit RETURN to continue
POLY: s-a-v l t 500 2000 50
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex29 y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 1000.00
...OK

Phase Region from 1000.00 for:
GAS
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global test at 1.28000E+03 .... OK
Global test at 1.38000E+03 .... OK
Global test at 1.48000E+03 .... OK
Global test at 1.58000E+03 .... OK
Global test at 1.68000E+03 .... OK
Global test at 1.78000E+03 .... OK
Global test at 1.88000E+03 .... OK
Global test at 1.98000E+03 .... OK
Terminating at 2000.00
Calculated 103 equilibria

Phase Region from 1000.00 for:
GAS
Global test at 9.20000E+02 .... OK
Global check of adding phase at 8.35809E+02
Calculated 19 equilibria

```

```

Phase Region from      835.809      for:
  GAS
  C_S
Global test at  7.60000E+02 .... OK
Global test at  6.60000E+02 .... OK
Global test at  5.60000E+02 .... OK
Terminating at  500.000
Calculated  37 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex29\tcex29.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

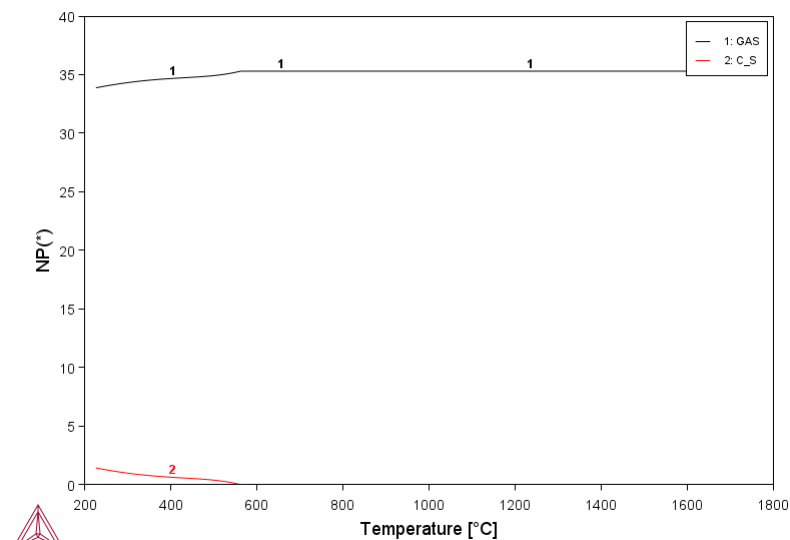
Setting automatic diagram axes

```

POST:
POST: @@ Plot the amount of phases (mainly gas)
POST: s-d-a x t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-l f
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 29a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 29a

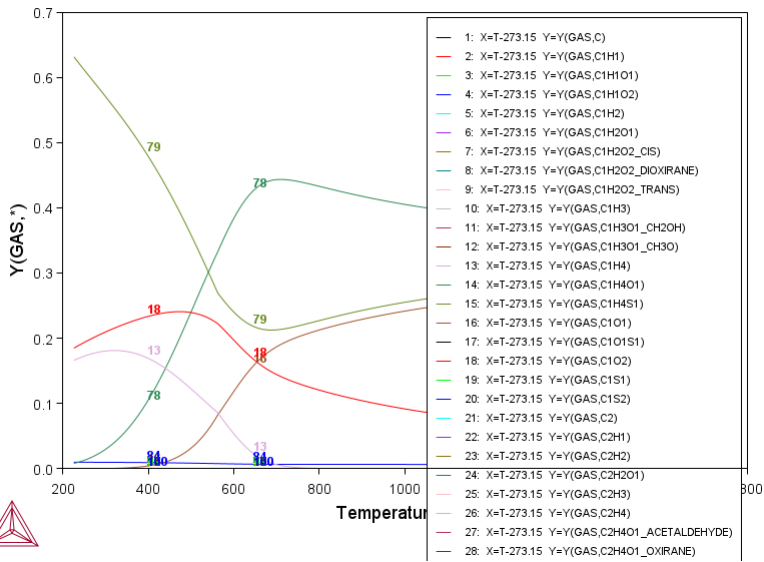


```

POST:
POST: Hit RETURN to continue
POST: @@ Plot gas speciation. y(gas,*) are partial
POST: @@ pressures expressed in bar (as total pressure
POST: @@ is one bar). Set labels on the lines.
POST: s-d-a y y(gas,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 29b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 29b

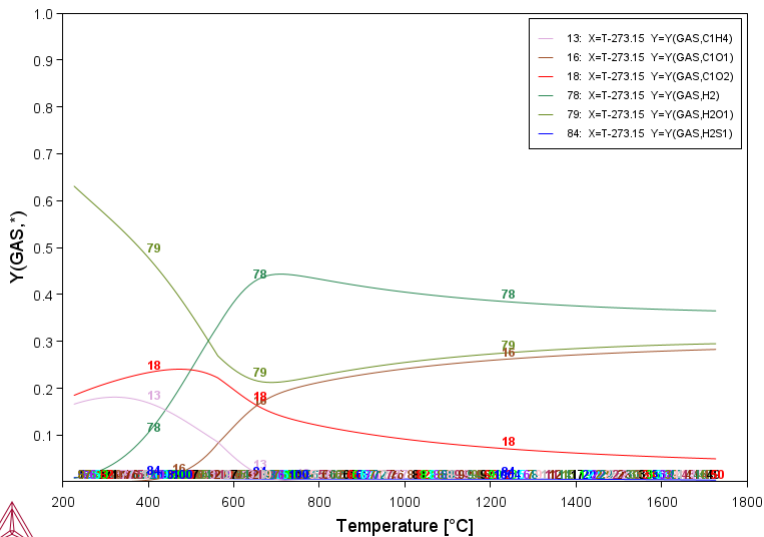


```

POST:Hit RETURN to continue
POST: @@ To avoid cluttered lables, change the scaling
POST: @@ so only major species are visible
POST: s-s y n 0.001 1
... the command in full is SET_SCALING_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 29b

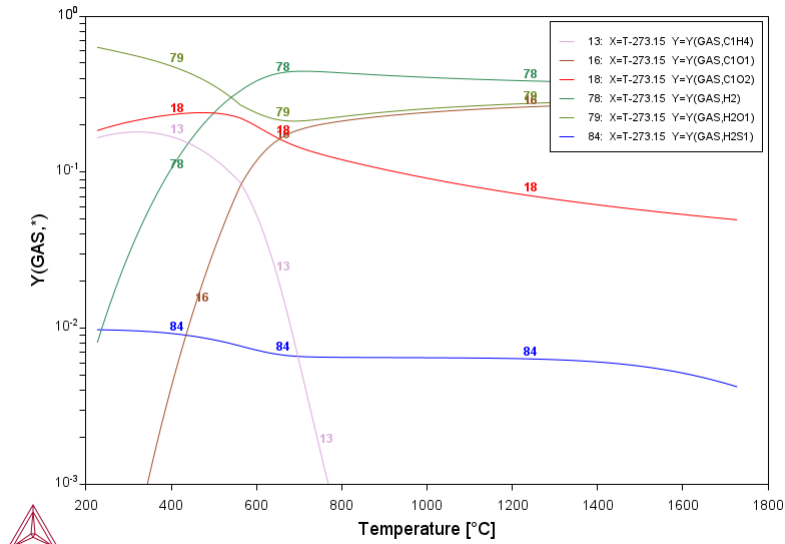


```

POST:Hit RETURN to continue
POST: @@ Set a logarithmic axis
POST: s-ax-ty
... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : y
AXIS TYPE /LINEAR/ : log
POST:
POST: set-title example 29c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 29c

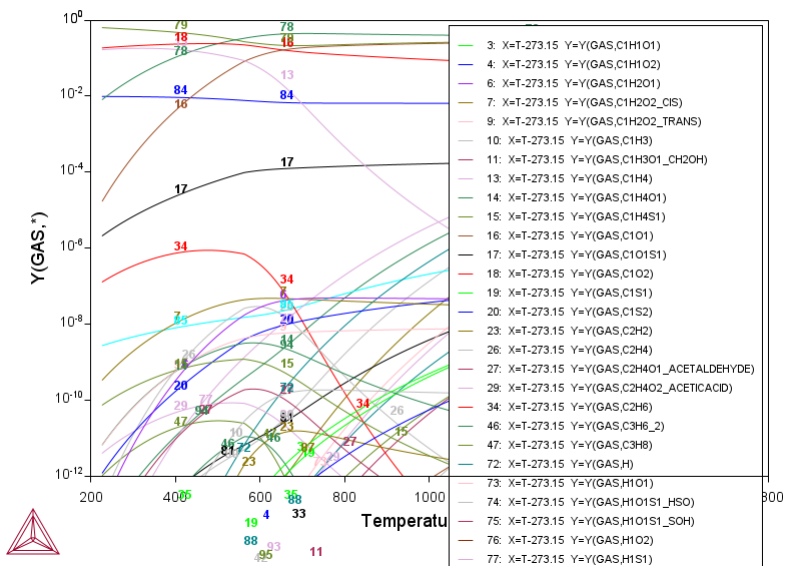


```

POST:
POST:Hit RETURN to continue
POST: @@ Set scaling
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 29d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 29d



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```


tcex30A

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex30A\tcex30A.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Scheil calculation for an Al-4Mg-2Si-2Cu alloy

SYS:

SYS: @@ This is the first of two examples showing how to

SYS: @@ do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy.

SYS: @@ In part A, you use the POLY3 module and the

SYS: @@ STEP_WITH_OPTIONS command with an EVALUATE setting.

SYS: @@ Then in part B you use the SCHEIL module commands to

SYS: @@ do the same thing.

SYS:

SYS: go da

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw user tcex30_cost2.TDB

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

09:17:08,920 [Thread-0] INFO TDBFileParser: USER_200751175_21, number of lines read: 880

09:17:09,435 [Thread-0] INFO DatabaseUtils: Parsing of USER_200751175_21 completed in 613 ms

TDB_USER: def-ele al cu mg si

AL CU

MG

SI DEFINED

TDB_USER: get

09:17:09,665 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_USER: go p-3

POLY version 3.32

POLY: s-c p=101325 n=1 t=1000 w(si)=0.02 w(mg)=0.04 w(cu)=0.02

POLY: c-e

Using global minimization procedure

09:17:10,398 [Thread-0] INFO Database: Preparing system for use: USER_200751175_21

09:17:11,371 [Thread-0] INFO Phase: Preparing phase for use: LIQUID

09:17:11,839 [Thread-0] INFO Phase: Preparing phase for use: AL12MG17

09:17:12,193 [Thread-0] INFO Phase: Preparing phase for use: ALCE_AMORPHOUS

09:17:12,477 [Thread-0] INFO Phase: Preparing phase for use: ALCUZN_T

09:17:12,812 [Thread-0] INFO Phase: Preparing phase for use: ALCU_DELTA

09:17:13,103 [Thread-0] INFO Phase: Preparing phase for use: ALCU_EPSILON

09:17:13,416 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ETA

09:17:13,721 [Thread-0] INFO Phase: Preparing phase for use: ALCU_PRIME

09:17:14,067 [Thread-0] INFO Phase: Preparing phase for use: ALCU_THETA

09:17:14,362 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ZETA

09:17:14,631 [Thread-0] INFO Phase: Preparing phase for use: ALLI

09:17:14,894 [Thread-0] INFO Phase: Preparing phase for use: ALMG_BETA

09:17:15,160 [Thread-0] INFO Phase: Preparing phase for use: ALMG_EPS

09:17:15,435 [Thread-0] INFO Phase: Preparing phase for use: ALMG_GAMMA

09:17:15,810 [Thread-0] INFO Phase: Preparing phase for use: ALMO

09:17:16,100 [Thread-0] INFO Phase: Preparing phase for use: ALM_D019

09:17:16,343 [Thread-0] INFO Phase: Preparing phase for use: ALND_AMORPHOUS

09:17:16,624 [Thread-0] INFO Phase: Preparing phase for use: ALTI

09:17:16,869 [Thread-0] INFO Phase: Preparing phase for use: BCC_B2

09:17:17,108 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2

09:17:17,413 [Thread-0] INFO Phase: Preparing phase for use: BCT_A5

09:17:17,666 [Thread-0] INFO Phase: Preparing phase for use: CBCC_A12

09:17:18,063 [Thread-0] INFO Phase: Preparing phase for use: CR3SI_A15

09:17:18,324 [Thread-0] INFO Phase: Preparing phase for use: CRSI2

09:17:18,668 [Thread-0] INFO Phase: Preparing phase for use: CU19SI6_ETA

09:17:19,075 [Thread-0] INFO Phase: Preparing phase for use: CU33SI7_DELTA

09:17:19,322 [Thread-0] INFO Phase: Preparing phase for use: CU4SI_EPSILON

09:17:19,572 [Thread-0] INFO Phase: Preparing phase for use: CU56SI11_GAMMA

09:17:19,833 [Thread-0] INFO Phase: Preparing phase for use: CU6Y

09:17:20,084 [Thread-0] INFO Phase: Preparing phase for use: CUB_A13

09:17:20,367 [Thread-0] INFO Phase: Preparing phase for use: CUB_A15

09:17:20,635 [Thread-0] INFO Phase: Preparing phase for use: CUMG2

09:17:20,868 [Thread-0] INFO Phase: Preparing phase for use: CUMGSI_SIGMA

09:17:21,125 [Thread-0] INFO Phase: Preparing phase for use: CUMGSI_TAU

09:17:21,356 [Thread-0] INFO Phase: Preparing phase for use: CUZN_GAMMA

09:17:21,620 [Thread-0] INFO Phase: Preparing phase for use: DIAMOND_A4

09:17:21,881 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1

09:17:22,197 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_D83

09:17:22,456 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_H

09:17:22,810 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3

09:17:23,064 [Thread-0] INFO Phase: Preparing phase for use: HCP_ZN

09:17:23,361 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C14

09:17:23,628 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C15

09:17:23,922 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C36

09:17:24,167 [Thread-0] INFO Phase: Preparing phase for use: MG24Y5

09:17:24,455 [Thread-0] INFO Phase: Preparing phase for use: MG2SI

09:17:24,773 [Thread-0] INFO Phase: Preparing phase for use: MG2Y

09:17:25,008 [Thread-0] INFO Phase: Preparing phase for use: MG2ZN11

09:17:25,280 [Thread-0] INFO Phase: Preparing phase for use: MG2ZN3

09:17:25,512 [Thread-0] INFO Phase: Preparing phase for use: MGY_GAMMA

```

09:17:25,751 [Thread-0] INFO Phase: Preparing phase for use: MGZN
09:17:26,035 [Thread-0] INFO Phase: Preparing phase for use: PHI
09:17:26,269 [Thread-0] INFO Phase: Preparing phase for use: QPHASE
09:17:26,500 [Thread-0] INFO Phase: Preparing phase for use: SIV3
09:17:26,794 [Thread-0] INFO Phase: Preparing phase for use: SPHASE
09:17:27,034 [Thread-0] INFO Phase: Preparing phase for use: TAU
09:17:27,346 [Thread-0] INFO Phase: Preparing phase for use: VPHASE
Calculated 26538 grid points in 17.376 s
Found the set of lowest grid points in 0.006 s
Calculated POLY solution 0.172 s, total time 17.554 s
POLY: l-e,,
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=101325, N=1, T=1000, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01
Total Gibbs energy -4.56562E+04, Enthalpy 3.06144E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              9.2731E-01  9.2000E-01  5.4982E-03 -4.3263E+04 SER
CU              8.5596E-03  2.0000E-02  5.9020E-07 -1.1925E+05 SER
MG              4.4759E-02  4.0000E-02  1.0064E-04 -7.6526E+04 SER
SI              1.9367E-02  2.0000E-02  1.1370E-03 -5.6367E+04 SER

LIQUID          Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:
AL 9.20000E-01 MG 4.00000E-02 CU 2.00000E-02 SI 2.00000E-02
POLY: @@ calculate liquidus temperature in order to choose
POLY: @@ a starting temperature where only liquid exists
POLY: c-st phase fcc_al=fix 0
POLY: s-c t=none
POLY: c-e
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 26538 grid points in 0.114 s
12 ITS, CPU TIME USED 1 SECONDS
POLY: l-e,,
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=101325, N=1, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
FIXED PHASES
FCC_A1=0
DEGREES OF FREEDOM 0

Temperature 897.74 K ( 624.59 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01
Total Gibbs energy -3.80281E+04, Enthalpy 2.73862E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              9.2731E-01  9.2000E-01  8.2190E-03 -3.5838E+04 SER
CU              8.5596E-03  2.0000E-02  5.5836E-07 -1.0747E+05 SER
MG              4.4759E-02  4.0000E-02  1.2754E-04 -6.6933E+04 SER
SI              1.9367E-02  2.0000E-02  2.2867E-03 -4.5388E+04 SER

LIQUID          Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:
AL 9.20000E-01 MG 4.00000E-02 SI 2.00000E-02 CU 2.00000E-02

FCC_A1          Status FIXED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
AL 9.85194E-01 MG 1.12509E-02 CU 1.91685E-03 SI 1.63879E-03
POLY: show t
T=897.74074
POLY:Hit RETURN to continue
POLY: s-c t
Value /897.7407448/: 900
POLY: c-st phase
Phase name(s): fcc_al
Status: /ENTERED/: ENTERED
Start value, number of mole formula units /0/: 0
POLY: c-e
Using global minimization procedure
Calculated 26538 grid points in 0.122 s
Found the set of lowest grid points in 0.007 s
Calculated POLY solution 0.061 s, total time 0.190 s
POLY: l-e,,
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=101325, N=1, T=900, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
DEGREES OF FREEDOM 0

Temperature 900.00 K ( 626.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01
Total Gibbs energy -3.81928E+04, Enthalpy 2.74567E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              9.2731E-01  9.2000E-01  8.1424E-03 -3.5998E+04 SER
CU              8.5596E-03  2.0000E-02  5.5930E-07 -1.0773E+05 SER
MG              4.4759E-02  4.0000E-02  1.2687E-04 -6.7141E+04 SER
SI              1.9367E-02  2.0000E-02  2.2488E-03 -4.5627E+04 SER

LIQUID          Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:
AL 9.20000E-01 MG 4.00000E-02 SI 2.00000E-02 CU 2.00000E-02
POLY: s-a-v 1 t
Min value /0/: 750 900 1
POLY:
POLY: ent var nl=1;
POLY: ent var nfcc=0;
POLY: ent var nl=np(liquid)*nl;
POLY: ent fun ns=l-nl;
POLY: ent var nfcc=nfcc+nl*np(fcc_al);
POLY: ent var wsi=w(liquid,si);
POLY: ent var wmg=w(liquid,mg);
POLY: ent var wcu=w(liquid,cu);
POLY: ent tab tab1

```

```

Variable(s): t nl ns nfcc
&
POLY: s-c w (si)=wsi w (mg)=wmg w (cu)=wcu
POLY: save tcex30a y
POLY:
POLY: step
Option? /NORMAL/: eva
Variable name(s): wsi wmg wcu
No initial equilibrium, using default
...OK

Phase Region from 900.000 for:
LIQUID
Global check of adding phase at 8.97741E+02
Calculated 5 equilibria

Phase Region from 897.741 for:
LIQUID
FCC_A1
Global test at 8.90000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 8.70000E+02 .... OK
Global test at 8.60000E+02 .... OK
Global check of adding phase at 8.57875E+02
Calculated 43 equilibria

Phase Region from 857.875 for:
LIQUID
FCC_A1
MG2SI
Global test at 8.50000E+02 .... OK
Global test at 8.40000E+02 .... OK
Global test at 8.30000E+02 .... OK
Global test at 8.20000E+02 .... OK
Global test at 8.10000E+02 .... OK
Global test at 8.00000E+02 .... OK
Global test at 7.90000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global check of adding phase at 7.78888E+02
Calculated 82 equilibria

Phase Region from 778.888 for:
LIQUID
ALCU_THETA
FCC_A1
MG2SI
Global check of adding phase at 7.73208E+02
Calculated 8 equilibria

Phase Region from 773.208 for:
LIQUID
ALCU_THETA
DIAMOND_A4
FCC_A1
MG2SI
Calculated 2 equilibria

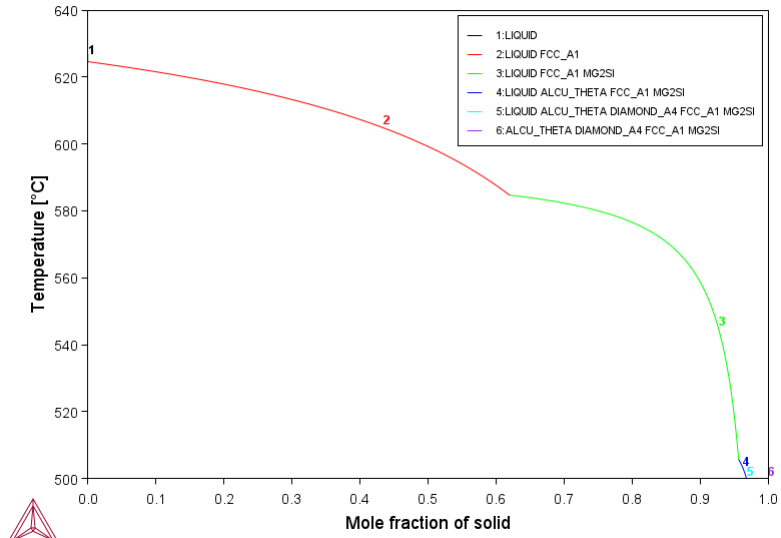
Phase Region from 773.208 for:
ALCU_THETA
DIAMOND_A4
FCC_A1
MG2SI
Global test at 7.66000E+02 .... OK
Global test at 7.56000E+02 .... OK
Terminating at 750.000
Calculated 27 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex30A\tcex30a.POLY3
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x tab1
COLUMN NUMBER /*/: 3
POST: s-d-a y t-c
POST:
POST: s-s-s y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 500 640
POST: s-lab b
POST: se-ax-te x n
AXIS TEXT : Mole fraction of solid
POST: set-title example 30Aa
POST: plot

```

example 30Aa



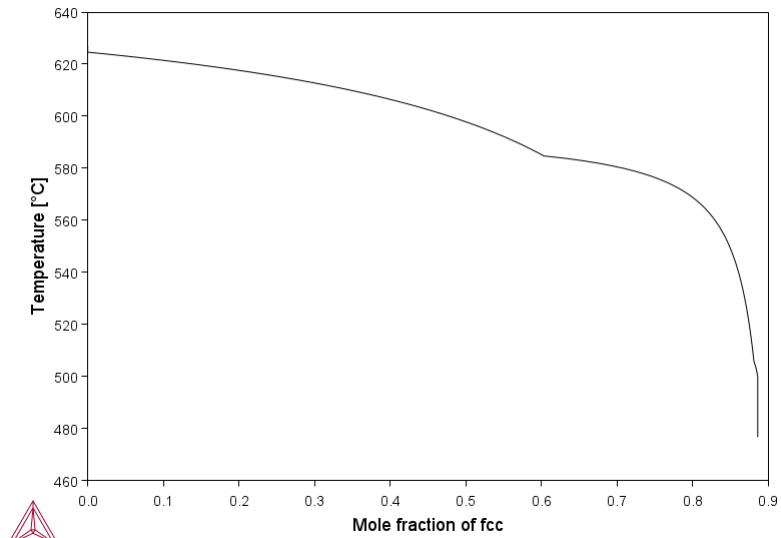
```

POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST:Hit RETURN to continue
POST: back
POLY: read,,
POLY: po
      POLY-3 POSTPROCESSOR VERSION 3.2

      Setting automatic diagram axes

POST: s-d-a x tab1
COLUMN NUMBER /*/: 4
POST: s-d-a y t-c
POST: se-ax-te x n
AXIS TEXT : Mole fraction of fcc
POST: set-title example 30Ab
POST:
POST: plot
  
```

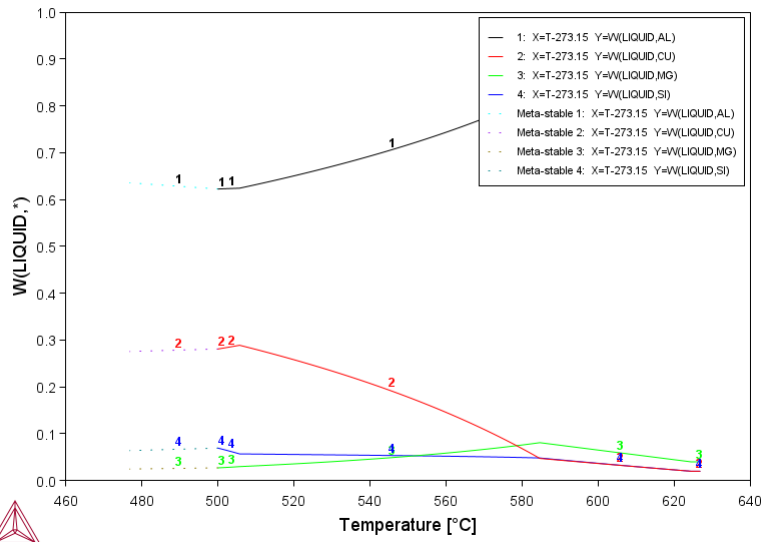
example 30Ab



```

POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST:Hit RETURN to continue
POST: s-d-a x t-c
POST: s-d-a y w(liquid,*),,
POST: set-title example 30Ac
POST: s-l d
POST:
POST: plot
  
```

example 30Ac



POST: SET_EXP_FILE_FORMAT 5
 POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 POST: SET_EXP_FILE_FORMAT 10
 POST:
 POST:
 POST: set-inter
 POST:

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex30B\tcex30B.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Scheil calculation for an Al-4Mg-2Si-2Cu alloy

SYS:

SYS: @@ This is the second of two examples showing how to

SYS: @@ do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy.

SYS: @@ In part A, you used the POLY3 module and the

SYS: @@ STEP_WITH_OPTIONS command with an Evaluate setting.

SYS:

SYS: @@ This is part B where you use the SCHEIL module commands

SYS: @@ to do the same thing.

SYS:

SYS: go scheil

SCHEIL: start

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: user tcex30_cost2.TDB

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

09:18:57,005 [Thread-0] INFO TDBFileParser: USER_796321178_21, number of lines read: 880

09:18:57,495 [Thread-0] INFO DatabaseUtils: Parsing of USER_796321178_21 completed in 570 ms

Major element or alloy: al

Composition input in mass (weight) percent? /Y/:

1st alloying element: mg 4 si 2 cu 2

Next alloying element:

Temperature (C) /2000/: 800

VA /- DEFINED

REINITIATING GES

AL DEFINED

MG DEFINED

SI DEFINED

CU DEFINED

This database has following phases for the defined system

LIQUID:L	AL12MG17	ALCE_AMORPHOUS
ALCUZN_T	ALCU_DELTA	ALCU_EPSILON
ALCU_ETA	ALCU_PRIME	ALCU_THETA
ALCU_ZETA	ALLI	ALMG_BETA
ALMG_EPS	ALMG_GAMMA	ALMO
ALM_D019	ALND_AMORPHOUS	ALTI
BCC_A2	BCC_B2	BCT_A5
CBCC_A12	CR3SI_A15	CRSI2
CU19SI6_ETA	CU33SI7_DELTA	CU4SI_EPSILON
CU56SI11_GAMMA	CU6Y	CUB_A13
CUB_A15	CUMG2	CUMGSI_SIGMA
CUMGSI_TAU	CUZN_GAMMA	DIAMOND_A4
FCC_A1	GAMMA_D83	GAMMA_H
HCP_A3	HCP_ZN	LAVES_C14
LAVES_C15	LAVES_C36	MG24Y5
MG2SI	MG2Y	MG2ZN11
MG2ZN3	MGY_GAMMA	MGZN
PHI	QPHASE	SIV3
SPHASE	TAU	VPHASE

Reject phase(s) /NONE/: *

LIQUID:L	AL12MG17	ALCE_AMORPHOUS
ALCUZN_T	ALCU_DELTA	ALCU_EPSILON
ALCU_ETA	ALCU_PRIME	ALCU_THETA
ALCU_ZETA	ALLI	ALMG_BETA
ALMG_EPS	ALMG_GAMMA	ALMO
ALM_D019	ALND_AMORPHOUS	ALTI
BCC_A2	BCC_B2	BCT_A5
CBCC_A12	CR3SI_A15	CRSI2
CU19SI6_ETA	CU33SI7_DELTA	CU4SI_EPSILON
CU56SI11_GAMMA	CU6Y	CUB_A13
CUB_A15	CUMG2	CUMGSI_SIGMA
CUMGSI_TAU	CUZN_GAMMA	DIAMOND_A4
FCC_A1	GAMMA_D83	GAMMA_H
HCP_A3	HCP_ZN	LAVES_C14
LAVES_C15	LAVES_C36	MG24Y5
MG2SI	MG2Y	MG2ZN11
MG2ZN3	MGY_GAMMA	MGZN
PHI	QPHASE	SIV3
SPHASE	TAU	VPHASE

Restore phase(s):: liquid fcc_a1 alcu_th mg2si diamond_a4 all12mg17

LIQUID:L FCC_A1 ALCU_THETA

MG2SI DIAMOND_A4 AL12MG17

RESTORED

Restore phase(s): /NONE/:

.....

The following phases are retained in this system:

LIQUID:L	AL12MG17	ALCU_THETA
DIAMOND_A4	FCC_A1	MG2SI

```

.....
OK? /Y/: Y
09:18:57,729 [Thread-0] INFO   JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Should any phase have a miscibility gap check? /N/: N
09:18:58,146 [Thread-0] INFO   Database: Preparing system for use: USER_796321178_21
09:18:59,158 [Thread-0] INFO   Phase: Preparing phase for use: LIQUID
09:18:59,603 [Thread-0] INFO   Phase: Preparing phase for use: AL12MG17
09:18:59,976 [Thread-0] INFO   Phase: Preparing phase for use: ALCU_THETA
09:19:00,269 [Thread-0] INFO   Phase: Preparing phase for use: DIAMOND_A4
09:19:00,607 [Thread-0] INFO   Phase: Preparing phase for use: FCC_A1
09:19:00,925 [Thread-0] INFO   Phase: Preparing phase for use: MG2SI
LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/:
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=1073.15, W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=100000, N=1
DEGREES OF FREEDOM 0
PHASE CHANGE AT 897.740742588
FCC_A1#1 forms
Testing POLY result by global minimization procedure
Calculated      5945 grid points in      0.030 s
CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

Phase Region from      897.831      for:
LIQUID
Terminating at      897.931
Calculated      4 equilibria

Phase Region from      897.831      for:
LIQUID
Global check of adding phase at      8.97741E+02
Calculated      3 equilibria

Phase Region from      897.741      for:
LIQUID
FCC_A1
Global test at      8.89831E+02 .... OK
Global test at      8.79831E+02 .... OK
Global test at      8.69831E+02 .... OK
Global test at      8.59831E+02 .... OK
Global check of adding phase at      8.57535E+02
Calculated      43 equilibria

Phase Region from      857.535      for:
LIQUID
FCC_A1
MG2SI
Global test at      8.49831E+02 .... OK
Global test at      8.39831E+02 .... OK
Global test at      8.29831E+02 .... OK
Global check of removing phase at      8.26196E+02
Calculated      34 equilibria

Phase Region from      826.196      for:
FCC_A1
MG2SI
Calculated      4 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_5608.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_5608.EXP
has been created to store the equilibrium solidification results.
CALCULATING SCHEIL SOLIDIFICATION
T(C)      fraction solid
624.6807      0.000000
PHASE REGION:LIQUID + FCC_A1
T(C)      fraction solid
624.5851      0.2038889E-03
623.5851      0.3538798E-01
622.5851      0.6842453E-01
621.5851      0.9949709E-01
620.5851      0.1287693
619.5851      0.1563873
618.5851      0.1824824
617.5851      0.2071723
616.5851      0.2305634
615.5851      0.2527515
614.5851      0.2738237
613.5851      0.2938587
612.5851      0.3129285
611.5851      0.3310983
610.5851      0.3484280
609.5851      0.3649722
608.5851      0.3807809
607.5851      0.3959003
606.5851      0.4103725
605.5851      0.4242366
604.5851      0.4375286
603.5851      0.4502817
602.5851      0.4625266
601.5851      0.4742918
600.5851      0.4856038
599.5851      0.4964872
598.5851      0.5069647
597.5851      0.5170577
596.5851      0.5267860
595.5851      0.5361681
594.5851      0.5452213

```

593.5851	0.5539619
592.5851	0.5624050
591.5851	0.5705648
590.5851	0.5784547
589.5851	0.5860871
588.5851	0.5934739
587.5851	0.6006261
586.5851	0.6075542
585.5851	0.6142679

PHASE REGION:LIQUID + FCC_A1 + MG2SI

T(C)	fraction solid
584.7245	0.6199090
583.7245	0.6576760
582.7245	0.6886411
581.7245	0.7144754
580.7245	0.7363465
579.7245	0.7550939
578.7245	0.7713365
577.7245	0.7855406
576.7245	0.7980640
575.7245	0.8091857
574.7245	0.8191265
573.7245	0.8280633
572.7245	0.8361395
571.7245	0.8434725
570.7245	0.8501596
569.7245	0.8562816
568.7245	0.8619067
567.7245	0.8670925
566.7245	0.8718879
565.7245	0.8763351
564.7245	0.8804703
563.7245	0.8843250
562.7245	0.8879265
561.7245	0.8912987
560.7245	0.8944628
559.7245	0.8974371
558.7245	0.9002382
557.7245	0.9028806
556.7245	0.9053773
555.7245	0.9077400
554.7245	0.9099790
553.7245	0.9121039
552.7245	0.9141230
551.7245	0.9160440
550.7245	0.9178738
549.7245	0.9196187
548.7245	0.9212845
547.7245	0.9228765
546.7245	0.9243993
545.7245	0.9258573
544.7245	0.9272547
543.7245	0.9285951
542.7245	0.9298819
541.7245	0.9311183
540.7245	0.9323071
539.7245	0.9334511
538.7245	0.9345527
537.7245	0.9356142
536.7245	0.9366378
535.7245	0.9376256
534.7245	0.9385793
533.7245	0.9395007
532.7245	0.9403914
531.7245	0.9412529
530.7245	0.9420867
529.7245	0.9428941
528.7245	0.9436762
527.7245	0.9444344
526.7245	0.9451697
525.7245	0.9458831
524.7245	0.9465756
523.7245	0.9472482
522.7245	0.9479016
521.7245	0.9485367
520.7245	0.9491543
519.7245	0.9497551
518.7245	0.9503399
517.7245	0.9509091
516.7245	0.9514636
515.7245	0.9520038
514.7245	0.9525303
513.7245	0.9530437
512.7245	0.9535444
511.7245	0.9540330
510.7245	0.9545099
509.7245	0.9549755
508.7245	0.9554302
507.7245	0.9558745
506.7245	0.9563086

PHASE REGION:LIQUID + ALCU_THETA + FCC_A1 + MG2SI

T(C)	fraction solid
505.7364	0.9567319
504.7364	0.9594803
503.7364	0.9618348
502.7364	0.9638799
501.7364	0.9656767
500.7364	0.9672706
500.0670	0.9682413

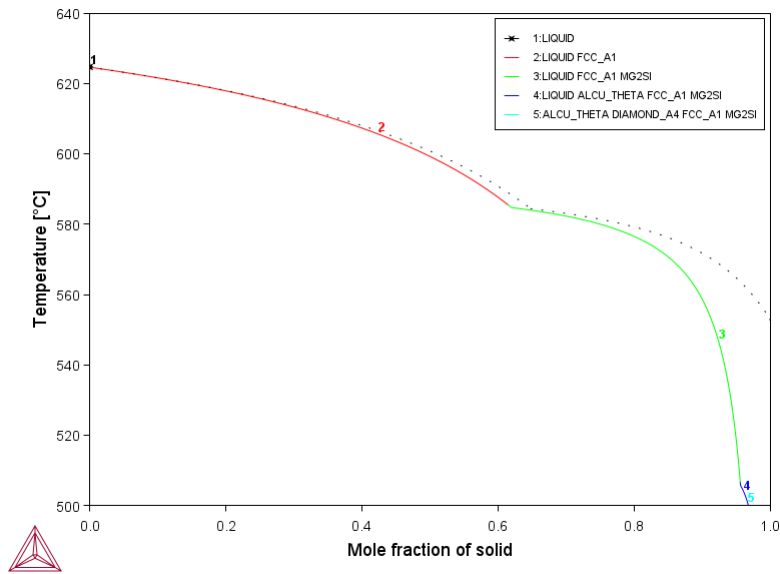
PHASE REGION:ALCU_THETA + DIAMOND_A4 + FCC_A1 + MG2SI

T(C)	fraction solid
500.0351	1.000000

Calculating properties ...

Liquidus temperature: 897.741 K

Solidus temperature: 773.185 K

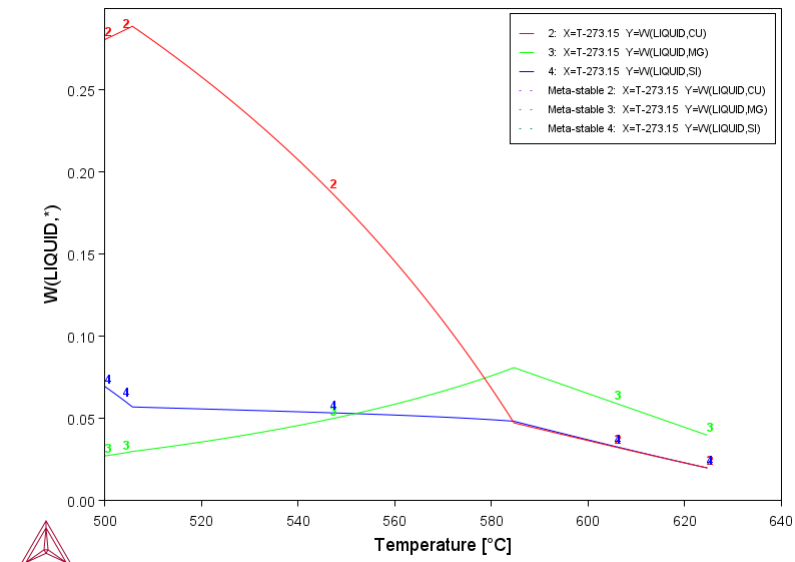


The following axis variables are available

T - Temperature in Celsius
 NL/BL/VL - Mole/mass/volume fraction of liquid
 NS/BS/VS - Mole/mass/volume fraction of all solid phases
 NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
 VS(ph) - Volume fraction of a solid phase
 W(ph,el) - Weight fraction of an element in a phase
 X(ph,el) - Mole fraction of an element in a phase
 Y(ph,el) - Site fraction of an element in a phase
 NN(ph,el) - Distribution of an element in a phase
 NH/BH - Heat release and Latent heat per mole/gram
 CP/BCP - Apparent heat capacity per mole/gram
 NV/NV(ph) - Molar volume of the system or a phase
 DS/DS(ph) - Average density of the system or a phase
 BT - Apparent volumetric TEC of the system
 DVIS(ph) - Dynamic viscosity of a phase
 KVIS(ph) - Kinematic viscosity of a phase
 SURF(ph) - Surface tension of a liquid phase
 ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
 ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
 THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
 "*" can be used as a wild character for "el" and "ph"

POST:
 POST: Hit RETURN to continue
 POST: s-d-a x t
 POST: s-d-a y w(liquid,*),,,,,,
 POST: s-s-s y n 0 0.3
 POST: set-lab F
 POST:
 POST: SET_EXP_FILE_FORMAT 5
 POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 POST: SET_EXP_FILE_FORMAT 10
 POST:
 POST: plot,,,,



POST:
POST: set-inter
POST:

tcex31

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tcex31.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Using the GES module to calculate CVM

SYS:

SYS: @@ This example calculates the CVM and compares it with the

SYS: @@ sublattices of a fictitious A B system. You also learn how

SYS: @@ to overlay diagrams from two calculations.

SYS:

SYS: @@ This example uses some GES commands that are not yet

SYS: @@ supported by GES6. Therefore, we enforce the use of GES5.

SYS: set-ges-version 5

SYS:

SYS: set-log ex31,,,

SYS:

SYS: go g

... the command in full is GOTO_MODULE

GIBBS ENERGY SYSTEM

GES5:

GES5: @@ Enter the elements and the reference states

GES5: e-e A B

... the command in full is ENTER_ELEMENT

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

GES5: a-e-d A

... the command in full is AMEND_ELEMENT_DATA

NEW STABLE ELEMENT REFERENCE /UNKNOWN/: FCC

NEW ATOMIC MASS /0/: 10

NEW H(298.15)-H(0) /0/: 0

NEW S(298.15) /0/: 0

Default element reference state symbol index /1/: 1

GES5: a-e-d B

... the command in full is AMEND_ELEMENT_DATA

NEW STABLE ELEMENT REFERENCE /BETA_RHOMBO_B/: FCC

NEW ATOMIC MASS /10.811/: 10

NEW H(298.15)-H(0) /1222/: 0

NEW S(298.15) /5.9/: 0

Default element reference state symbol index /1/: 1

GES5:

GES5: @@ =====

GES5: @@ These species represent the clusters. 4 clusters A3B are

GES5: @@ needed as the B atom can be on 4 different sublattices etc.

GES5:

GES5: e-sp S0 A

... the command in full is ENTER_SPECIES

GES5: e-sp S11 A.75B.25

... the command in full is ENTER_SPECIES

GES5: e-sp S12 A.75B.25

... the command in full is ENTER_SPECIES

GES5: e-sp S13 A.75B.25

... the command in full is ENTER_SPECIES

GES5: e-sp S14 A.75B.25

... the command in full is ENTER_SPECIES

GES5: e-sp S21 A.5B.5

... the command in full is ENTER_SPECIES

GES5: e-sp S22 A.5B.5

... the command in full is ENTER_SPECIES

GES5: e-sp S23 A.5B.5

... the command in full is ENTER_SPECIES

GES5: e-sp S24 A.5B.5

... the command in full is ENTER_SPECIES

GES5: e-sp S25 A.5B.5

... the command in full is ENTER_SPECIES

GES5: e-sp S26 A.5B.5

... the command in full is ENTER_SPECIES

GES5: e-sp S31 A.25B.75

... the command in full is ENTER_SPECIES

GES5: e-sp S32 A.25B.75

... the command in full is ENTER_SPECIES

GES5: e-sp S33 A.25B.75

... the command in full is ENTER_SPECIES

GES5: e-sp S34 A.25B.75

... the command in full is ENTER_SPECIES

GES5: e-sp S4 B

... the command in full is ENTER_SPECIES

GES5:

GES5: @@ =====

GES5: @@ This function describes the bond energy A-B at equiatomic

GES5: @@ composition.

GES5: e-sy fun UIJ

... the command in full is ENTER_SYMBOL

LOW TEMPERATURE LIMIT /298.15/: 298.15

FUNCTION: -100*R;

HIGH TEMPERATURE LIMIT /6000/: 6000

ANY MORE RANGES /N/: N

GES5:

GES5: @@ These functions describe the end-member energies at

GES5: @@ A3B, A2B2 and AB3 respectively.

GES5: @@ In the simplest case, like here, they are just the

GES5: @@ bond energy multiplied with 3, 4 and 3, respectively.

```

GES5: e-sy fun GA3B1,,3*UIJ,,,
... the command in full is ENTER_SYMBOL
GES5: e-sy fun GA2B2,,4*UIJ,,,
... the command in full is ENTER_SYMBOL
GES5: e-sy fun GA1B3,,3*UIJ,,,
... the command in full is ENTER_SYMBOL
GES5:
GES5: @@ =====
GES5: @@ This is the FCC phase with CVM for both LRO and SRO
GES5: e-ph CVM_TET
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S4
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES5: E-PAR G(C,S11),,GA3B1,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S12),,GA3B1,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S13),,GA3B1,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S14),,GA3B1,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S21),,GA2B2,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S22),,GA2B2,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S23),,GA2B2,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S24),,GA2B2,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S25),,GA2B2,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S26),,GA2B2,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S31),,GA1B3,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(C,S32),,GA1B3,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(C,S33),,GA1B3,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(C,S34),,GA1B3,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: l-d,,,
... the command in full is LIST_DATA

```

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT DATE 2025- 5-12
FROM DATABASE: User data 2025.05.12

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT REFERENCE	MASS	H298-H0	S298
1 A	FCC		1.0000E+01	0.0000E+00	0.0000E+00
2 B	FCC		1.0000E+01	0.0000E+00	0.0000E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 S0	A
4 S11	A0.75B0.25
5 S12	A0.75B0.25
6 S13	A0.75B0.25
7 S14	A0.75B0.25
8 S21	A0.5B0.5
9 S22	A0.5B0.5
10 S23	A0.5B0.5
11 S24	A0.5B0.5
12 S25	A0.5B0.5
13 S26	A0.5B0.5
14 S31	A0.25B0.75
15 S32	A0.25B0.75
16 S33	A0.25B0.75
17 S34	A0.25B0.75
18 S4	B

CVM_TET
CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
S4

```

G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3

```

```

G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

```

```

SYMBOL      STATUS      VALUE/FUNCTION
FUNCTION R      298.15      8.314510000000000      ; 6000 N REF0 !
  2 RTLN      20000000 +R*T*LN(1E-05*P)
103 UIJ      20000000 -100*R
104 GA3B1      20000000 +3*UIJ
105 GA2B2      20000000 +4*UIJ
106 GA1B3      20000000 +3*UIJ

```

```

GES5:
GES5:Hit RETURN to continue
GES5:
GES5: @@ =====
GES5: @@ This is an FCC phase with no SRO but LRO
GES5: @@ described with the sublattice model
GES5:

```

```

GES5: E-PH LRO
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 4
NUMBER OF SITES IN SUBLATTICE 1 /1/: .25
NUMBER OF SITES IN SUBLATTICE 2 /1/: .25
NUMBER OF SITES IN SUBLATTICE 3 /1/: .25
NUMBER OF SITES IN SUBLATTICE 4 /1/: .25
CONSTITUENTS IN SUBLATTICE 1
NAME OF CONSTITUENT: A B;
CONSTITUENTS IN SUBLATTICE 2
NAME OF CONSTITUENT: A B;
CONSTITUENTS IN SUBLATTICE 3
NAME OF CONSTITUENT: A B;
CONSTITUENTS IN SUBLATTICE 4
NAME OF CONSTITUENT: A B;
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO

```

```

GES5:
GES5: E-PAR G(L,A:A:A:B),,GA3B1,,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,A:A:B:A),,GA3B1,,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,B:A:A:A),,GA3B1,,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,A:B:B:B),,GA1B3,,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:B:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(L,B:A:B:B),,GA1B3,,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(L,B:B:A:B),,GA1B3,,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:A:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(L,A:A:B:B),,GA2B2,,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,A:B:A:B),,GA2B2,,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,B:A:A:B),,GA2B2,,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:A:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,A:B:B:A),,GA2B2,,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,B:A:B:A),,GA2B2,,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,B:B:A:A),,GA2B2,,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: 1-p-d lro
... the command in full is LIST_PHASE_DATA

```

```

LRO
EXCESS MODEL IS REDLICH-KISTER MUGGIANU
4 SUBLATTICES, SITES .25: .25: .25: .25
CONSTITUENTS: A,B : A,B : A,B : A,B

```

```

G(LRO,A:A:A:A;0)-G(FCC,A;0) = 0.0
G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:B:A;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,B:B:B;0)-G(FCC,B;0) = 0.0

```

```

GES5:
GES5: @@ =====
GES5: @@ This is the FCC phase with no SRO and no LRO. The regular
GES5: @@ parameter is simply 12 times the bond energy as the ;1 and ;2
GES5: @@ parameters cancel when GA1B3=GA3B1=0.75*GA2B2
GES5:
GES5: e-ph fcc_a1
... the command in full is ENTER_PHASE

```

```

TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES5:
GES5: e-par 1(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;0)
GES5: e-par 1(fcc,a,b;1),,2*GA3B1-2*GA1B3;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;1)
GES5: e-par 1(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;2)
GES5: l-p-d fcc
... the command in full is LIST_PHASE_DATA

FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3
GES5:
GES5: @@ Finally, add together the LRO phase with the disordered FCC
GES5: @@ Note that the parameters in LRO give zero contribution
GES5: @@ when the phase is disordered
GES5:
GES5: amend-phase LRO dis FCC
... the command in full is AMEND_PHASE_DESCRIPTION
GES5:
GES5: @@
GES5: @@ This is the way to set CVM entropy calculation
GES5: am-ph cvm stat 02204030
... the command in full is AMEND_PHASE_DESCRIPTION
GES5:
GES5: l-p-d cvm
... the command in full is LIST_PHASE_DATA

CVM_TET
$ CVM-SRO ENTROPY CONTRIBUTION
CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
S4

G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0
GES5:
GES5:Hit RETURN to continue
GES5:
GES5: @@ We need 3 CVM phases for the L10, L12 and disordered states
GES5: am-ph cvm
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
Creating a new composition set CVM_TET#2
GIVE FOR COMPOSITION SET 2
Major constituent(s) for sublattice 1: /$/: s11
Creating a new composition set CVM_TET#2
GIVE FOR COMPOSITION SET 3
Major constituent(s) for sublattice 1: /$/: none
GES5:
GES5: am-ph cvm maj
... the command in full is AMEND_PHASE_DESCRIPTION
Composition set /1/: 1
Major constituent(s) for sublattice 1: /S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S/: S25
GES5:
GES5: @@ Also for the sublattice phase we need 3 composition sets
GES5: am-ph lro
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
Creating a new composition set LRO#2
GIVE FOR COMPOSITION SET 2
Major constituent(s) for sublattice 1: /A B/: *
Major constituent(s) for sublattice 2: /A B/: *
Major constituent(s) for sublattice 3: /A B/: *
Major constituent(s) for sublattice 4: /A B/: *
Creating a new composition set LRO#2
GIVE FOR COMPOSITION SET 3
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: B
Major constituent(s) for sublattice 4: /A B/: B
GES5: am-ph lro
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: maj
Composition set /1/: 1
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: A
Major constituent(s) for sublattice 4: /A B/: B
GES5:

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```

GES5: l-d,,,,
... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT      DATE 2025- 5-12
FROM DATABASE: User data 2025.05.12

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT STABLE ELEMENT REFERENCE  MASS          H298-H0      S298
1 A    FCC                    1.0000E+01  0.0000E+00  0.0000E+00
2 B    FCC                    1.0000E+01  0.0000E+00  0.0000E+00

SPECIES                                STOICHIOMETRY
1 A                                A
2 B                                B
3 S0                               A
4 S11                             A0.75B0.25
5 S12                             A0.75B0.25
6 S13                             A0.75B0.25
7 S14                             A0.75B0.25
8 S21                             A0.5B0.5
9 S22                             A0.5B0.5
10 S23                            A0.5B0.5
11 S24                            A0.5B0.5
12 S25                            A0.5B0.5
13 S26                            A0.5B0.5
14 S31                            A0.25B0.75
15 S32                            A0.25B0.75
16 S33                            A0.25B0.75
17 S34                            A0.25B0.75
18 S4                              B

CVM_TET
$ CVM-SRO ENTROPY CONTRIBUTION
  CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
  S4

  G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
  G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  CONSTITUENTS: A,B

  G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
  G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
  L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
  L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
  L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3

LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES .25: .25: .25: .25
  CONSTITUENTS: A,B : A,B : A,B : A,B

  G(LRO,A:A:A:A;0) = 0.0
  G(LRO,B:A:A:A;0) = +GA3B1
  G(LRO,A:B:A:A;0) = +GA3B1
  G(LRO,B:B:A:A;0) = +GA2B2
  G(LRO,A:A:B:A;0) = +GA3B1
  G(LRO,B:A:B:A;0) = +GA2B2
  G(LRO,A:B:B:A;0) = +GA2B2
  G(LRO,B:B:B:A;0) = +GA1B3
  G(LRO,A:A:A:B;0) = +GA3B1
  G(LRO,B:A:A:B;0) = +GA2B2
  G(LRO,A:B:A:B;0) = +GA2B2
  G(LRO,B:B:A:B;0) = +GA1B3
  G(LRO,A:A:B:B;0) = +GA2B2
  G(LRO,B:A:B:B;0) = +GA1B3
  G(LRO,A:B:B:B;0) = +GA1B3
  G(LRO,B:B:B:B;0) = 0.0

SYMBOL      STATUS      VALUE/FUNCTION
FUNCTION R   298.15      8.314510000000000 ; 6000 N REF0 !
2 RTLNPN    20000000 +R*T*LN(1E-05*P)
103 UIJ     20000000 -100*R
104 GA3B1    20000000 +3*UIJ
105 GA2B2    20000000 +4*UIJ
106 GA1B3    20000000 +3*UIJ

GES5:Hit RETURN to continue
GES5:
GES5: @@ =====
GES5: @@ Now start the calculation
GES5: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:
POLY: @@ Turn global minimization off
POLY: set-min-op

```

```

... the command in full is SET_MINIMIZATION_OPTIONS
This command is DEPRECATED and to be removed in the future!
Settings for global minimization:
Use global minimization /Y/: n
Settings for general calculations:
Force positive definite Phase Hessian /Y/: n
Control minimization step size /Y/:
POLY:
POLY: L-C
... the command in full is LIST_CONDITIONS
DEGREES OF FREEDOM 4
POLY: S-C T=60 P=1E5 N=1 X(B)=.4
... the command in full is SET_CONDITION
POLY: @@
POLY: @@ First calculate just with the full CVM phases
POLY: ch-st ph *=sus
... the command in full is CHANGE_STATUS
POLY: ch-st ph cvm cvm#2 cvm#3=ent 1
... the command in full is CHANGE_STATUS
POLY: @@
POLY: @@ L10 ordering, setting start composition essential
POLY: @@ The initial fraction of each species is bascially
POLY: @@ calculated as the product of the site fraction on
POLY: @@ each sublattice.
POLY: s-s-c cvm
... the command in full is SET_START_CONSTITUTION
Y(CVM_TET#1,S0) /1/: .002
Y(CVM_TET#1,S11) /1/: 1.16e-3
Y(CVM_TET#1,S12) /1/: 1.76e-1
Y(CVM_TET#1,S13) /1/: 1.16e-3
Y(CVM_TET#1,S14) /1/: 1.76e-1
Y(CVM_TET#1,S21) /1/: 7.56e-3
Y(CVM_TET#1,S22) /1/: 5e-5
Y(CVM_TET#1,S23) /1/: 7.56e-3
Y(CVM_TET#1,S24) /1/: 7.56e-3
Y(CVM_TET#1,S25) /1/: 6.08e-1
Y(CVM_TET#1,S26) /1/: 7.56e-3
Y(CVM_TET#1,S31) /1/: 1.76e-3
Y(CVM_TET#1,S32) /1/: 2e-5
Y(CVM_TET#1,S33) /1/: 1.76e-3
Y(CVM_TET#1,S34) /1/: 2e-5
Y(CVM_TET#1,S4) /1/: 4e-7
POLY:
POLY: @@ L12 ordering
POLY: s-s-c cvm#2
... the command in full is SET_START_CONSTITUTION
Y(CVM_TET#2,S0) /1/: .002
Y(CVM_TET#2,S11) /1/: .46
Y(CVM_TET#2,S12) /1/: .0078
Y(CVM_TET#2,S13) /1/: .0078
Y(CVM_TET#2,S14) /1/: .0078
Y(CVM_TET#2,S21) /1/: .168
Y(CVM_TET#2,S22) /1/: .168
Y(CVM_TET#2,S23) /1/: .168
Y(CVM_TET#2,S24) /1/: .0012
Y(CVM_TET#2,S25) /1/: .0012
Y(CVM_TET#2,S26) /1/: .0012
Y(CVM_TET#2,S31) /1/: 5e-6
Y(CVM_TET#2,S32) /1/: .002
Y(CVM_TET#2,S33) /1/: .002
Y(CVM_TET#2,S34) /1/: .002
Y(CVM_TET#2,S4) /1/: 1e-6
POLY:
POLY: s-s-c cvm#3 *
... the command in full is SET_START_CONSTITUTION
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,
15 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xnp
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=60, P=100000, N=1, X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 60.00 K ( -213.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -3.10213E+03, Enthalpy -2.96850E+03, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A      6.0000E-01  6.0000E-01  2.0465E-02 -1.9401E+03 SER
B      4.0000E-01  4.0000E-01  6.0538E-05 -4.8452E+03 SER

CVM_TET#1      Status ENTERED      Driving force 0.0000E+00
Moles 5.6950E-01, Mass 5.6950E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.89207E-01 B 4.10793E-01
Constitution:
S25 5.78440E-01 S26 1.28068E-02 S31 4.13398E-03 S22 2.56479E-04
S14 1.76120E-01 S24 1.28068E-02 S0 3.76373E-03 S32 1.15932E-04
S12 1.76120E-01 S21 1.28068E-02 S11 2.78465E-03 S34 1.15932E-04
S23 1.28068E-02 S33 4.13398E-03 S13 2.78465E-03 S4 3.67798E-06

CVM_TET#2      Status ENTERED      Driving force 0.0000E+00
Moles 4.3050E-01, Mass 4.3050E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.14278E-01 B 3.85722E-01
Constitution:
S11 4.21306E-01 S12 1.38900E-02 S34 4.69234E-03 S24 3.19866E-03
S22 1.69717E-01 S13 1.38900E-02 S32 4.69234E-03 S26 3.19866E-03
S21 1.69717E-01 S14 1.38900E-02 S0 4.13973E-03 S31 5.05554E-05
S23 1.69717E-01 S33 4.69234E-03 S25 3.19866E-03 S4 8.90403E-06

CVM_TET#3      Status ENTERED      Driving force -2.3482E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.09605E-01 B 3.90395E-01
Constitution:
S13 1.09346E-01 S26 8.57142E-02 S22 8.57142E-02 S32 7.93976E-03
S14 1.09346E-01 S25 8.57142E-02 S21 8.57142E-02 S34 7.93976E-03

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S12 1.09346E-01 S24 8.57142E-02 S0 1.64839E-02 S33 7.93976E-03
S11 1.09346E-01 S23 8.57142E-02 S31 7.93976E-03 S4 8.69093E-05
POLY:Hit RETURN to continue
POLY:
POLY: s-c t=40
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
14 ITS, CPU TIME USED 0 SECONDS
POLY: s-s-c cvm#3 *
... the command in full is SET_START_CONSTITUTION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
18 ITS, CPU TIME USED 0 SECONDS
POLY: L-E
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNP/:
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=40, P=100000, N=1, X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 40.00 K ( -233.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -3.06232E+03, Enthalpy -2.98938E+03, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
A                6.0000E-01  6.0000E-01  4.1519E-03 -1.8239E+03 SER
B                4.0000E-01  4.0000E-01  3.7621E-07 -4.9199E+03 SER

CVM_TET#1      Status ENTERED      Driving force 0.0000E+00
Moles 6.6953E-01, Mass 6.6953E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.88358E-01 B 4.11642E-01
Constitution:
S25 6.26368E-01 S24 4.57470E-03 S33 6.44301E-04 S22 1.02379E-05
S12 1.76201E-01 S26 4.57470E-03 S31 6.44301E-04 S32 4.02672E-06
S14 1.76201E-01 S23 4.57470E-03 S13 4.60814E-04 S34 4.02672E-06
S21 4.57470E-03 S0 7.03194E-04 S11 4.60814E-04 S4 2.24689E-08

CVM_TET#2      Status ENTERED      Driving force 0.0000E+00
Moles 3.3047E-01, Mass 3.3047E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.23586E-01 B 3.76414E-01
Constitution:
S11 4.81572E-01 S12 4.56422E-03 S32 7.57611E-04 S26 4.03145E-04
S23 1.66859E-01 S14 4.56422E-03 S34 7.57611E-04 S24 4.03145E-04
S22 1.66859E-01 S13 4.56422E-03 S0 6.77145E-04 S31 4.66624E-07
S21 1.66859E-01 S33 7.57611E-04 S25 4.03145E-04 S4 4.50770E-08

CVM_TET#3      Status ENTERED      Driving force -6.0046E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.15517E-01 B 3.84483E-01
Constitution:
S24 1.46218E-01 S13 1.44857E-01 S21 2.79748E-02 S32 1.40187E-03
S25 1.46205E-01 S14 1.44849E-01 S11 2.54012E-02 S34 1.40110E-03
S26 1.46097E-01 S22 2.79941E-02 S31 6.70812E-03 S33 1.40093E-03
S12 1.44923E-01 S23 2.79926E-02 S0 6.52643E-03 S4 5.09667E-05
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 1 x(b) 0 .5,,
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 t 0 100,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex31a y
... the command in full is SAVE_WORKSPACES
POLY: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.116E-01 4.000E+01
CVM_TET#1
** CVM_TET#2
*** Buffer saved on file:
c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tce
x31a.POLY3
Terminating at diagram limit
CALCULATED 27 EQUILIBRIA

Phase region boundary 2 at: 4.116E-01 4.000E+01
CVM_TET#1
** CVM_TET#2
CALCULATED 26 EQUILIBRIA

Phase region boundary 2 at: 4.240E-01 8.061E+01
CVM_TET#1
** CVM_TET#2
CVM_TET#3

Phase region boundary 2 at: 4.147E-01 8.061E+01
** CVM_TET#2
CVM_TET#3
*** SORRY CANNOT CONTINUE *** 4

CALCULATED 95 EQUILIBRIA

Phase region boundary 2 at: 4.240E-01 8.061E+01
CVM_TET#1
** CVM_TET#3
Terminating at diagram limit
CALCULATED 24 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tcex31a.POLY3
CPU time for mapping 1 seconds
POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x m-f b

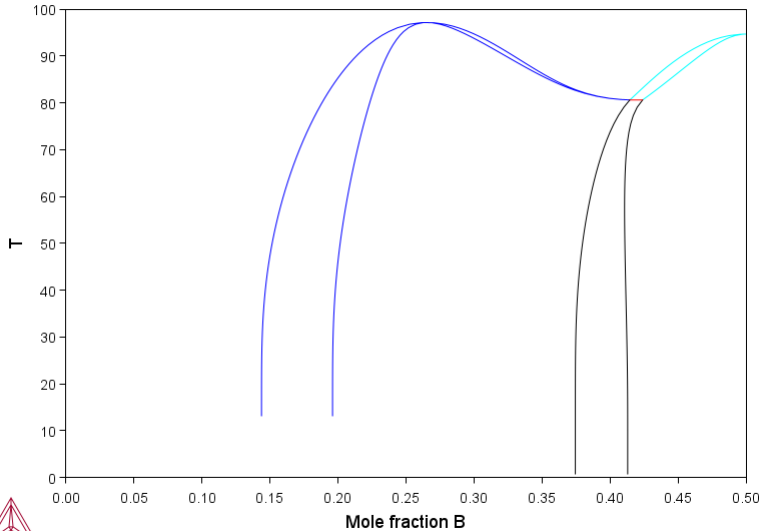
```

```

... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s-x n 0 0.5
... the command in full is SET_SCALING_STATUS
POST: s-s-y n 0 100
... the command in full is SET_SCALING_STATUS
POST: set-title example 31a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 31a



```

POST:
POST:
POST:Hit RETURN to continue
POST:
POST: @@ Make an Experimental data file to overlay the next
POST: @@ calculation
POST: make tcex31 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: @@
POLY: @@ It is interesting to compare with a CEF without any
POLY: @@ SRO contribution. This is the classical FCC ordering
POLY: @@ diagram first calculated manually by W Shockley,
POLY: @@ J Chem Phys, 6, (1938) p 130.
POLY: read tcex31a
... the command in full is READ_WORKSPACES
POLY: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: c-st p *=sus
... the command in full is CHANGE_STATUS
POLY: c-st p lro lro#2 lro#3=ent 0
... the command in full is CHANGE_STATUS
POLY: s-c t=70 x(b)=.4
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
29 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=70, P=100000, N=1., X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 70.00 K ( -203.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -3.08055E+03, Enthalpy -2.95310E+03, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A               6.0000E-01  6.0000E-01  4.7333E-02 -1.7755E+03 SER
B               4.0000E-01  4.0000E-01  1.7400E-04 -5.0382E+03 SER

LRO#1          ORD      Status ENTERED Driving force 0.0000E+00
Moles 2.6762E-01, Mass 2.6762E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.74559E-01 B 3.25441E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.99309E-01 B 1.00691E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.99309E-01 B 1.00691E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.99309E-01 B 1.00691E-01
Sublattice 4, Number of sites 2.5000E-01
B 9.99692E-01 A 3.08116E-04

LRO#2          DISORD Status ENTERED Driving force -4.6485E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.45965E-01 B 3.54035E-01
Constitution:

```

```

Sublattice 1, Number of sites 2.5000E-01
A 6.45965E-01 B 3.54035E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.45965E-01 B 3.54035E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.45965E-01 B 3.54035E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.45965E-01 B 3.54035E-01

LRO#3          ORD      Status ENTERED   Driving force 0.0000E+00
Moles 7.3238E-01, Mass 7.3238E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.72756E-01 B 4.27244E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.99661E-01 B 3.38612E-04
Sublattice 2, Number of sites 2.5000E-01
A 9.99661E-01 B 3.38612E-04
Sublattice 3, Number of sites 2.5000E-01
B 8.54150E-01 A 1.45850E-01
Sublattice 4, Number of sites 2.5000E-01
B 8.54150E-01 A 1.45850E-01
POLY:Hit RETURN to continue
POLY:
POLY: s-s-c lro#3
... the command in full is SET_START_CONSTITUTION
Y(LRO#3,A) /.9996613878/:
Y(LRO#3,B) /3.386121641E-04/:
Y(LRO#3,A#2) /.9996613878/:
Y(LRO#3,B#2) /3.386121641E-04/:
Y(LRO#3,A#3) /.1458499446/: 0.0001
Y(LRO#3,B#3) /.8541500554/: 0.9999
Y(LRO#3,A#4) /.1458499446/: .6
Y(LRO#3,B#4) /.8541500554/: .4
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
19 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=70, P=100000, N=1., X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 70.00 K ( -203.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -3.09267E+03, Enthalpy -2.98506E+03, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A                6.0000E-01  6.0000E-01 4.1721E-02 -1.8489E+03 SER
B                4.0000E-01  4.0000E-01 1.9961E-04 -4.9583E+03 SER

LRO#1          ORD      Status ENTERED   Driving force -3.9680E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.68666E-01 B 3.31334E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.91452E-01 B 1.08548E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.91452E-01 B 1.08548E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.91452E-01 B 1.08548E-01
Sublattice 4, Number of sites 2.5000E-01
B 9.99690E-01 A 3.09940E-04

LRO#2          DISORD Status ENTERED   Driving force -4.9687E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.39146E-01 B 3.60854E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01

LRO#3          ORD      Status ENTERED   Driving force 0.0000E+00
Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 0.0000E+00 Mole fractions:
A 6.00000E-01 B 4.00000E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.98449E-01 B 1.55066E-03
Sublattice 2, Number of sites 2.5000E-01
A 9.98449E-01 B 1.55066E-03
Sublattice 3, Number of sites 2.5000E-01
B 9.92271E-01 A 7.72920E-03
Sublattice 4, Number of sites 2.5000E-01
B 6.04628E-01 A 3.95372E-01
POLY:Hit RETURN to continue
POLY:
POLY: s-c x(b)=.33
... the command in full is SET_CONDITION
POLY: s-s-c lro *
... the command in full is SET_START_CONSTITUTION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
20 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=70, P=100000, N=1., X(B)=0.33
DEGREES OF FREEDOM 0

Temperature 70.00 K ( -203.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -2.85605E+03, Enthalpy -2.74060E+03, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A                6.7000E-01  6.7000E-01 5.7336E-02 -1.6639E+03 SER
B                3.3000E-01  3.3000E-01 1.1554E-04 -5.2765E+03 SER

```

```

LRO#1          ORD      Status ENTERED      Driving force  0.0000E+00
Moles 7.8876E-02, Mass 7.8876E-01, Volume fraction 0.0000E+00  Mole fractions:
A  6.87496E-01 B  3.12504E-01
Constitution:
Sublattice 1,  Number of sites  2.5000E-01
A  9.16558E-01 B  8.34422E-02
Sublattice 2,  Number of sites  2.5000E-01
A  9.16558E-01 B  8.34422E-02
Sublattice 3,  Number of sites  2.5000E-01
A  9.16558E-01 B  8.34422E-02
Sublattice 4,  Number of sites  2.5000E-01
B  9.99689E-01 A  3.11152E-04

LRO#2          DISORD Status ENTERED      Driving force -4.8130E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
A  6.61498E-01 B  3.38502E-01
Constitution:
Sublattice 1,  Number of sites  2.5000E-01
A  6.61498E-01 B  3.38502E-01
Sublattice 2,  Number of sites  2.5000E-01
A  6.61498E-01 B  3.38502E-01
Sublattice 3,  Number of sites  2.5000E-01
A  6.61498E-01 B  3.38502E-01
Sublattice 4,  Number of sites  2.5000E-01
A  6.61498E-01 B  3.38502E-01

LRO#3          ORD      Status ENTERED      Driving force  0.0000E+00
Moles 9.2112E-01, Mass 9.2112E+00, Volume fraction 0.0000E+00  Mole fractions:
A  6.68502E-01 B  3.31498E-01
Constitution:
Sublattice 1,  Number of sites  2.5000E-01
A  9.82295E-01 B  1.77045E-02
Sublattice 2,  Number of sites  2.5000E-01
A  9.82295E-01 B  1.77045E-02
Sublattice 3,  Number of sites  2.5000E-01
B  9.99255E-01 A  7.44800E-04
Sublattice 4,  Number of sites  2.5000E-01
A  7.08671E-01 B  2.91329E-01
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 2 t 0 250 5
... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: save tcex31c y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: add -1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
No 1 -1 T=70, P=100000, N=1., X(B)=0.33
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: map -
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  3.315E-01  7.000E+01
** LRO#1
LRO#3
*** SORRY CANNOT CONTINUE ***  4

CALCULATED  42 EQUILIBRIA

Phase region boundary  2 at:  3.315E-01  7.000E+01
** LRO#1
LRO#3
Terminating at diagram limit
CALCULATED  68 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tcex31c.POLY3
CPU time for mapping  1 seconds
POLY: @@ Add the A2/L1_2 line
POLY: read tcex31c
... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:
POLY: s-c x(b)=.15 t=110
... the command in full is SET_CONDITION
POLY: s-a-s f
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
34 ITS, CPU TIME USED  0 SECONDS
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=110, P=100000, N=1., X(B)=0.15
DEGREES OF FREEDOM 0

```

Temperature 110.00 K (-163.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -1.66707E+03, Enthalpy -1.39975E+03, Volume 0.00000E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
A	8.5000E-01	8.5000E-01	7.3635E-01	-2.7991E+02	SER
B	1.5000E-01	1.5000E-01	2.9909E-05	-9.5277E+03	SER

LRO#1 ORD Status ENTERED Driving force 0.0000E+00
Moles 7.2552E-01, Mass 7.2552E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.40743E-01 B 1.59257E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 4, Number of sites 2.5000E-01
B 5.6112E-01 A 4.38888E-01

LRO#2 DISORD Status ENTERED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.74469E-01 B 1.25531E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 4, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01

LRO#3 DISORD Status ENTERED Driving force 0.0000E+00
Moles 2.7448E-01, Mass 2.7448E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.74469E-01 B 1.25531E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 4, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01

POLY:Hit RETURN to continue

POLY:

POLY: list-ini-eq

... the command in full is LIST_INITIAL_EQUILIBRIA

POLY:

POLY:

POLY:Hit RETURN to continue

POLY:

POLY: map -

Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE

Generating start point 1

Generating start point 2

Phase region boundary 1 at: 1.593E-01 1.100E+02

LRO#1

** LRO#3

MAPPING TERMINATED 1

CALCULATED 59 EQUILIBRIA

Phase region boundary 2 at: 1.593E-01 1.100E+02

LRO#1

** LRO#3

Terminating at diagram limit

CALCULATED 69 EQUILIBRIA

*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tcex31c.POLY3

CPU time for mapping 0 seconds

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-s x n 0 .5

... the command in full is SET_SCALING_STATUS

POST: @@ Usually some 2nd order lines also appear

POST: set-title example 31b

POST:

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

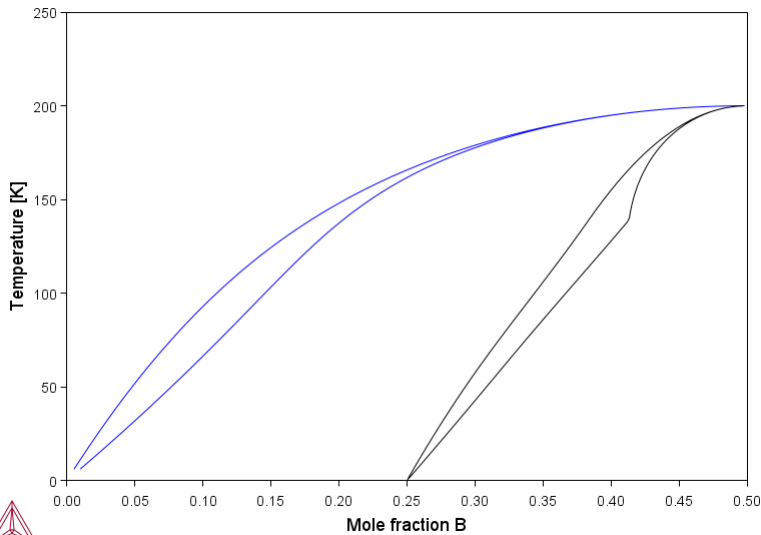
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 31b

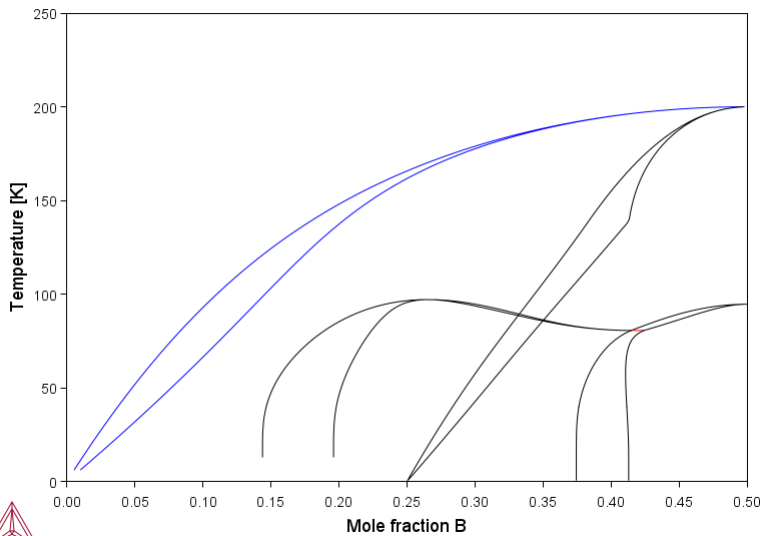


```

POST:
POST:
POST:Hit RETURN to continue
POST:
POST: a-e-d y tcex31 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 31c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 31c



```

POST:
POST:Hit RETURN to continue
POST:
POST: ba
... the command in full is BACK
POLY: read tcex31c
... the command in full is READ_WORKSPACES
POLY: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES5: @@ Now add a reciprocal parameter to LRO which describes
GES5: @@ the SRO contribution. The default value of this is
GES5: @@ the bond energy. One can have 3 different parameters
GES5: @@ depending on if one is at 25%B, 50%B or 75%B. Here
GES5: @@ we just take the same value.
GES5:
GES5: e-sym f GSROAA,,UIJ;,,,,
... the command in full is ENTER_SYMBOL
GES5: e-sym f GSROAB,,UIJ;,,,,
... the command in full is ENTER_SYMBOL
GES5: e-sym f GSROBB,,UIJ;,,,,
... the command in full is ENTER_SYMBOL
GES5:
GES5: e-par l(lro,a,b:a,b:*),,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,A,B:A,B:*:0)
GES5: e-par l(lro,a,b:*:a,b*),,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,A,B:*:A,B:*:0)
GES5: e-par l(lro,a,b:*:a,b),,GSROAB;,,,,

```

```

... the command in full is ENTER_PARAMETER
L(LRO,A,B:*:A,B;0)
GES5: e-par l(lro,*:a,b:a,b:*),,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,*:A,B:A,B:*;0)
GES5: e-par l(lro,*:a,b:*:a,b),,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,*:A,B:*:A,B;0)
GES5: e-par l(lro,*:a,b:a,b),,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,*:A,B:A,B;0)
GES5: l-p-d lro
... the command in full is LIST_PHASE_DATA

LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES .25: .25: .25: .25
  CONSTITUENTS: A,B : A,B : A,B : A,B

  G(LRO,A:A:A;0) = 0.0
  G(LRO,B:A:A;0) = +GA3B1
  G(LRO,A:B:A;0) = +GA3B1
  G(LRO,B:B:A;0) = +GA2B2
  G(LRO,A:A:B;0) = +GA3B1
  G(LRO,B:A:B;0) = +GA2B2
  G(LRO,A:B:B;0) = +GA2B2
  G(LRO,B:B:B;0) = +GA1B3
  G(LRO,A:A:B;0) = +GA3B1
  G(LRO,B:A:B;0) = +GA2B2
  G(LRO,A:B:B;0) = +GA2B2
  G(LRO,B:B:B;0) = +GA1B3
  G(LRO,A:A:B;0) = +GA2B2
  G(LRO,B:A:B;0) = +GA1B3
  G(LRO,A:B:B;0) = +GA1B3
  G(LRO,B:B:B;0) = +GA1B3
  G(LRO,B:B:B;0) = 0.0
  G(LRO,A:A:*:0) = 0.0
  G(LRO,A:*:A;0) = 0.0
  G(LRO,A:*:*:A;0) = 0.0
  G(LRO,*:A:A;0) = 0.0
  G(LRO,*:A:*:A;0) = 0.0
  G(LRO,*:*:A;0) = 0.0
  L(LRO,A,B:A,B:*:0) = +GSROAB
  L(LRO,A,B:*:A,B;0) = +GSROAB
  L(LRO,A,B:*:*:A,B;0) = +GSROAB
  L(LRO,*:A,B:A,B;0) = +GSROAB
  L(LRO,*:A,B:*:A,B;0) = +GSROAB
  L(LRO,*:*:A,B:A,B;0) = +GSROAB
GES5:
GES5:Hit RETURN to continue
GES5:
GES5: @@ These reciprocal parameters do not give any contribution to
GES5: @@ the disordered state as the contribution from the ordered
GES5: @@ phase is zero there. But it is in the disordered state that
GES5: @@ the SRO contribution to the Gibbs energy is most important.
GES5: @@ We must add regular solution parameters to the FCC phase
GES5: @@ giving the same contribution. These can be derived by
GES5: @@ setting all site-fractions for the same element equal,
GES5: @@ i.e. the disordered state.
GES5:
GES5: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3+
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;0)
& 0.375*GSROAA+0.75*GSROAB+0.375*GSROBB;,,,,,
GES5: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3+0.75*GSROAA-0.75*GSROBB;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;1)
GES5: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;2)
GES5: e-par l(fcc,a,b;3),,-0.75*GSROAA+0.75*GSROBB;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;3)
GES5: e-par l(fcc,a,b;4),,-0.375*GSROAA+0.75*GSROAB-0.375*GSROBB;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;4)
GES5: l-p-d fcc
... the command in full is LIST_PHASE_DATA

FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  CONSTITUENTS: A,B

  G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
  G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
  L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3+.375*GSROAA+.75*GSROAB
  +.375*GSROBB
  L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3+.75*GSROAA-.75*GSROBB
  L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB
  L(FCC_A1,A,B;3) = -.75*GSROAA+.75*GSROBB
  L(FCC_A1,A,B;4) = -.375*GSROAA+.75*GSROAB-.375*GSROBB
GES5:
GES5:Hit RETURN to continue
GES5:
GES5: ba
... the command in full is BACK
POLY: c-st p lro#3=e 0
... the command in full is CHANGE_STATUS
POLY: l-c
... the command in full is LIST_CONDITIONS
T=70, P=100000, N=1., X(B)=0.33
DEGREES OF FREEDOM 0
POLY:
POLY: s-c t=40
... the command in full is SET_CONDITION
POLY: s-a-s f
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM

```

```

Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL MINIMIZATION Y,,,,,,,,,
  24 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=40, P=100000, N=1., X(B)=0.33
DEGREES OF FREEDOM 0

Temperature 40.00 K ( -233.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -2.81177E+03, Enthalpy -2.73484E+03, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
A      6.7000E-01  6.7000E-01  5.5303E-03 -1.7286E+03 SER
B      3.3000E-01  3.3000E-01  2.8612E-07 -5.0109E+03 SER

LRO#1      ORD      Status ENTERED      Driving force 0.0000E+00
Moles 9.1974E-01, Mass 9.1974E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.79151E-01 B 3.20849E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 4, Number of sites 2.5000E-01
B 9.99993E-01 A 6.81574E-06

LRO#2      DISORD Status ENTERED      Driving force -3.8166E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.26318E-01 B 3.73682E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01

LRO#3      ORD      Status ENTERED      Driving force 0.0000E+00
Moles 8.0263E-02, Mass 8.0263E-01, Volume fraction 0.0000E+00 Mole fractions:
A 5.65144E-01 B 4.34856E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.99996E-01 B 4.15407E-06
Sublattice 2, Number of sites 2.5000E-01
A 9.99996E-01 B 4.15407E-06
Sublattice 3, Number of sites 2.5000E-01
B 8.69708E-01 A 1.30292E-01
Sublattice 4, Number of sites 2.5000E-01
B 8.69708E-01 A 1.30292E-01
POLY:Hit RETURN to continue
POLY:
POLY: save tcex31d y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 3.208E-01 4.000E+01
LRO#1
** LRO#3
TOO LONG JUMP IN AXIS, SKIPPING NODE
MAPPING TERMINATED 1
CALCULATED 31 EQUILIBRIA

Phase region boundary 2 at: 3.208E-01 4.000E+01
LRO#1
** LRO#3
CALCULATED 22 EQUILIBRIA

Phase region boundary 2 at: 3.685E-01 7.734E+01
LRO#1
LRO#2
** LRO#3

Phase region boundary 2 at: 4.193E-01 7.734E+01
** LRO#2
LRO#3
Terminating at diagram limit
CALCULATED 23 EQUILIBRIA

Phase region boundary 2 at: 3.685E-01 7.734E+01
LRO#1
** LRO#2
Terminating at diagram limit
CALCULATED 90 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tcex31d.POLY3
CPU time for mapping 1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: set-title example 31d
POST: s-s y n
... the command in full is SET_SCALING_STATUS

```

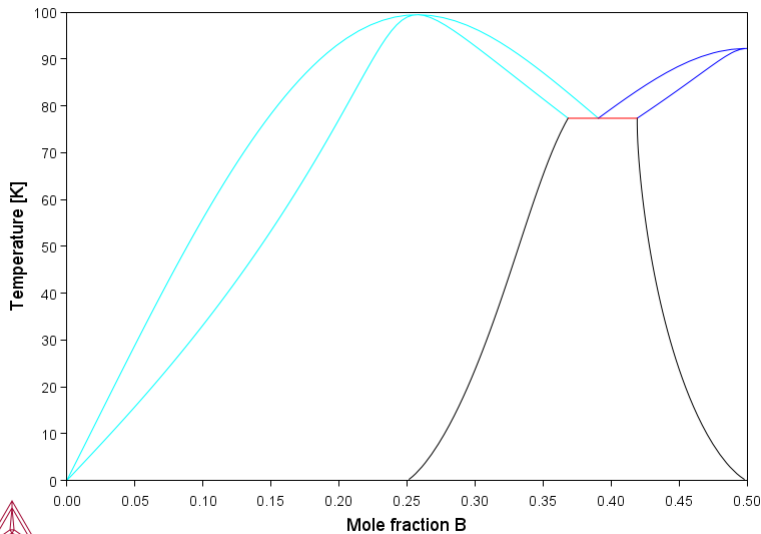


```

MIN VALUE : 0 100
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 31d

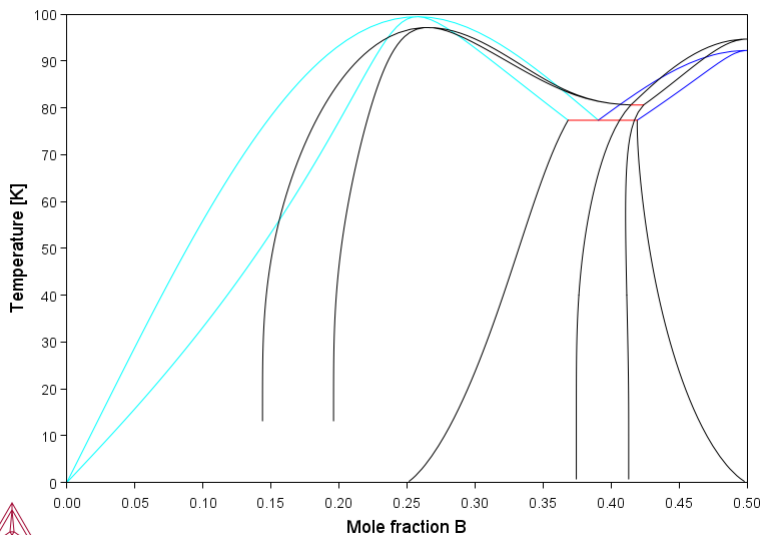


```

POST:
POST:Hit RETURN to continue
POST:
POST: a-e-d y tcex31 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-title example 31e
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 31e



```

POST:
POST: @@ It actually turns out, that this is not the stable phase diagram,
POST: @@ but rather a meta-stable diagram. Thanks to Nathalie Dupin for
POST: @@ pointing this out to us :)
POST: @@ The calculation of the stable phase diagram is not entirely trivial.
POST: @@ It requires switching GLOBAL on again and also a Global test interval of 1.
POST: @@ This is done like shown below and will noticeably increase calculation time.
POST:
POST:Hit RETURN to continue
POST:
POST: ba
... the command in full is BACK
POLY: s-c x(b)=0.4 t=70
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
17 ITS, CPU TIME USED 0 SECONDS
POLY: adv g y 2000
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY: adv step,1,,,
... the command in full is ADVANCED_OPTIONS

```

```

Settings for MAP and STEP:
Settings for MAP:
POLY: s-a-s y
... the command in full is SET_ALL_START_VALUES
Old start values kept
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1360 grid points in 0.034 s
Found the set of lowest grid points in 0.001 s
Calculated POLY solution 0.078 s, total time 0.113 s
POLY: save tcex3le_stable y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Trying global minimization! 3
Working hard
Working hard
Trying global minimization! 3
Working hard
Trying global minimization! 3
Working hard
Working hard
Working hard
Working hard
Working hard
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Trying global minimization! 3
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12

Phase region boundary 1 at: 1.244E-02 5.000E+00
LRO#1
** LRO#2
Calculated. 37 equilibria

Phase region boundary 2 at: 3.796E-01 7.734E+01
LRO#1
** LRO#2
** LRO#3

Phase region boundary 3 at: 4.050E-01 7.734E+01
LRO#1
** LRO#3
Calculated.. 16 equilibria
Terminating at axis limit.

Phase region boundary 4 at: 3.939E-01 7.734E+01
LRO#2
** LRO#3
Calculated 18 equilibria

Phase region boundary 5 at: 3.796E-01 7.734E+01
LRO#1
** LRO#2
Calculated 55 equilibria

Phase region boundary 6 at: 1.244E-02 5.000E+00
LRO#1
** LRO#2
Calculated. 37 equilibria
Terminating at known equilibrium

Phase region boundary 7 at: 1.244E-02 5.000E+00
LRO#1
** LRO#2
Calculated. 37 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 1.244E-02 5.000E+00
LRO#1
** LRO#2
Calculated. 37 equilibria
Terminating at known equilibrium

Phase region boundary 9 at: 1.415E-01 6.228E+01
** LRO#1
LRO#2
Calculated 35 equilibria

Phase region boundary 10 at: 1.415E-01 6.228E+01
** LRO#1
LRO#2
Calculated. 23 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 1.244E-02 5.000E+00
** LRO#1
LRO#2

```

```

Calculated.          37 equilibria
Terminating at known equilibrium

Phase region boundary 12 at:  1.244E-02  5.000E+00
** LRO#1
   LRO#2
Calculated.          37 equilibria
Terminating at known equilibrium

Phase region boundary 13 at:  4.840E-01  9.148E+01
** LRO#1
   LRO#2
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 14 at:  4.840E-01  9.148E+01
** LRO#1
   LRO#2
Calculated..         3 equilibria
Terminating at axis limit.

Phase region boundary 15 at:  4.965E-01  9.199E+01
** LRO#1
   LRO#2
Calculated.         19 equilibria
Terminating at known equilibrium

Phase region boundary 16 at:  4.430E-01  8.500E+01
** LRO#1
   LRO#2
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  4.430E-01  8.500E+01
** LRO#1
   LRO#2
Calculated..        10 equilibria
Terminating at axis limit.

Phase region boundary 18 at:  4.962E-01  9.201E+01
** LRO#1
   LRO#2
Calculated.         19 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tcex31e_stable.POLY3
CPU time for mapping          37 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

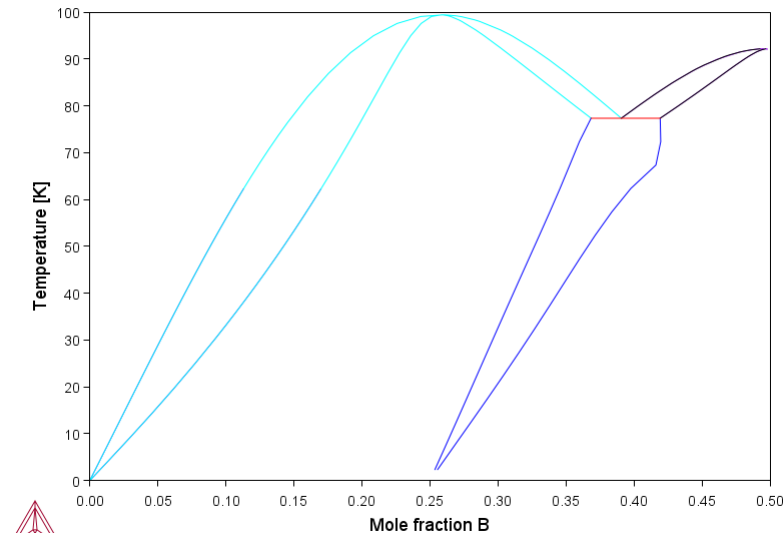
Setting automatic diagram axes

```

POST: set-title example 31e-stable
POST: s-s-s y n 0 100
... the command in full is SET_SCALING_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 31e-stable



```

POST:
POST: @@ There is still a tiny part of the phase diagram missing
POST: @@ At M-F B = 0.25.
POST: @@ This gap can be filled by some more fine tuning:
POST: @@ 1. making a finer step interval in the mapping
POST: @@ 2. increase the gridpoints for GLOBAL to 4000
POST: @@ Note, that there might be other combinations that will
POST: @@ work. Finding good solutions is simply a matter of experience
POST: @@ and trial-and-error... If you find a good solution, you are
POST: @@ always welcomed to let us know: support@thermocalc.com
POST:
POST: Hit RETURN to continue
POST:
POST: ba
... the command in full is BACK
POLY: s-a-v 1 X(B) 0 0.5 0.0005
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 t 0 100 1
... the command in full is SET_AXIS_VARIABLE

```

```

POLY: adv g y 4000
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY: adv step,10,,,,
... the command in full is ADVANCED_OPTIONS
Settings for MAP and STEP:
Settings for MAP:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Trying global minimization! 3
Trying global minimization! 3
Generating start point 5
Generating start point 6
Trying global minimization! 3
Trying global minimization! 3
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Trying global minimization! 3
Generating start point 11
Generating start point 12
Trying global minimization! 3
Generating start point 13
Generating start point 14
Trying global minimization! 3
Generating start point 15
Generating start point 16

Phase region boundary 1 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated 19 equilibria

Phase region boundary 2 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated. 756 equilibria

Phase region boundary 3 at: 3.796E-01 7.734E+01
** LRO#1
LRO#2
** LRO#3

Phase region boundary 4 at: 3.939E-01 7.734E+01
LRO#2
** LRO#3
Calculated 31 equilibria

Phase region boundary 5 at: 3.939E-01 7.734E+01
LRO#2
** LRO#3
Calculated 20 equilibria

Phase region boundary 6 at: 4.050E-01 7.734E+01
LRO#1
** LRO#3
Calculated.. 191 equilibria
Terminating at axis limit.

Phase region boundary 7 at: 3.796E-01 7.734E+01
** LRO#1
LRO#2
Calculated 774 equilibria

Phase region boundary 8 at: 1.384E-01 6.081E+01
** LRO#1
LRO#2
Calculated 290 equilibria

Phase region boundary 9 at: 1.384E-01 6.081E+01
** LRO#1
LRO#2
Calculated. 484 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated 19 equilibria

Phase region boundary 11 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated. 756 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 4.992E-01 9.224E+01
** LRO#1
LRO#2
Calculated. 190 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 4.992E-01 9.224E+01

```

```

** LRO#1
LRO#2
Calculated..          3 equilibria
Terminating at axis limit.

Phase region boundary 14 at:  4.997E-01  9.224E+01
** LRO#1
LRO#2
Calculated.          191 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  3.158E-01  3.367E+01
** LRO#2
LRO#3
Calculated          157 equilibria

Phase region boundary 16 at:  3.158E-01  3.367E+01
** LRO#2
LRO#3
Calculated.          163 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  3.815E-01  6.633E+01
LRO#2
** LRO#3
Calculated          270 equilibria

Phase region boundary 18 at:  3.815E-01  6.633E+01
LRO#2
** LRO#3
Calculated.          26 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  3.212E-01  9.073E+01
LRO#1
** LRO#2
Calculated          654 equilibria

Phase region boundary 20 at:  3.212E-01  9.073E+01
LRO#1
** LRO#2
Calculated.          118 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  4.996E-01  9.224E+01
LRO#1
** LRO#2
Calculated.          191 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  4.996E-01  9.224E+01
LRO#1
** LRO#2
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 23 at:  4.996E-01  9.224E+01
LRO#1
** LRO#2
Calculated.          199 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex31\tcex31e_stable.POLY3
CPU time for mapping          79 seconds

```

```

POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

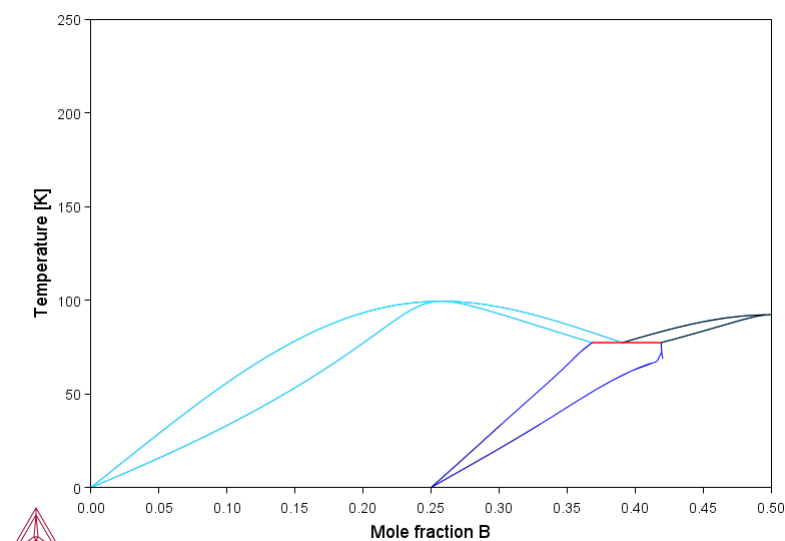
```

Setting automatic diagram axes

```

POST: pl,,,
... the command in full is PLOT_DIAGRAM
example 31e-stable

```

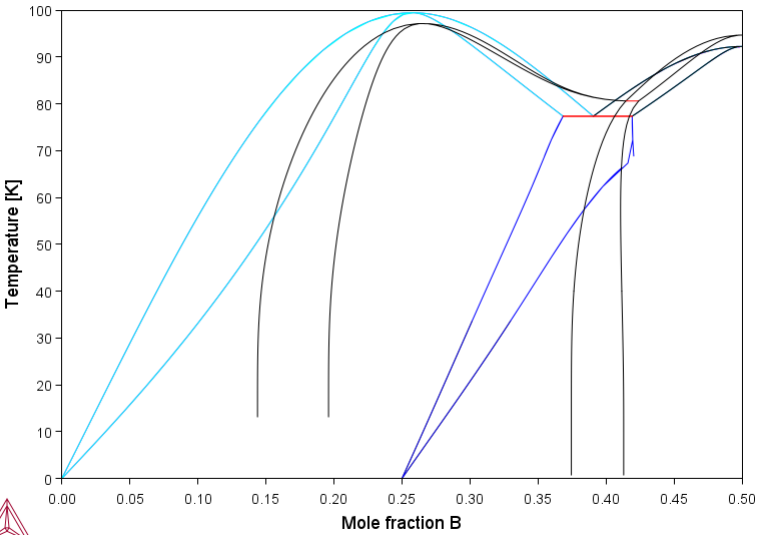


```

POST: a-e-d y tcex31 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: s-s-s y n 0 100
... the command in full is SET_SCALING_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```

... the command in full is PLOT_DIAGRAM
example 31e-stable



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tcex32

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex32\tcex32.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating oxide layers on steel

SYS:

SYS: @@ This example calculates oxide layers on a steel

SYS:

SYS: @@ Note that a TCOX license is

SYS: @@ required to run the example.

SYS:

SYS: set-log ex32,,,

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw tcex12

... the command in full is SWITCH_DATABASE

Current database: Metal Oxide Solutions v12.0

VA /- DEFINED

PEROVSKITE:I REJECTED

TDB_TCOX12: d-sys fe cr c v mn si o

... the command in full is DEFINE_SYSTEM

FE CR C

V MN SI

O DEFINED

TDB_TCOX12: get

... the command in full is GET_DATA

09:23:54,642 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set IONIC_LIQ#2

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set IONIC_LIQ#3

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

MN+4 IN NIMNO3:I SUBLATTICE 1 REJECTED

CR+3 IN GARNET:I SUBLATTICE 3 REJECTED

FE+3 IN GARNET:I SUBLATTICE 3 REJECTED

VA IN NB2O5:I SUBLATTICE 2 REJECTED

VA IN RUTILE:I SUBLATTICE 2 REJECTED

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

FE+3 IN ALPO4_S1:I SUBLATTICE 1 REJECTED

MN+3 IN ALPO4_S1:I SUBLATTICE 1 REJECTED

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_TCOX12:

TDB_TCOX12: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: s-c b(cr)=16 b(v)=.1 b(c)=1 b(mn)=.3 b(si)=.3 t=1073 p=1e5 b=100

... the command in full is SET_CONDITION

POLY: l-c

... the command in full is LIST_CONDITIONS

B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=100000, B=100

DEGREES OF FREEDOM 1

POLY:Hit RETURN to continue

POLY:

POLY: @@ We have atomic oxygen as a component. Later we use the

POLY: @@ partial pressure of O2 as output. The state variable

POLY: @@ LNACR is the chemical potential divided by RT, usual

POLY: @@ values are between -40 and 0

POLY: @@ To improve convergence we first choose a very low value

POLY:

POLY: s-c lnacr(o)=-50

... the command in full is SET_CONDITION

POLY: s-r-s o gas * 1e5

... the command in full is SET_REFERENCE_STATE

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 45875 grid points in 1.011 s

106 ITS, CPU TIME USED 9 SECONDS

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

```

Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0  , database: TCOX12

Conditions:
B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=100000, B=100,
  LNACR(O)=-50
DEGREES OF FREEDOM 0

Temperature 1073.00 K ( 799.85 C), Pressure 1.000000E+05
Number of moles of components 1.88275E+00, Mass in grams 1.00000E+02
Total Gibbs energy -9.42381E+04, Enthalpy 4.96931E+04, Volume 1.34230E-05

Component      Moles      W-Fraction Activity Potential Ref.stat
C               8.3257E-02   1.0000E-02 6.0029E-03 -4.5638E+04 SER
CR             3.0772E-01   1.6000E-01 2.2693E-03 -5.4317E+04 SER
FE             1.4737E+00   8.2300E-01 4.5659E-03 -4.8079E+04 SER
MN             5.4607E-03   3.0000E-03 8.6742E-06 -1.0398E+05 SER
O              4.6959E-12   7.5130E-13 1.9287E-22 -4.4607E+05 GAS
SI             1.0682E-02   3.0000E-03 6.0839E-10 -1.8932E+05 SER
V              1.9631E-03   1.0000E-03 1.0285E-07 -1.4355E+05 SER

BCC_A2          Status ENTERED      Driving force 0.0000E+00
Moles 1.5657E+00, Mass 8.6625E+01, Volume fraction 8.5605E-01 Mass fractions:
FE 9.16292E-01 SI 3.46321E-03 V 1.35768E-04 O 8.67303E-13
CR 7.73672E-02 MN 2.68313E-03 C 5.86710E-05

M7C3_D101       Status ENTERED      Driving force 0.0000E+00
Moles 1.8521E-01, Mass 7.4807E+00, Volume fraction 8.1843E-02 Mass fractions:
CR 7.60041E-01 C 8.92121E-02 MN 2.88836E-03 O 0.00000E+00
FE 1.40049E-01 V 7.80948E-03 SI 5.42131E-11

M23C6_D84       Status ENTERED      Driving force 0.0000E+00
Moles 1.3181E-01, Mass 5.8944E+00, Volume fraction 6.2107E-02 Mass fractions:
CR 6.12851E-01 C 5.55686E-02 V 5.05875E-03 SI 0.00000E+00
FE 3.18723E-01 MN 7.79845E-03 O 0.00000E+00

POLY:
POLY: @@ Vary the normalized chemical potential of oxygen
POLY: @@ between -15 and -50
POLY: s-a-v 1 lnacr(o)
... the command in full is SET_AXIS_VARIABLE
Min value /O/: -50
Max value /I/: -15
Increment /.875/: 0.5
POLY: save tcex32 y
... the command in full is SAVE_WORKSPACES
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value -50.0000
...OK

Phase Region from -50.0000 for:
BCC_A2
M23C6_D84
M7C3_D101
Global test at -4.60000E+01 .... OK
Global test at -4.10000E+01 .... OK
Global test at -3.60000E+01 .... OK
Global check of adding phase at -3.16386E+01
Calculated 39 equilibria

Phase Region from -31.6386 for:
BCC_A2
M23C6_D84
M7C3_D101
RHODONITE
Global check of adding phase at -3.15084E+01
Calculated 3 equilibria

Phase Region from -31.5084 for:
BCC_A2
M23C6_D84
M7C3_D101
RHODONITE
SPINEL
Global check of adding phase at -3.14620E+01
Calculated 4 equilibria

Phase Region from -31.4620 for:
BCC_A2
M23C6_D84
M7C3_D101
QUARTZ
RHODONITE
SPINEL
Global check of removing phase at -3.14619E+01
Calculated 2 equilibria

Phase Region from -31.4619 for:
BCC_A2
M23C6_D84
M7C3_D101
QUARTZ
SPINEL
Global check of adding phase at -3.06418E+01
Calculated 4 equilibria

Phase Region from -30.6418 for:
BCC_A2
CORUNDUM
M23C6_D84
M7C3_D101
QUARTZ
SPINEL
Global check of removing phase at -3.06418E+01
Calculated 2 equilibria

Phase Region from -30.6418 for:
BCC_A2
CORUNDUM
M7C3_D101
QUARTZ
SPINEL
Global check of adding phase at -3.01021E+01

```


Calculated 7 equilibria

Phase Region from -30.1021 for:

BCC_A2
CORUNDUM
FCC_A1
M7C3_D101
QUARTZ
SPINEL

Global check of removing phase at -3.00993E+01

Calculated 3 equilibria

Phase Region from -30.0993 for:

CORUNDUM
FCC_A1
M7C3_D101
QUARTZ
SPINEL

Global check of adding phase at -2.93536E+01

Calculated 10 equilibria

Phase Region from -29.3536 for:

CEMENTITE_D011
CORUNDUM
FCC_A1
M7C3_D101
QUARTZ
SPINEL

Global check of removing phase at -2.93427E+01

Calculated 3 equilibria

Phase Region from -29.3427 for:

CEMENTITE_D011
CORUNDUM
FCC_A1
QUARTZ
SPINEL

Global test at -2.85000E+01 OK

Global check of adding phase at -2.81889E+01

Calculated 14 equilibria

Phase Region from -28.1889 for:

CEMENTITE_D011
CORUNDUM
FCC_A1
GRAPHITE
QUARTZ
SPINEL

Global check of removing phase at -2.81889E+01

Calculated 2 equilibria

Phase Region from -28.1889 for:

CORUNDUM
FCC_A1
GRAPHITE
QUARTZ
SPINEL

Global check of removing phase at -2.67786E+01

Calculated 6 equilibria

Phase Region from -26.7786 for:

FCC_A1
GRAPHITE
QUARTZ
SPINEL

Global check of adding phase at -2.32959E+01

Calculated 10 equilibria

Phase Region from -23.2959 for:

GAS
FCC_A1
GRAPHITE
QUARTZ
SPINEL

Global check of removing phase at -2.32959E+01

Calculated 3 equilibria

Phase Region from -23.2959 for:

FCC_A1
GRAPHITE
QUARTZ
SPINEL

Global check of adding phase at -2.32959E+01

Calculated 3 equilibria

Phase Region from -23.2959 for:

GAS
FCC_A1
GRAPHITE
QUARTZ
SPINEL

Calculated 3 equilibria

Sorry cannot continue 0 189 1 -2.3295895E+01

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex32\tcex32.POLY3

POLY:

POLY:

POLY: @@ Additional start value is required for the calculation of the whole curve

POLY: s-c lnacr(o)=-15

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Using already calculated grid

122 ITS, CPU TIME USED 1 SECONDS

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/:

Output from POLY-3, equilibrium = 1, label A0 , database: TCOX12

Conditions:

B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3000000002, B(SI)=0.3, T=1073,

P=100000, B=100., LNACR(O)=-15

DEGREES OF FREEDOM 0

Temperature 1073.00 K (799.85 C), Pressure 1.000000E+05
Number of moles of components 3.21117E+00, Mass in grams 1.00000E+02
Total Gibbs energy -6.95780E+05, Enthalpy -4.88543E+05, Volume 7.44899E-03

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	8.3257E-02	1.0000E-02	1.0979E-07	-1.4296E+05	SER
CR	3.0772E-01	1.6000E-01	2.0699E-14	-2.8110E+05	SER
FE	9.4031E-01	5.2513E-01	7.2944E-07	-1.2607E+05	SER
MN	5.4607E-03	3.0000E-03	1.8050E-15	-3.0287E+05	SER
O	1.8618E+00	2.9787E-01	3.0590E-07	-1.3382E+05	GAS
SI	1.0682E-02	3.0000E-03	2.8207E-24	-4.8377E+05	SER
V	1.9631E-03	1.0000E-03	7.5558E-19	-3.7226E+05	SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 2.4961E-01, Mass 3.6614E+00, Volume fraction 9.9715E-01 Mass fractions:
O 7.26881E-01 FE 9.83660E-17 CR 2.08046E-18 SI 1.05412E-19
C 2.73119E-01 V 4.97537E-17 MN 1.94360E-19

Constitution:

C1O2	9.98014E-01	C3O2	7.12414E-25	C4	1.00000E-30
C1O1	1.98609E-03	O1V1	2.23272E-25	SI	1.00000E-30
O2	9.35762E-14	MN1O2	9.61561E-26	C3	1.00000E-30
O	3.83114E-16	C2O1	1.61643E-27	C2SI3	1.00000E-30
FE	7.41038E-17	O1O4	7.08722E-28	C2SI2	1.00000E-30
O2V1	4.29523E-17	CR2O3	6.88113E-28	C2SI1	1.00000E-30
FE1O1	3.20822E-18	FE2	2.51602E-28	SI2	1.00000E-30
CR1O2	1.63386E-18	CR2O2	3.28756E-30	C2	1.00000E-30
MN	1.55338E-19	C	1.00000E-30	C1SI4	1.00000E-30
FE1O2	1.47213E-19	CR2	1.00000E-30	C1SI3	1.00000E-30
CR1O3	1.25504E-19	CR2O1	1.00000E-30	C1SI2	1.00000E-30
O1SI1	8.50205E-20	O2SI2	1.00000E-30	C1SI1	1.00000E-30
O2SI1	8.00397E-20	O3	1.00000E-30	SI3	1.00000E-30
CR1O1	2.48192E-22	C60	1.00000E-30	V	1.00000E-30
MN1O1	2.45336E-22	C5FE1O5	1.00000E-30		
CR	2.30535E-24	C5	1.00000E-30		

SPINEL Status ENTERED Driving force 0.0000E+00
Moles 2.9295E+00, Mass 9.5697E+01, Volume fraction 2.8177E-03 Mass fractions:
FE 5.48748E-01 CR 1.67195E-01 V 1.04497E-03 SI 0.00000E+00
O 2.79878E-01 MN 3.13490E-03 C 0.00000E+00

QUARTZ Status ENTERED Driving force 0.0000E+00
Moles 3.2046E-02, Mass 6.4180E-01, Volume fraction 3.3996E-05 Mass fractions:
O 5.32563E-01 C 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
SI 4.67437E-01 V 0.00000E+00 FE 0.00000E+00

POLY:

POLY: sh lnacr(o)

... the command in full is SHOW_VALUE
LNACR(O)=-15

POLY: @@ List the activity of O2

POLY: show lnacr(o2,gas)

... the command in full is SHOW_VALUE
LNACR(O2,GAS)=-30

POLY:Hit RETURN to continue

POLY:

POLY: @@ Vary the normalized chemical potential of oxygen

POLY: @@ between -15 and -50 again to calculate the whole curve

POLY: s-a-v 1 lnacr(o)

... the command in full is SET_AXIS_VARIABLE

Min value /-50/: -50

Max value /-15/: -15

Increment /.875/: 0.5

POLY:

POLY: step

... the command in full is STEP_WITH_OPTIONS

Option? /NORMAL/: NORMAL

No initial equilibrium, using default

Step will start from axis value -15.0000

...OK

Phase Region from -15.0000 for:

GAS
QUARTZ
SPINEL

Global check of adding phase at -1.70864E+01

Calculated 7 equilibria

Phase Region from -17.0864 for:

GAS
OLIVINE
QUARTZ
SPINEL

Global check of removing phase at -1.70927E+01

Calculated 3 equilibria

Phase Region from -17.0927 for:

GAS
OLIVINE
SPINEL

Global check of adding phase at -2.09633E+01

Calculated 10 equilibria

Phase Region from -20.9633 for:

GAS
HALITE
OLIVINE
SPINEL

Global test at -2.17000E+01 OK

Global check of adding phase at -2.17921E+01

Calculated 11 equilibria

Phase Region from -21.7921 for:

GAS
BCC A2
HALITE
OLIVINE
SPINEL

Global check of removing phase at -2.17937E+01

Calculated 3 equilibria

Phase Region from -21.7937 for:

GAS
BCC A2
OLIVINE
SPINEL

Global check of adding phase at -2.23245E+01
Calculated 4 equilibria

Phase Region from -22.3245 for:

GAS
BCC_A2
FCC_A1
OLIVINE
SPINEL

Global check of removing phase at -2.23245E+01
Calculated 2 equilibria

Phase Region from -22.3245 for:

GAS
FCC_A1
OLIVINE
SPINEL

Global check of adding phase at -2.31503E+01
Calculated 5 equilibria

Phase Region from -23.1503 for:

GAS
FCC_A1
OLIVINE
QUARTZ
SPINEL

Global check of removing phase at -2.31608E+01
Calculated 3 equilibria

Phase Region from -23.1608 for:

GAS
FCC_A1
QUARTZ
SPINEL

Global check of adding phase at -2.32959E+01
Calculated 3 equilibria

Phase Region from -23.2959 for:

GAS
FCC_A1
GRAPHITE
QUARTZ
SPINEL

Global check of removing phase at -2.32959E+01
Calculated 3 equilibria

Phase Region from -23.2959 for:

GAS
FCC_A1
QUARTZ
SPINEL

Global check of adding phase at -2.32959E+01
Calculated 3 equilibria

Phase Region from -23.2959 for:

GAS
FCC_A1
GRAPHITE
QUARTZ
SPINEL

Calculated 3 equilibria
Sorry cannot continue 0 189 1 -2.3295995E+01

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex32\tcex32.POLY3

POLY:

POLY: po

... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

POST:

POST: s-d-a x acr(o2,gas)

... the command in full is SET_DIAGRAM_AXIS

POST: s-d-a y bpw(*)

... the command in full is SET_DIAGRAM_AXIS

COLUMN NUMBER /*/: *

POST: s-a-ty

... the command in full is SET_AXIS_TYPE

AXIS (X, Y OR Z) : x

AXIS TYPE /LINEAR/: log

POST: set-title example 32a

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

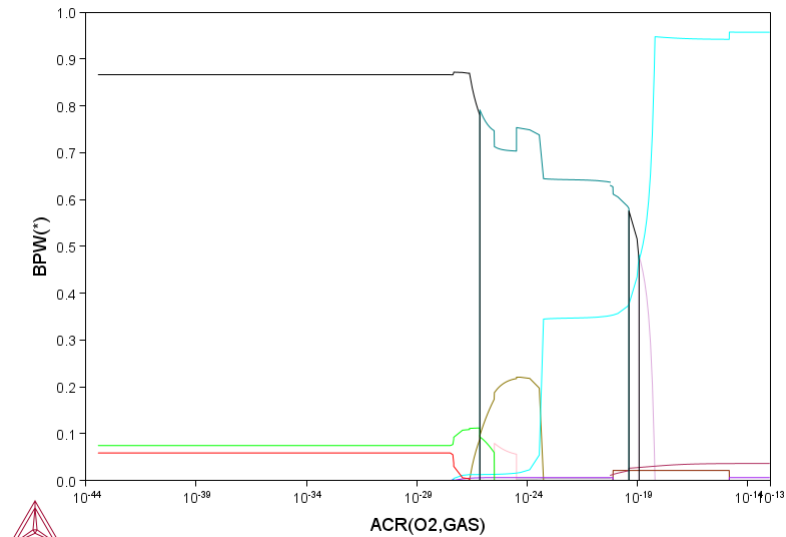
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 32a

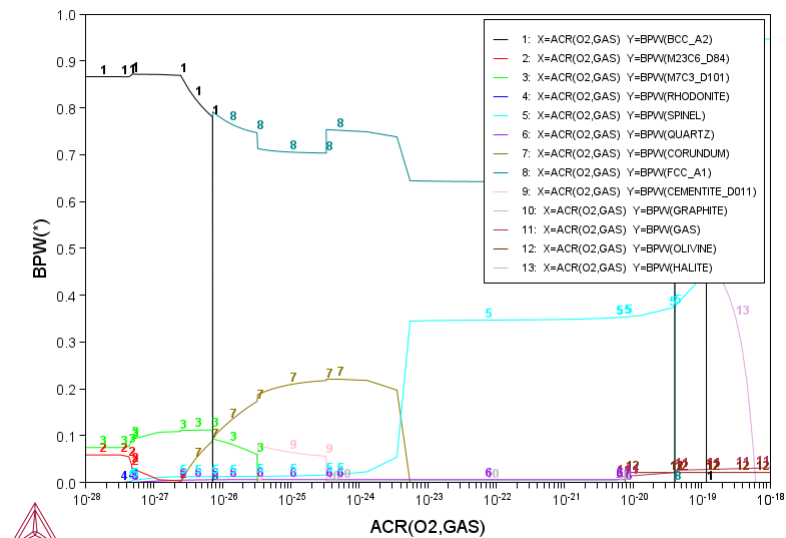


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-lab f
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s x n 1e-28 1e-18
... the command in full is SET_SCALING_STATUS
POST: set-title example 32b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 32b

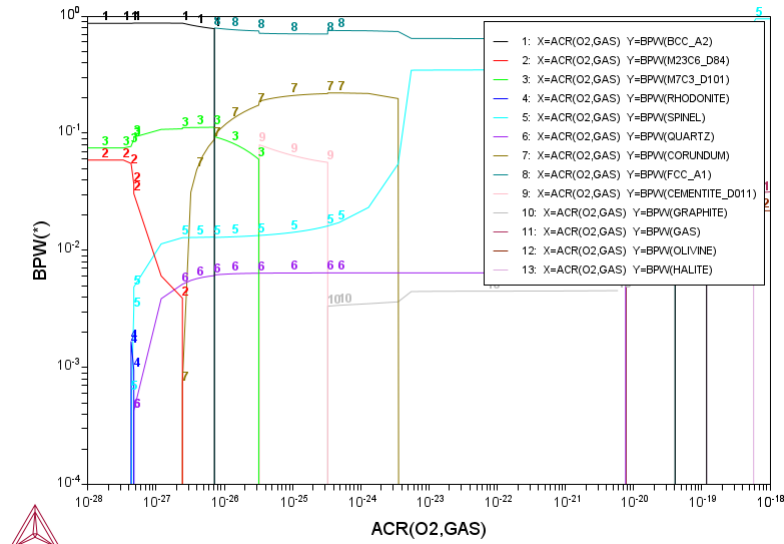


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-a-ty y
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: s-s y n 1e-4 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 32c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 32c

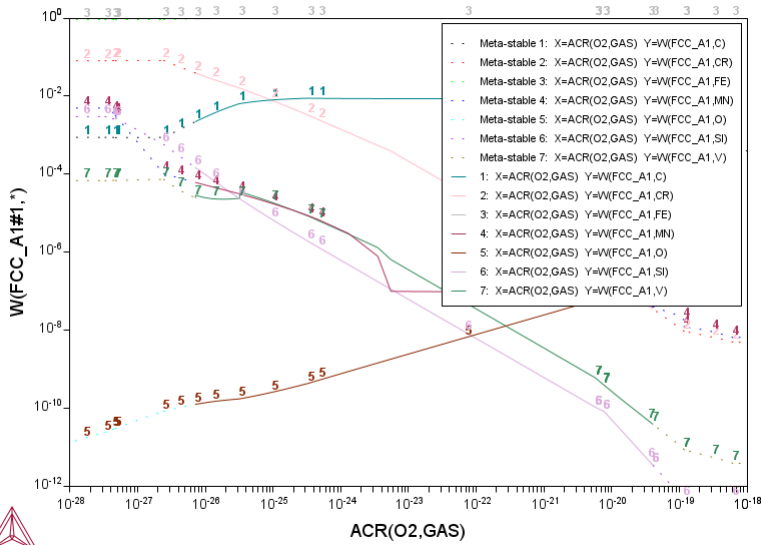


```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ Finally plot how the composition of FCC varies.
POST: s-d-a y w(fcc_a1#1,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 32d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 32d



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex33

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex33\tcex33.TCM.test"

SYS: set-echo

SYS: @@

SYS: @@

SYS: @@ Benchmark calculation for Fe-Cr-C isopleth

SYS: @@

SYS: set-log ex33,,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw FEDEMO

... the command in full is SWITCH_DATABASE

Current database: Iron Demo Database v6.0

VA /- DEFINED

TDB_FEDEMO: d-sys fe cr c

... the command in full is DEFINE_SYSTEM

FE CR C

DEFINED

TDB_FEDEMO: rej ph /all

... the command in full is REJECT

GAS:G	LIQUID:L	BCC_A2
C14 LAVES	CBCC_A12	CEMENTITE_D011
CHI_A12	CUB_A13	DIAMOND_A4
FCC_A1	GRAPHITE_A9	HCP_A3
KSI_CARBIDE	M23C6_D84	M3C2_D510
M5C2	M7C3_D101	SIGMA_D8B

REJECTED

TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 graphite sigma cementite m23 m7 m3c2

... the command in full is RESTORE

LIQUID:L	FCC_A1	BCC_A2
GRAPHITE_A9	SIGMA_D8B	CEMENTITE_D011
M23C6_D84	M7C3_D101	M3C2_D510

RESTORED

TDB_FEDEMO: get

... the command in full is GET_DATA

09:25:35,669 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set FCC_A1#2

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_FEDEMO: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: s-c t=1200,p=1e5,n=1 w(cr)=.13 w(c)=.01

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 10193 grid points in 0.383 s

Found the set of lowest grid points in 0.002 s

Calculated POLY solution 0.113 s, total time 0.498 s

POLY: s-a-v 1 w(c) 0 .02

... the command in full is SET_AXIS_VARIABLE

Increment /5E-04/: 5E-04

POLY: s-a-v 2 t 800 2000

... the command in full is SET_AXIS_VARIABLE

Increment /30/: 30

POLY: save tcex33 y

... the command in full is SAVE_WORKSPACES

POLY: map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 6.615E-03 8.100E+02
  BCC_A2
  M23C6_D84
  ** M7C3_D101
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 6.665E-03 8.000E+02
  BCC_A2
  M23C6_D84
  ** M7C3_D101
Calculated. 11 equilibria

Phase region boundary 3 at: 5.191E-03 1.088E+03
  BCC_A2
  ** FCC_A1#1
  M23C6_D84
  ** M7C3_D101

Phase region boundary 4 at: 5.191E-03 1.088E+03
  BCC_A2
  ** FCC_A1#1
  M23C6_D84
Calculated. 12 equilibria

Phase region boundary 5 at: 1.203E-04 1.127E+03
  BCC_A2
  ** FCC_A1#1
  ** M23C6_D84

Phase region boundary 6 at: 1.203E-04 1.127E+03
  BCC_A2
  ** FCC_A1#1
Calculated 18 equilibria

Phase region boundary 7 at: 1.203E-04 1.127E+03
  BCC_A2
  ** M23C6_D84
Calculated.. 12 equilibria
Terminating at axis limit.

Phase region boundary 8 at: 1.203E-04 1.127E+03
  BCC_A2
  FCC_A1#1
  ** M23C6_D84
Calculated. 3 equilibria

Phase region boundary 9 at: 1.027E-03 1.162E+03
  ** BCC_A2
  FCC_A1#1
  ** M23C6_D84

Phase region boundary 10 at: 1.027E-03 1.162E+03
  FCC_A1#1
  ** M23C6_D84
Calculated. 9 equilibria

Phase region boundary 11 at: 3.934E-03 1.328E+03
  FCC_A1#1
  ** M23C6_D84
  ** M7C3_D101

Phase region boundary 12 at: 3.934E-03 1.328E+03
  FCC_A1#1
  ** M23C6_D84
  M7C3_D101
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 3.934E-03 1.328E+03
  FCC_A1#1
  ** M7C3_D101
Calculated. 19 equilibria

Phase region boundary 14 at: 1.106E-02 1.554E+03
  ** LIQUID
  FCC_A1#1
  ** M7C3_D101

Phase region boundary 15 at: 1.106E-02 1.554E+03
  LIQUID
  FCC_A1#1
  ** M7C3_D101
Calculated.. 20 equilibria
Terminating at axis limit.

```

Phase region boundary 16 at: 1.106E-02 1.554E+03
 ** LIQUID
 FCC_A1#1
 Calculated. 16 equilibria

Phase region boundary 17 at: 5.090E-03 1.667E+03
 ** LIQUID
 ** BCC_A2
 FCC_A1#1

Phase region boundary 18 at: 5.090E-03 1.667E+03
 ** LIQUID
 BCC_A2
 FCC_A1#1
 Calculated. 8 equilibria

Phase region boundary 19 at: 2.029E-03 1.685E+03
 ** LIQUID
 BCC_A2
 ** FCC_A1#1

Phase region boundary 20 at: 2.029E-03 1.685E+03
 ** LIQUID
 BCC_A2
 Calculated 24 equilibria

Phase region boundary 21 at: 2.029E-03 1.685E+03
 BCC_A2
 ** FCC_A1#1
 Calculated 26 equilibria

Phase region boundary 22 at: 2.029E-03 1.685E+03
 LIQUID
 BCC_A2
 ** FCC_A1#1
 Calculated. 17 equilibria

Phase region boundary 23 at: 9.895E-03 1.706E+03
 LIQUID
 ** BCC_A2
 ** FCC_A1#1

Phase region boundary 24 at: 9.895E-03 1.706E+03
 LIQUID
 ** FCC_A1#1
 Calculated.. 22 equilibria
 Terminating at axis limit.

Phase region boundary 25 at: 9.895E-03 1.706E+03
 LIQUID
 ** BCC_A2
 Calculated 32 equilibria

Phase region boundary 26 at: 9.895E-03 1.706E+03
 LIQUID
 ** BCC_A2
 FCC_A1#1
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 5.090E-03 1.667E+03
 ** BCC_A2
 FCC_A1#1
 Calculated. 18 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 1.106E-02 1.554E+03
 ** LIQUID
 FCC_A1#1
 M7C3_D101
 Calculated.. 20 equilibria
 Terminating at axis limit.

Phase region boundary 29 at: 3.934E-03 1.328E+03
 FCC_A1#1
 M23C6_D84
 ** M7C3_D101
 Calculated. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 1.027E-03 1.162E+03
 ** BCC_A2
 FCC_A1#1
 M23C6_D84
 Calculated. 14 equilibria
 Terminating at known equilibrium

Phase region boundary 31 at: 6.464E-03 1.088E+03
 BCC_A2
 ** FCC_A1#1
 M7C3_D101
 Calculated.. 29 equilibria
 Terminating at axis limit.

Phase region boundary 32 at: 7.028E-03 1.088E+03
 ** BCC_A2
 FCC_A1#1
 M7C3_D101
 Calculated.. 28 equilibria
 Terminating at axis limit.

Phase region boundary 33 at: 6.464E-03 1.088E+03
 BCC_A2
 ** M23C6_D84
 M7C3_D101
 Calculated.. 11 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 34 at: 6.615E-03 8.100E+02
 BCC_A2
 M23C6_D84
 ** M7C3_D101
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 35 at: 5.000E-04 1.122E+03
 BCC_A2
 ** FCC_A1#1
 M23C6_D84
 Calculated. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 36 at: 5.000E-04 1.122E+03
 BCC_A2
 ** FCC_A1#1
 M23C6_D84
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 37 at: 6.833E-03 1.055E+03
 BCC_A2
 ** M23C6_D84
 M7C3_D101
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 38 at: 6.833E-03 1.055E+03
 BCC_A2
 ** M23C6_D84
 M7C3_D101
 Calculated.. 12 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 39 at: 1.317E-02 1.076E+03
 BCC_A2
 ** FCC_A1#1
 M7C3_D101
 Calculated. 15 equilibria
 Terminating at known equilibrium

Phase region boundary 40 at: 1.317E-02 1.076E+03
 BCC_A2
 ** FCC_A1#1
 M7C3_D101
 Calculated.. 15 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 41 at: 1.943E-02 8.100E+02
 BCC_A2
 M3C2_D510
 ** M7C3_D101
 Calculated.. 3 equilibria
 Terminating at axis limit.

Phase region boundary 42 at: 1.941E-02 8.000E+02
 BCC_A2
 M3C2_D510
 ** M7C3_D101
 Calculated. 19 equilibria

Phase region boundary 43 at: 1.973E-02 8.151E+02
 BCC_A2
 ** GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101

Phase region boundary 44 at: 1.973E-02 8.151E+02
 BCC_A2
 ** GRAPHITE_A9
 M3C2_D510
 Calculated.. 2 equilibria
 Terminating at axis limit.

Phase region boundary 45 at: 2.266E-02 8.151E+02
 BCC_A2
 ** GRAPHITE_A9
 M7C3_D101

Phase region boundary 46 at: 7.607E-01 8.151E+02
 ** BCC_A2
 GRAPHITE_A9
 M7C3_D101

Phase region boundary 47 at: 2.266E-02 8.151E+02
 BCC_A2
 ** M3C2_D510
 M7C3_D101

Phase region boundary 48 at: 7.607E-01 8.151E+02
 GRAPHITE_A9
 ** M3C2_D510
 M7C3_D101

Phase region boundary 49 at: 1.943E-02 8.100E+02
 BCC_A2
 M3C2_D510
 ** M7C3_D101
 Calculated. 22 equilibria
 Terminating at known equilibrium

Phase region boundary 50 at: 1.950E-02 8.204E+02
 BCC_A2
 M3C2_D510
 ** M7C3_D101
 Calculated.. 7 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 51 at: 1.950E-02 8.204E+02
 BCC_A2
 M3C2_D510
 ** M7C3_D101
 Calculated. 8 equilibria
 Terminating at known equilibrium

Phase region boundary 52 at: 8.289E-04 1.203E+03
 ** BCC_A2
 FCC_A1#1

```

Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 53 at:  8.289E-04  1.203E+03
** BCC_A2
   FCC_A1#1
Calculated.          17 equilibria
Terminating at known equilibrium

Phase region boundary 54 at:  6.104E-03  1.203E+03
   FCC_A1#1
** M23C6_D84
   M7C3_D101
Calculated.           5 equilibria
Terminating at known equilibrium

Phase region boundary 55 at:  6.104E-03  1.203E+03
   FCC_A1#1
** M23C6_D84
   M7C3_D101
Calculated.           7 equilibria
Terminating at known equilibrium

Phase region boundary 56 at:  1.148E-03  1.597E+03
   BCC_A2
** FCC_A1#1
Calculated            26 equilibria

Phase region boundary 57 at:  1.148E-03  1.597E+03
   BCC_A2
** FCC_A1#1
Calculated.           4 equilibria
Terminating at known equilibrium

Phase region boundary 58 at:  8.870E-03  1.597E+03
** LIQUID
   FCC_A1#1
Calculated.           7 equilibria
Terminating at known equilibrium

Phase region boundary 59 at:  8.870E-03  1.597E+03
** LIQUID
   FCC_A1#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 60 at:  5.000E-04  1.788E+03
   LIQUID
** BCC_A2
Calculated            22 equilibria

Phase region boundary 61 at:  5.000E-04  1.788E+03
   LIQUID
** BCC_A2
Calculated.           20 equilibria
Terminating at known equilibrium

Phase region boundary 62 at:  6.833E-03  1.733E+03
   LIQUID
** BCC_A2
Calculated            26 equilibria

Phase region boundary 63 at:  6.833E-03  1.733E+03
   LIQUID
** BCC_A2
Calculated.           8 equilibria
Terminating at known equilibrium

Phase region boundary 64 at:  1.317E-02  1.688E+03
   LIQUID
** FCC_A1#1
Calculated.           8 equilibria
Terminating at known equilibrium

Phase region boundary 65 at:  1.317E-02  1.688E+03
   LIQUID
** FCC_A1#1
Calculated..          15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 66 at:  1.950E-02  1.652E+03
   LIQUID
** FCC_A1#1
Calculated.           21 equilibria
Terminating at known equilibrium

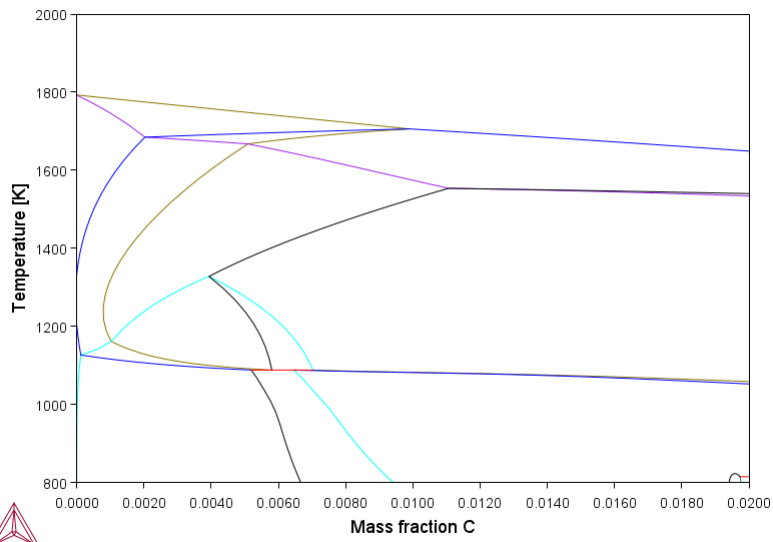
Phase region boundary 67 at:  1.950E-02  1.652E+03
   LIQUID
** FCC_A1#1
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex33\tcex33.POLY3
CPU time for mapping          11 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: set-title example 33a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 33a



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tcex34

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex34\tcex34.TCM"

SYS: set-echo

SYS:

SYS: @@ The Al-Zn phase diagram and its G curve

SYS:

SYS: @@ This example uses the BINARY module to calculate

SYS: @@ the phase diagram and G curves in the Al-Zn system.

SYS:

SYS: go bin

THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED

First element: al zn

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase_Diagram

VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
REINITIATING GES
AL ZN DEFINED
GAS:G LIQUID:L IONIC_LIQUID:Y
FCC_A1 BCC_A2 A2_BCC
HCP_A3 HCP_ZN DIAMOND_A4
BCT_A5 TETRAGONAL_A6 RHOMBOHEDRAL_A7
CBCC_A12 CUB_A13 B32_ALLI
B3_ZINCBLLENDE C14_LAVES C15_LAVES
C16_AL2CU C36_LAVES D019_ALIM3
D513_AL3NI2 D82_FEZN_GAMMA L10_ALTI
AGZN_ZETA AL5FE4 ALCE_AMORPHOUS
ALCU_ETA FEZN4 FEZN_DELTA

FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
HCP_ZN RESTORED

09:26:43,687 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Creating a new composition set FCC_A1#2
The condition X(ZN)=.1234 created
The condition T=612.43 created

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Forcing automatic start values
Automatic start values will be set
Start points provided by database
Version S mapping is selected

Organizing start points

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 5.345E-01 5.000E+02
** FCC_A1#1
HCP_ZN
Calculated.. 10 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 5.027E-01 3.000E+02
** FCC_A1#1
HCP_ZN
Calculated. 13 equilibria

Phase region boundary 3 at: 5.626E-01 5.504E+02
** FCC_A1#1
** FCC_A1#2
HCP_ZN

Phase region boundary 4 at: 7.872E-01 5.504E+02
** FCC_A1#1
HCP_ZN
Calculated. 6 equilibria

Phase region boundary 5 at: 8.211E-01 6.540E+02
** LIQUID

```

** FCC_A1#1
HCP_ZN

Phase region boundary 6 at: 9.263E-01 6.540E+02
** LIQUID
HCP_ZN
Calculated 17 equilibria

Phase region boundary 7 at: 7.783E-01 6.540E+02
** LIQUID
FCC_A1#1
Calculated 73 equilibria

Phase region boundary 8 at: 3.658E-01 5.504E+02
** FCC_A1#1
FCC_A1#2
Calculated 27 equilibria

Phase region boundary 9 at: 5.345E-01 5.000E+02
** FCC_A1#1
HCP_ZN
Calculated. 5 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping 3 seconds
POSTPROCESSOR VERSION 3.2

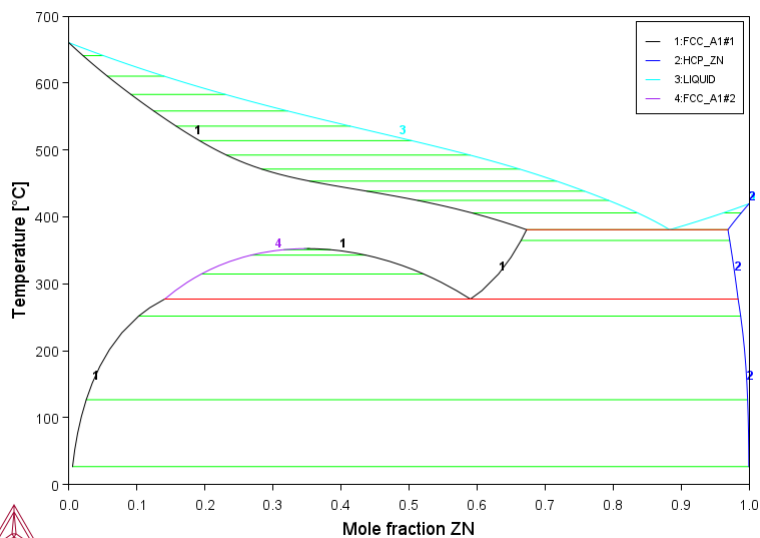
```

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

AL ZN

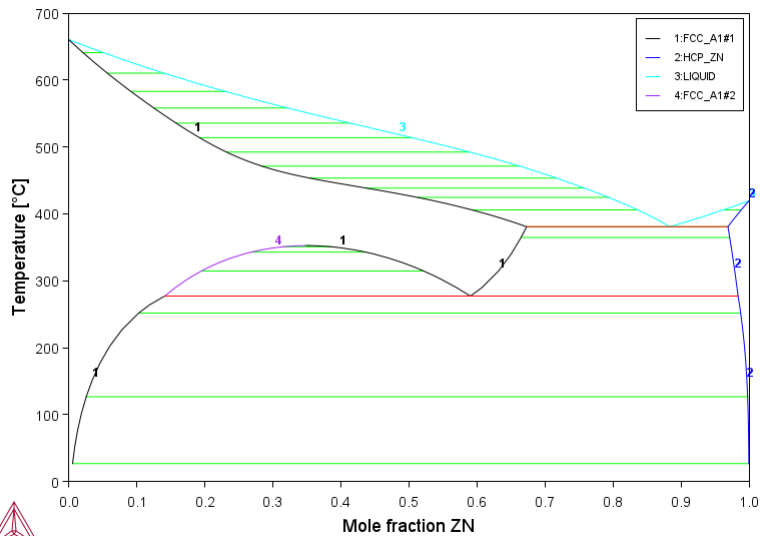


```

POST: set-title example 34a
POST: plot

```

example 34a



```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot a G curve at 573 K!
POST: back
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
SYS: go bin
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED

```

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED

First element: al zn

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G

Temperature (C): /1000/: 300

VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
REINITIATING GES
AL ZN DEFINED
GAS:G LIQUID:L IONIC LIQUID:Y
FCC_A1 BCC_A2 A2_BCC
HCP_A3 HCP_ZN DIAMOND_A4
BCT_A5 TETRAGONAL_A6 RHOMBOHEDRAL_A7
CBCC_A12 CUB_A13 B32_ALLI
B3_ZINCBLLENDE C14_LAVES C15_LAVES
C16_AL2CU C36_LAVES D019_ALIM3
D513_AL3NI2 D82_FEZN_GAMMA L10_ALTI
AGZN_ZETA AL5FE4 ALCE_AMORPHOUS
ALCU_ETA FEZN4 FEZN_DELTA
FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
HCP_ZN RESTORED
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Creating a new composition set FCC_A1#2

The condition X(ZN)=.1234 created

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

Forcing automatic start values

Automatic start values will be set

Phase Region from 0.502463 for:

LIQUID
FCC_A1#1
FCC_A1#2
HCP_A3
HCP_ZN

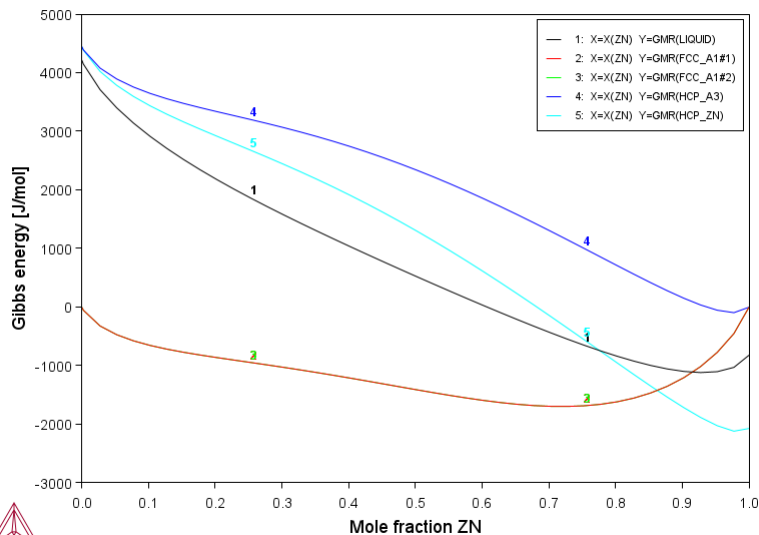
Phase Region from 0.502463 for:

LIQUID
FCC_A1#1
FCC_A1#2
HCP_A3
HCP_ZN

*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\GCURVE_002.POLY3

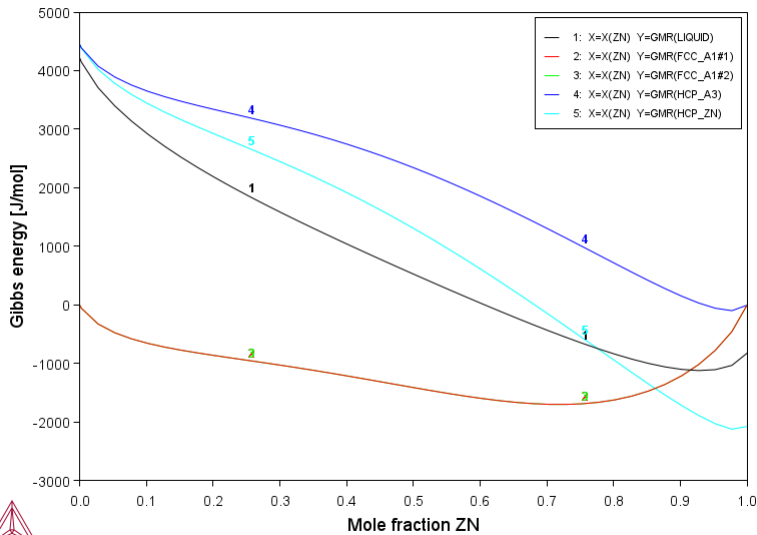
POSTPROCESSOR VERSION 3.2

AL ZN



POST:
POST: set-title example 34b
POST:
POST: plot

example 34b



```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot an activity (A) curve at 573 K
POST: back
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
SYS: go bin
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

VA /- DEFINED
BCC_B2 /- DEFINED FCC_L12 FCC_L102
D021_HCP REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: A
Temperature (C): /1000/: 300
VA /- DEFINED
BCC_B2 /- DEFINED FCC_L12 FCC_L102
D021_HCP REJECTED
REINITIATING GES .....
AL ZN DEFINED
GAS:G LIQUID:L IONIC_LIQUID:Y
FCC_A1 BCC_A2 A2_BCC
HCP_A3 HCP_ZN DIAMOND_A4
BCT_A5 TETRAGONAL_A6 RHOMBOHEDRAL_A7
CBCC_A12 CUB_A13 B32_ALLI
B3_ZINCBLENDE C14_LAVES C15_LAVES
C16_AL2CU C36_LAVES D019_AL1M3
D513_AL3NI2 D82_FEZN_GAMMA L10_ALTI
AGZN_ZETA AL5FE4 ALCE_AMORPHOUS
ALCU_ETA FEZN4 FEZN_DELTA
FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
HCP_ZN RESTORED
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Creating a new composition set FCC_A1#2
The condition X(ZN)=.1234 created

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Forcing automatic start values
Automatic start values will be set
No initial equilibrium, using default
Step will start from axis value 0.123400
...OK

Phase Region from 0.123400 for:
FCC_A1#1
Global Test at 3.23400E-01 .. Backtracking to find phase change for FCC_A1#2
Global test at 1.48400E-01 .... OK
Global check of adding phase at 1.70853E-01
Calculated 5 equilibria

Phase Region from 0.170853 for:
FCC_A1#1
FCC_A1#2
Global Test at 3.48400E-01 .... OK
Global check of removing phase at 5.51861E-01
Calculated 19 equilibria

Phase Region from 0.551861 for:

```

```

FCC_A1#2
Global check of adding phase at 6.18456E-01
Calculated 5 equilibria

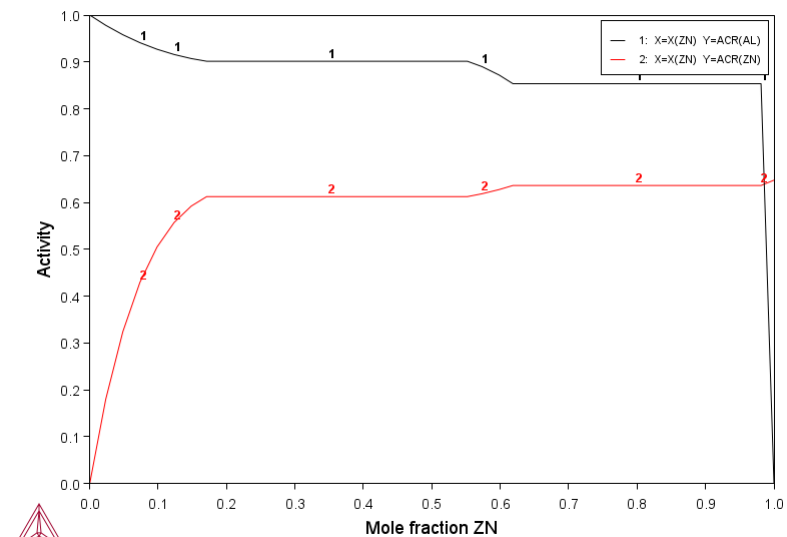
Phase Region from 0.618456 for:
FCC_A1#2
HCP_ZN
Global test at 7.98400E-01 .... OK
Global check of removing phase at 9.81102E-01
Calculated 18 equilibria

Phase Region from 0.981102 for:
HCP_ZN
Terminating at 1.00000
Calculated 4 equilibria

Phase Region from 0.123400 for:
FCC_A1#1
Terminating at 0.100000E-11
Calculated 8 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\GCURVE_002.POLY3
POSTPROCESSOR VERSION 3.2

```

AL ZN

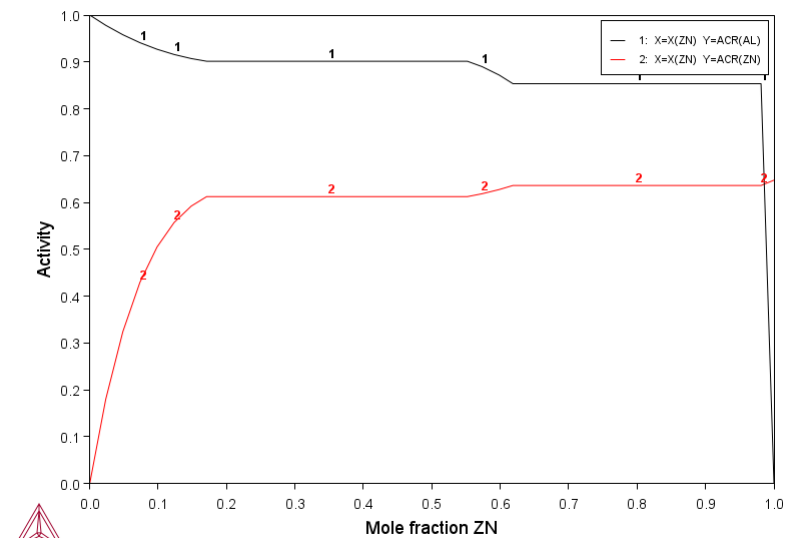


```

POST:
POST: set-title example 34c
POST:
POST: plot

```

example 34c



```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot a Phase fraction (F) curve for
POST: @@ x(zn)=.5. The miscibility gap is found now
POST: back
Current database: Steels/Fe-Alloys v11.0

```

```

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
SYS: go bin
Current database: Steels/Fe-Alloys v11.0

```

```

VA /- DEFINED
DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

```

```

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

```

```

VA /- DEFINED
BCC B2 FCC_L12 FCC_L102
D021_HCP REJECTED

```



```

First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: F
Fraction of: zn /.5/: .5
VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
REINITIATING GES .....
AL ZN DEFINED
GAS:G LIQUID:L IONIC_LIQUID:Y
FCC_A1 BCC_A2 A2_BCC
HCP_A3 HCP_ZN DIAMOND_A4
BCT_A5 TETRAGONAL_A6 RHOMBOHEDRAL_A7
CBCC_A12 CUB_A13 B32_ALLI
B3_ZINCBLLENDE C14_LAVES C15_LAVES
C16_AL2CU C36_LAVES D019_ALIM3
D513_AL3NI2 D82_FEZN_GAMMA L10_ALTI
AGZN_ZETA AL5FE4 ALCE_AMORPHOUS
ALCU_ETA FEZN4 FEZN_DELTA
FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
HCP_ZN RESTORED
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
Creating a new composition set FCC_A1#2
Forcing automatic start values
Automatic start values will be set
No initial equilibrium, using default
Step will start from axis value 1000.00
...OK

Phase Region from 1000.00 for:
LIQUID
Global test at 9.20000E+02 .... OK
Global test at 8.20000E+02 .... OK
Global check of adding phase at 7.88048E+02
Calculated 24 equilibria

Phase Region from 788.048 for:
LIQUID
FCC_A1#1
Global test at 7.26000E+02 .... OK
Global test at 7.06000E+02 .... OK
Global check of removing phase at 7.00299E+02
Calculated 23 equilibria

Phase Region from 700.299 for:
FCC_A1#1
Global test at 6.28000E+02 .... OK
Global test at 5.28000E+02 .. Backtracking to find phase change for FCC_A1#2
Global test at 6.18000E+02 .... OK
Global test at 5.98000E+02 .... OK
Global check of adding phase at 5.96831E+02
Calculated 15 equilibria

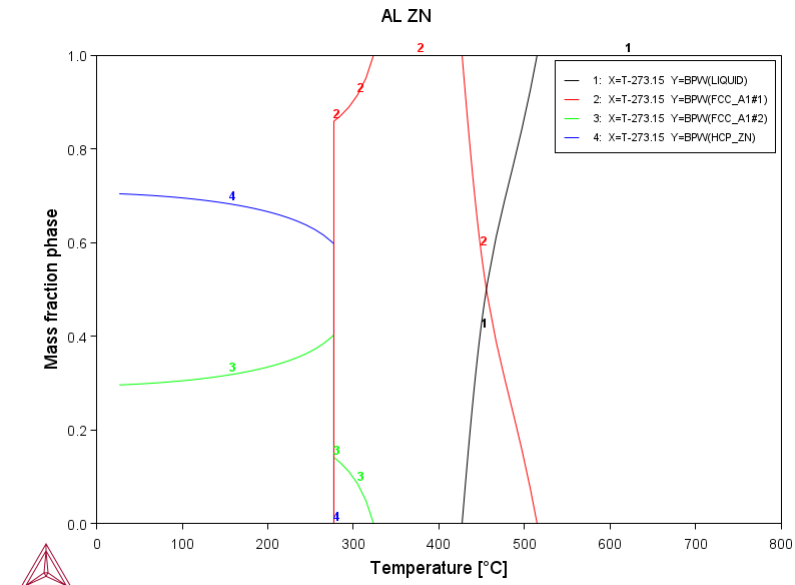
Phase Region from 596.831 for:
FCC_A1#1
FCC_A1#2
Global check of adding phase at 5.50386E+02
Calculated 7 equilibria

Phase Region from 550.386 for:
FCC_A1#1
FCC_A1#2
HCP_ZN
Calculated 2 equilibria

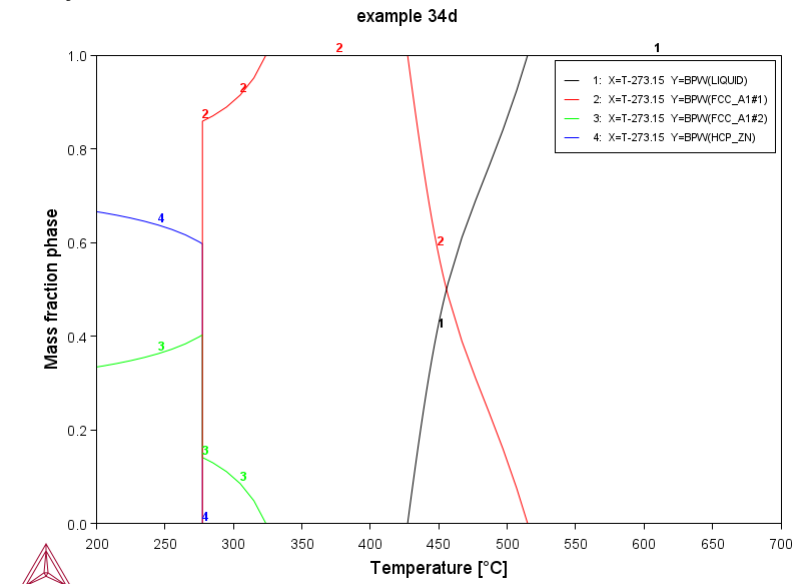
Phase Region from 550.386 for:
FCC_A1#2
HCP_ZN
Global test at 4.78000E+02 .... OK
Global test at 3.78000E+02 .... OK
Terminating at 300.000
Calculated 29 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\PFCURVE_002.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```



POST: s-s x n 200 700
POST: set-title example 34d
POST: plot



POST: set-inter

tcex35

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex35\tcex35.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a potential diagram using

SYS: @@ the POTENTIAL module.

SYS:

SYS: @@ There are no commands for this module, you

SYS: @@ just follow the prompts.

SYS:

SYS: go pot

Simple potential phase diagram calculation module

Database: /POT/: SUBDEMO

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Substance Demo Database v1.0

VA /- DEFINED

Matrix element: /FE/: FE

First potential species: /SI02/: C101

Second potential species: /O2/: O2

Temperature: /1000/: 1000

VA /- DEFINED

REINITIATING GES

FE C O

DEFINED

09:27:55,773 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

This command is DEPRECATED and to be removed in the future!

Please use ADVANCED_OPTIONS instead of SPECIAL_OPTIONS

The condition LNACR(C101,GAS)=-140.8589 created

The condition LNACR(O2,GAS)=-140.8589 created

Normal POLY minimization, not global

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Working hard

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Phase region boundary 1 at: -4.633E+01 -1.409E+02

FE_S

** GRAPHITE

Calculated.. 81 equilibria

Terminating at axis limit.

Phase region boundary 2 at: -1.259E+02 -3.000E+02

FE_S

** GRAPHITE

Calculated. 126 equilibria

Phase region boundary 3 at: -9.383E-01 -5.007E+01

** FE101_S

FE_S

** GRAPHITE

Phase region boundary 4 at: -9.383E-01 -5.007E+01

** FE101_S

FE_S

Calculated.. 151 equilibria

Terminating at axis limit.

Phase region boundary 5 at: -9.383E-01 -5.007E+01

** FE101_S

GRAPHITE

Calculated. 2 equilibria

Phase region boundary 6 at: -3.398E-01 -4.887E+01

** GAS

** FE101_S

GRAPHITE

Phase region boundary 7 at: -3.398E-01 -4.887E+01

** GAS

GRAPHITE

+++++

Phase region boundary 8 at: -3.398E-01 -4.887E+01

** GAS

FE101_S

Calculated. 7 equilibria

Phase region boundary 9 at: -3.272E+00 -4.059E+01

```

** GAS
FE101_S
** MAGNETITE

Phase region boundary 10 at: -3.272E+00 -4.059E+01
FE101_S
** MAGNETITE
Calculated.. 150 equilibria
Terminating at axis limit.

Phase region boundary 11 at: -3.272E+00 -4.059E+01
GAS
** MAGNETITE
Calculated.. 10 equilibria

Phase region boundary 12 at: -1.174E+01 -2.359E+01
GAS
** HEMATITE
** MAGNETITE

Phase region boundary 13 at: -1.174E+01 -2.359E+01
GAS
** HEMATITE
Calculated.. 168 equilibria
Terminating at axis limit.

Phase region boundary 14 at: -1.174E+01 -2.359E+01
** HEMATITE
MAGNETITE
Calculated.. 146 equilibria
Terminating at axis limit.

Phase region boundary 15 at: -4.633E+01 -1.409E+02
FE_S
** GRAPHITE
Calculated.. 47 equilibria
Terminating at known equilibrium

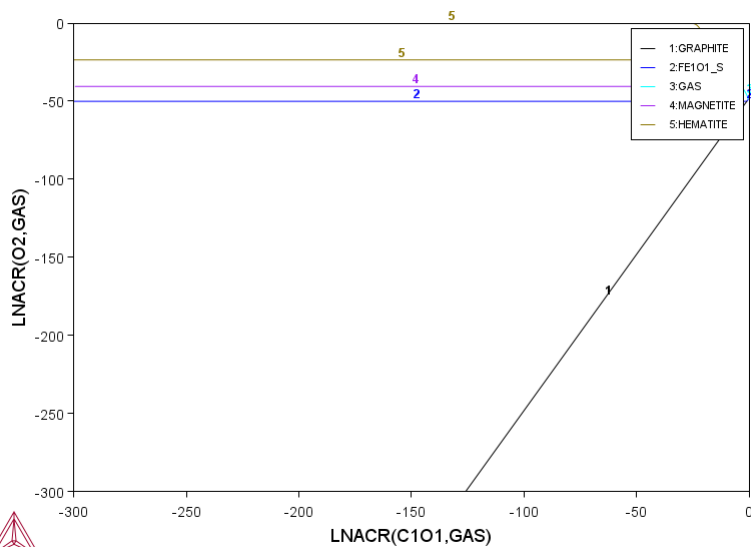
Phase region boundary 16 at: -1.409E+02 -5.007E+01
** FE101_S
FE_S
Calculated.. 81 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 17 at: -1.409E+02 -5.007E+01
** FE101_S
FE_S
Calculated.. 71 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex35\POT.POLY3
CPU time for mapping 6 seconds
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

FE C101 O2; Database: SUBDEMO

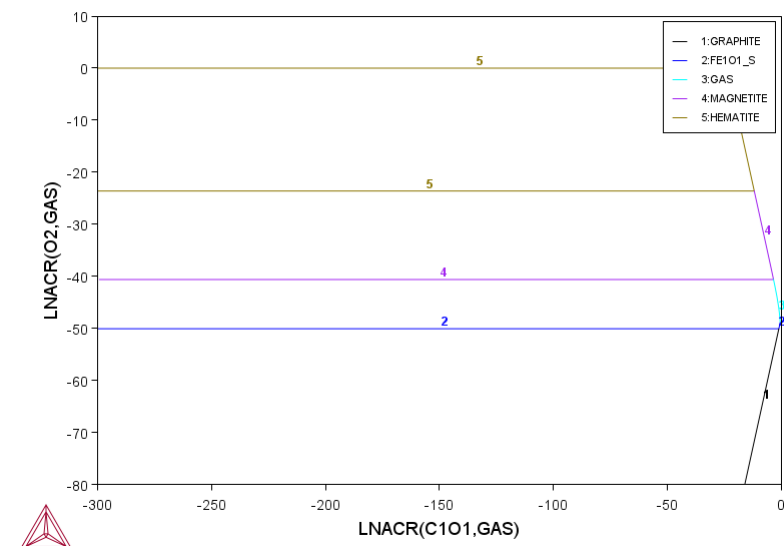


```

POST: s-s y n -80 10
POST: set-title example 35a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```

example 35a



POST:
POST: set-inter
POST:

tcex36a

SYS>About

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Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36a.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Assessment. The use of the PARROT module

SYS:

SYS: @@ This is the setup file for Windows systems

SYS:

SYS: @@ First the elements and phases must be entered in G-E-S module

SYS: GO G

GIBBS ENERGY SYSTEM
09:29:19,876 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

GES6: ENTER-ELEMENT A B

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

GES6: AMEND-ELEMENT-DATA A BCC 20 0 0 1

GES6: AMEND-ELEMENT-DATA B BCC 50 0 0 1

GES6: ENTER-PHASE LIQUID L 1 A B; N N

GES6: ENTER-PHASE BCC,, 1 A B; N N

GES6: ENTER-PHASE FCC,, 1 A B; N N

GES6: ENTER-PHASE A2B,, 2 2 1 A; B; N N

CONSTITUENTS IN SUBLATTICE 1

CONSTITUENTS IN SUBLATTICE 2

GES6: @@ There is a miscibility gap in the bcc, this must be stated here

GES6: AMEND_PHASE BCC COMPOSITION_SETS 2 B

Creating a new composition set BCC#2

GES6: @@ We can also set the major constituent of the first composition set

GES6: AMEND_PHASE BCC MAJOR 1 A

GES6:

GES6: @@ The FCC phase is stable only for element B

GES6: AMEND_PHASE FCC MAJOR 1 B

GES6: @@ The parameters can be entered in the PARROT module

GES6: GO PAR

PARROT VERSION 5.3

Global minimization used as test only

PARROT: ENTER-PARAMETER G(BCC,A) 500 0; 2000 N

G(BCC,A;0)-G(BCC,A;0)

PARROT: ENTER-PARAMETER G(BCC,B) 500 0; 2000 N

G(BCC,B;0)-G(BCC,B;0)

PARROT: ENTER-PARAMETER G(LIQUID,A) 500 14000-10*T; 2000 N

G(LIQUID,A;0)-G(BCC,A;0)

PARROT: ENTER-PARAMETER G(LIQUID,B) 500 18000-12*T; 2000 N

G(LIQUID,B;0)-G(BCC,B;0)

PARROT: ENTER-PARAMETER G(FCC,B) 500 3300-3*T; 2000 N

G(FCC,B;0)-G(BCC,B;0)

PARROT: ENTER-PARAMETER G(FCC,A) 500 408; 2000 N

G(FCC,A;0)-G(BCC,A;0)

PARROT: ENTER-PARAMETER G(A2B) 500 V1+V2*T+V3*T*LOG(T); 2000 N

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0)

PARROT: ENTER-PARAMETER G(LIQUID,A,B;0) 500 V11+V12*T; 2000 N

G(LIQUID,A,B;0)

PARROT: ENTER-PARAMETER G(LIQUID,A,B;1) 500 V13+V14*T; 2000 N

G(LIQUID,A,B;1)

PARROT: ENTER-PARAMETER G(BCC,A,B;0) 500 V15+V16*T; 2000 N

G(BCC,A,B;0)

PARROT: ENTER-PARAMETER G(BCC,A,B;1) 500 V17+V18*T; 2000 N

G(BCC,A,B;1)

PARROT: ENTER-PARAMETER G(FCC,A,B;0) 500 V19+V20*T; 2000 N

G(FCC,A,B;0)

PARROT: ENTER-PARAMETER G(FCC,A,B;1) 500 V21+V22*T; 2000 N

G(FCC,A,B;1)

PARROT:

PARROT: @@ Everything is saved to an unformatted work file by the Create command

PARROT: CREATE tcex36

PARROT:

PARROT:Hit RETURN to continue

PARROT:

PARROT: @@ The experimental data file is compiled to the work file.

PARROT: COMPILE tcex36 screen Y exp36

POP files may include graphics information using the GRAPHICS_PLOT command. A file name for generating an ".exp" file must be given.

\$

\$ POP file for assessment example

\$

\$ Enter some constants used later.

ENTER_SYMBOL CONSTANT DX=0.02,P0=101325,DH=500,DT=10

\$

\$ Eutectic point at A rich side from ref #2.

\$ T=1193 K, 40.8 w/o B in liquid, 13 w/o B in bcc.

\$ In a binary system one must have four conditions if P is not fixed.

\$ We obtain this by fixing the pressure and that three phases must be stable.

\$ The amount of the fixed phases is irrelevant here

CREATE_NEW_EQUILIBRIUM 1,1

CHANGE_STATUS PHASE LIQUID,BCC,A2B=FIX 1

SET-CONDITION P=P0

EXPERIMENT T=1193:DT,W(LIQ,B)=.408:DX,W(BCC,B)=.13:DX

GRAPHICS 1 .408 1193 MS5

GRAPHICS 1 .13 1193 DS5

GRAPHICS 1 .555 1193 DS5

LABEL AINV

```

SET-ALT X(A2B,A)=.6666667
SET_ALL_START 1193 Y
Automatic start values will be set
$
$ Congrent melting temperature for A2B 1341 K.
$ We will include the enthalpy of transformation also and this
$ requires a function.
ENTER_SYMBOL FUNCTION HTR=HM(LIQUID)-HM(A2B);
$
$ Note how one specifies that this is a congruent transformation!
CREATE_NEW EQUILIBRIUM 2,1
CHANGE_STATUS PHASE LIQ,A2B=FIX 1
SET-CONDITION P=P0,X(LIQ,B)-X(A2B,B)=0
EXPERIMENT T=1341:DT
EXPERIMENT HTR=3727:500
GRAPHICS 1 .555 1341 MS7
LABEL AINV
SET-ALT X(A)=.6666667
SET_ALL_START 1341 Y
Automatic start values will be set
$
$ Eutectic point at B rich side.
$ T=1049 K, 27 w/o A in liquid, 9.3 w/o A in bcc.
CREATE_NEW EQUILIBRIUM 3,1
CHANGE_STATUS PHASE LIQ,BCC,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=1049:DT,W(LIQ,A)=.27:DX,W(BCC,A)=.093:DX
SET-ALT X(A2B,A)=.66666667
GRAPHICS 1 .907 1049 MS5
GRAPHICS 1 .73 1049 DS5
GRAPHICS 1 .555 1049 DS5
LABEL AINV
SET_ALL_START 1049 Y
Automatic start values will be set
$
$ Peritectic point. T=1203 K, 19 w/o A in liquid, 6.9 w/o A in bcc,
$ 6.0 w/o A in fcc.
CREATE_NEW EQUILIBRIUM 4,1
CHANGE_STATUS PHASE LIQ,BCC,FCC=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=1203:DT,W(LIQ,A)=.19:DX,W(BCC,A)=.069:DX,W(FCC,A)=.06:DX
GRAPHICS 1 .81 1203 MS5
GRAPHICS 1 .931 1203 DS5
GRAPHICS 1 .94 1203 DS5
LABEL AINV
SET_ALL_START 1203 Y
Automatic start values will be set
$
$ Eutectoid transformation of A2B -> BCC1 + BCC2, from ref #3
$ T=726, 3.7 at/o B in A, 11.4 at/o A in B
$ Note that miscibility gaps are indicated by using # after the phase
$ name and then give an integer.
CREATE_NEW EQUILIBRIUM 5,1
CHANGE_STATUS PHASE BCC#1,BCC#2,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=726:DT,X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
SET-ALT X(A2B,A)=.6666667
GRAPHICS 1 0.09 726 MS5
GRAPHICS 1 0.95 726 DS5
LABEL AINV
SET_ALL_START 726 Y
Automatic start values will be set
$
$ It is sometimes useful to decribe an invariant equilibria as
$ three tie-lines between each pair of phases at the same temperature.
$ In this case it helps to add a tie-line across the miscibility gap
$ at the invariant temperature.
CREATE_NEW EQUILIBRIUM 6,1
CHANGE_STATUS PHASE BCC#1,BCC#2=FIX 1
SET-CONDITION P=P0 T=726
EXPERIMENT X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
LABEL AINV
SET_ALL_START Y
Automatic start values will be set
$
$ From ref #4 the liquidus at the B rich end:
$ The table values are referenced inside the table_head using @<column>
TABLE_HEAD 10
CREATE_NEW EQUILIBRIUM 0010,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1594,P=P0
EXPERIMENT W(LIQ,A)=0.02:DX
LABEL ALF
GRAPHICS 1 .98 1594 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW EQUILIBRIUM 0011,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1548,P=P0
EXPERIMENT W(LIQ,A)=0.042:DX
LABEL ALF
GRAPHICS 1 .958 1548 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW EQUILIBRIUM 0012,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1499,P=P0
EXPERIMENT W(LIQ,A)=0.065:DX
LABEL ALF
GRAPHICS 1 .935 1499 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW EQUILIBRIUM 0013,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1438,P=P0
EXPERIMENT W(LIQ,A)=0.093:DX
LABEL ALF
GRAPHICS 1 .907 1438 MS5
SET_ALL_START Y
Automatic start values will be set

$
$ From ref #5 we have the following tie-lines
TABLE_HEAD 20
CREATE_NEW EQUILIBRIUM 0020,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1

```

```

SET-CONDITION T=1413,P=P0
EXPERIMENT W(LIQ,A)=.104:DX,W(FCC,A)=.038:DX
GRAPHICS 1 .896 1413 MS9
GRAPHICS 1 .962 1413 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.104,Y(FCC,A)=.038
CREATE_NEW_EQUILIBRIUM 0021,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1337,P=P0
EXPERIMENT W(LIQ,A)=.136:DX,W(FCC,A)=.047:DX
GRAPHICS 1 .864 1337 MS9
GRAPHICS 1 .953 1337 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.136,Y(FCC,A)=.047
CREATE_NEW_EQUILIBRIUM 0022,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1213,P=P0
EXPERIMENT W(LIQ,A)=.187:DX,W(FCC,A)=.059:DX
GRAPHICS 1 .813 1213 MS9
GRAPHICS 1 .941 1213 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.187,Y(FCC,A)=.059
CREATE_NEW_EQUILIBRIUM 0023,1
CHANGE_STATUS PHASE LIQ,BCC=FIX 1
SET-CONDITION T=1100,P=P0
EXPERIMENT W(LIQ,A)=.245:DX,W(BCC,A)=.085:DX
GRAPHICS 1 .755 1100 MS9
GRAPHICS 1 .915 1100 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.245,Y(BCC,A)=.085

$
$ Thermochemical data
$ Activities of B in liquid (reference state fcc) at 1573 K.
$ The command SET_REFERENCE_STATE is used for this as the default
$ reference state for B is BCC.
$
$ Note that we have set an uncertainty on the fraction (condition) also.
TABLE_HEAD 100
CREATE_NEW_EQUILIBRIUM 0100,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.90:DX
SET_REFERENCE_STATE B FCC,,,,
09:29:22,603 [Thread-0] INFO Database: Preparing system for use: UNKNOWN_1747042159750
09:29:23,537 [Thread-0] INFO Phase: Preparing phase for use: FCC
EXPERIMENT ACR(B)=.94:DX
GRAPHICS 3 .90 .94 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0101,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.80:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.84:DX
GRAPHICS 3 .80 .84 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0102,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.70:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.74:DX
GRAPHICS 3 .70 .74 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0103,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.60:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.64:DX
GRAPHICS 3 .60 .64 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0104,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.50:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.54:DX
GRAPHICS 3 .50 .54 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0105,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.40:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.44:DX
GRAPHICS 3 .40 .44 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0106,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.30:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.34:DX
GRAPHICS 3 .30 .34 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0107,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.20:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.23:DX
GRAPHICS 3 .20 .23 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0108,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.10:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.12:DX
GRAPHICS 3 .10 .12 MS1
LABEL AA

$
$ Enthalpy of mixing at 1773 K (reference state: liquid)
TABLE_HEAD 110

```



```

CREATE_NEW_EQUILIBRIUM 0110,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.9
SET_REFERENCE_STATE A LIQ * 1E5
09:29:23,902 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-1964:DH
GRAPHICS 2 .9 -1964 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0111,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.8
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-3500:DH
GRAPHICS 2 .8 -3500 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0112,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.7
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-4588:DH
GRAPHICS 2 .7 -4588 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0113,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.6
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5239:DH
GRAPHICS 2 .6 -5239 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0114,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.5
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5454:DH
GRAPHICS 2 .5 -5454 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0115,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.4
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5233:DH
GRAPHICS 2 .4 -5233 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0116,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.3
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-4575:DH
GRAPHICS 2 .3 -4575 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0117,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.2
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-3481:DH
GRAPHICS 2 .2 -3481 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0118,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.1
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-1950:DH
GRAPHICS 2 .1 -1950 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set

$
$ Heat of melting for the compound. T=1341. H(liq)-H(A2B)=3727 J/mol.
$ This datum has already been used.
$
$ Do not forget the following line!
SAVE_WORKSPACES
PARROT:
PARROT: @@
PARROT: @@ Next file shows how to choose a rough start guess of the coefficients
PARROT: @@ and run the actual assessment. The values below are the final result.
PARROT: @@ S-O-V 1 20450,,,,,
PARROT: @@ S-O-V 2 -30.386,,,,,,
PARROT: @@ S-O-V 3 0.131,,,,,
PARROT: @@ S-O-V 11 -21817,,,,,
PARROT: @@ S-O-V 12 15.34,,,,,,
PARROT: @@ S-O-V 15 24212,,,,,,
PARROT: @@ S-O-V 16 -8.328,,,,,,
PARROT: @@ S-O-V 17 3105,,,,,
PARROT: @@ S-O-V 19 22030,,,,,
PARROT: @@ S-O-V 20 -6.981,,,,,,
PARROT: @@ Save the start guess on the work file
PARROT: s-o-v 1 0
PARROT: s-o-v 2 0

```

PARROT: s-o-v 11 0
PARROT: s-o-v 12 0
PARROT: s-o-v 15 0
PARROT: s-o-v 16 0
PARROT: s-o-v 17 0
PARROT: s-o-v 19 0
PARROT: s-o-v 20 0
PARROT:
PARROT: save
PARROT: @@ Now execute tcex36b.TCM to continue the assessment example
PARROT:Hit RETURN to continue
PARROT: mac tcex36b.TCM
PARROT: s-s-f tcex36
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V2	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V11	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V12	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V15	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V16	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V17	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V19	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V20	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

PARROT: @@ Set alt mode to start
PARROT: s-alt Y
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix	phases or comments
09:29:24,384	[Thread-0]	INFO					Phase: Preparing phase for use: A2B
09:29:24,670	[Thread-0]	INFO					Phase: Preparing phase for use: BCC
1	AINV	*alt*	1.0	1193.0			LIQUID A2B BCC
2	AINV	*alt*	1.0	1341.0			LIQUID A2B
3	AINV	*alt*	1.0	1049.0			LIQUID A2B BCC
4	AINV	*alt*	1.0	1203.0			LIQUID BCC FCC
5	AINV	*alt*	1.0	726.0			A2B BCC BCC#2
6	AINV	*alt*	1.0	726.0			BCC BCC#2
Failed using alternate for FCC#1							
10	ALF	*alt*	1.0	1594.0			LIQUID FCC
Failed using alternate for FCC#1							
11	ALF	*alt*	1.0	1548.0			LIQUID FCC
Failed using alternate for FCC#1							
12	ALF	*alt*	1.0	1499.0			LIQUID FCC
Failed using alternate for FCC#1							
13	ALF	*alt*	1.0	1438.0			LIQUID FCC
20	ATIE	*alt*	1.0	1413.0			LIQUID FCC
21	ATIE	*alt*	1.0	1337.0			LIQUID FCC
22	ATIE	*alt*	1.0	1213.0			LIQUID FCC
23	ATIE	*alt*	1.0	1100.0			LIQUID BCC
100	AA	5	1.	1573.0			LIQUID
101	AA	4	1.	1573.0			LIQUID
102	AA	2	1.	1573.0			LIQUID
103	AA	3	1.	1573.0			LIQUID
104	AA	4	1.	1573.0			LIQUID
105	AA	6	1.	1573.0			LIQUID
106	AA	8	1.	1573.0			LIQUID
107	AA	9	1.	1573.0			LIQUID
108	AA	11	1.	1573.0			LIQUID
110	AH	8	1.	1773.0			LIQUID
111	AH	6	1.	1773.0			LIQUID
112	AH	5	1.	1773.0			LIQUID
113	AH	3	1.	1773.0			LIQUID
114	AH	2	1.	1773.0			LIQUID
115	AH	3	1.	1773.0			LIQUID
116	AH	5	1.	1773.0			LIQUID
117	AH	7	1.	1773.0			LIQUID
118	AH	8	1.	1773.0			LIQUID

Number of alternate equilibria 14
ED_EXP: @@ Equilibria with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
Changed weight on 4 equilibria.

ED_EXP: c-a
Eq Lab Iter Weight Temp Exp Fix phases or comments
118 AH 2 1. 1773.0 LIQUID
ED_EXP: save
ED_EXP: @@ Save changes of weights before leaving the editor
ED_EXP: ba
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:29:25

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)

```
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V2	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V11	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V12	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V15	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V16	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V17	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V19	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V20	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.22023362E+03
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 3.21114110E+01

Number of alternate equilibria 10

SYMBOL	STATUS	VALUE/FUNCTION
FUNCTION R	298.15	8.31451000000000
2 RTLN P	20000000	+R*T*LN(1E-05*P)

; 6000 N REF0 !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)				
1 Alternate equilibrium calc				1.81
2 Alternate equilibrium calc				0.39
2 HTR=3727	1.5333E+04	5.00E+02	1.1606E+04	23.21 *
3 Alternate equilibrium calc				1.32
4 Alternate equilibrium calc				1.56
5 Alternate equilibrium calc				4.14
6 Alternate equilibrium calc				3.83
20 Alternate equilibrium calc				0.87
21 Alternate equilibrium calc				0.97
22 Alternate equilibrium calc				1.14
23 Alternate equilibrium calc				1.20
100 ACR(B)=0.94	0.9382	2.89E-02	-1.8474E-03	-6.3948E-02
101 ACR(B)=0.84	0.8339	2.89E-02	-6.0866E-03	-0.2107
102 ACR(B)=0.74	0.7297	2.89E-02	-1.0326E-02	-0.3574
103 ACR(B)=0.64	0.6254	2.89E-02	-1.4565E-02	-0.5042
104 ACR(B)=0.54	0.5212	2.89E-02	-1.8804E-02	-0.6509
105 ACR(B)=0.44	0.4170	2.89E-02	-2.3043E-02	-0.7976
106 ACR(B)=0.34	0.3127	2.89E-02	-2.7282E-02	-0.9444
107 ACR(B)=0.23	0.2085	2.89E-02	-2.1522E-02	-0.7450
108 ACR(B)=0.12	0.1042	2.89E-02	-1.5761E-02	-0.5455
110 HMR(LIQUID)=-1964	0.000	5.00E+02	1964.	3.928
111 HMR(LIQUID)=-3500	3.6380E-12	5.00E+02	3500.	7.000 *
112 HMR(LIQUID)=-4588	-3.6380E-12	5.00E+02	4588.	9.176 *
113 HMR(LIQUID)=-5239	0.000	5.00E+02	5239.	10.48 *
114 HMR(LIQUID)=-5454	1.8190E-12	5.00E+02	5454.	10.91 *
115 HMR(LIQUID)=-5233	5.4570E-12	5.00E+02	5233.	10.47 *
116 HMR(LIQUID)=-4575	3.6380E-12	5.00E+02	4575.	9.150 *
117 HMR(LIQUID)=-3481	-3.6380E-12	5.00E+02	3481.	6.962 *
118 HMR(LIQUID)=-1950	0.000	5.00E+02	1950.	3.900

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Note only one error from alternate calculations.

PARROT: @@ This error represents the difference in chemical

PARROT: @@ potentials of the phases.

PARROT: @@ Experiments with just one phase is calculated as normal.

PARROT: @@ Next command supresses the listing of parameters.

PARROT: s-o-l 1 Y Y N n N

PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:29:25

*** SUCCESSFUL OPTIMIZATION. ***

NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N

MINIMUM SAVE ON FILE: Y

ERROR FOR INEQUALITIES = 1.00000000E+00

RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04

ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

-- OPTIMIZING VARIABLES --

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V2	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V11	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V12	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V15	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V16	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V17	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V19	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V20	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.22023362E+03
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 3.21114110E+01

Number of alternate equilibria 10

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1	Alternate equilibrium calc				1.81	
2	Alternate equilibrium calc				0.39	
2	HTR=3727	1.5333E+04	5.00E+02	1.1606E+04	23.21	*
3	Alternate equilibrium calc				1.32	
4	Alternate equilibrium calc				1.56	
5	Alternate equilibrium calc				4.14	
6	Alternate equilibrium calc				3.83	
20	Alternate equilibrium calc				0.87	
21	Alternate equilibrium calc				0.97	
22	Alternate equilibrium calc				1.14	
23	Alternate equilibrium calc				1.20	
100	ACR(B)=0.94	0.9382	2.89E-02	-1.8474E-03	-6.3948E-02	
101	ACR(B)=0.84	0.8339	2.89E-02	-6.0866E-03	-0.2107	
102	ACR(B)=0.74	0.7297	2.89E-02	-1.0326E-02	-0.3574	
103	ACR(B)=0.64	0.6254	2.89E-02	-1.4565E-02	-0.5042	
104	ACR(B)=0.54	0.5212	2.89E-02	-1.8804E-02	-0.6509	
105	ACR(B)=0.44	0.4170	2.89E-02	-2.3043E-02	-0.7976	
106	ACR(B)=0.34	0.3127	2.89E-02	-2.7282E-02	-0.9444	
107	ACR(B)=0.23	0.2085	2.89E-02	-2.1522E-02	-0.7450	
108	ACR(B)=0.12	0.1042	2.89E-02	-1.5761E-02	-0.5455	
110	HMR(LIQUID)=-1964	0.000	5.00E+02	1964.	3.928	
111	HMR(LIQUID)=-3500	3.6380E-12	5.00E+02	3500.	7.000	*
112	HMR(LIQUID)=-4588	-3.6380E-12	5.00E+02	4588.	9.176	*
113	HMR(LIQUID)=-5239	0.000	5.00E+02	5239.	10.48	*
114	HMR(LIQUID)=-5454	1.8190E-12	5.00E+02	5454.	10.91	*
115	HMR(LIQUID)=-5233	5.4570E-12	5.00E+02	5233.	10.47	*
116	HMR(LIQUID)=-4575	3.6380E-12	5.00E+02	4575.	9.150	*
117	HMR(LIQUID)=-3481	-3.6380E-12	5.00E+02	3481.	6.962	*
118	HMR(LIQUID)=-1950	0.000	5.00E+02	1950.	3.900	

PARROT:

PARROT: @@ Now optimize

PARROT: opt 30

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

AT THE		0	TH	ITERATION WE HAVE THE SUM OF SQUARES	1.22023362E+03
1	0.0000E+00	2	0.0000E+00	3 0.0000E+00	4 0.0000E+00
6	0.0000E+00	7	0.0000E+00	8 0.0000E+00	9 0.0000E+00

AT THE		1	ST	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 0.0000E+00	4 0.0000E+00
6	0.0000E+00	7	0.0000E+00	8 0.0000E+00	9 0.0000E+00

AT THE		2	ND	ITERATION WE HAVE THE SUM OF SQUARES	1.22026107E+03
1	1.0000E-04	2	1.0000E-04	3 0.0000E+00	4 0.0000E+00
6	0.0000E+00	7	0.0000E+00	8 0.0000E+00	9 0.0000E+00

AT THE		3	RD	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 1.0000E-04	4 0.0000E+00
6	0.0000E+00	7	0.0000E+00	8 0.0000E+00	9 0.0000E+00

AT THE		4	TH	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 0.0000E+00	4 1.0000E-04
6	0.0000E+00	7	0.0000E+00	8 0.0000E+00	9 0.0000E+00

AT THE		5	TH	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 0.0000E+00	4 0.0000E+00
6	0.0000E+00	7	0.0000E+00	8 0.0000E+00	9 0.0000E+00

AT THE		6	TH	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 0.0000E+00	4 0.0000E+00
6	1.0000E-04	7	0.0000E+00	8 0.0000E+00	9 0.0000E+00

AT THE		7	TH	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 0.0000E+00	4 0.0000E+00
6	0.0000E+00	7	1.0000E-04	8 0.0000E+00	9 0.0000E+00

AT THE		8	TH	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 0.0000E+00	4 0.0000E+00
6	0.0000E+00	7	0.0000E+00	8 1.0000E-04	9 0.0000E+00

AT THE		9	TH	ITERATION WE HAVE THE SUM OF SQUARES	1.22023056E+03
1	1.0000E-04	2	0.0000E+00	3 0.0000E+00	4 0.0000E+00
6	0.0000E+00	7	0.0000E+00	8 0.0000E+00	9 1.0000E-04

```

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21799230E+03
1 1.5669E-03 2 -1.4577E-02 3 -1.7138E-13 4 -7.2597E-13 5 -2.0195E-12
6 -8.0197E-13 7 -4.7694E-14 8 -2.6978E-12 9 -1.7138E-13

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21756040E+03
1 1.6143E-02 2 -1.3110E-02 3 -1.8571E-12 4 -7.8664E-12 5 -2.1882E-11
6 -8.6898E-12 7 -5.1679E-13 8 -2.9232E-11 9 -1.8571E-12

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21666912E+03
1 4.5292E-02 2 -1.6084E-02 3 -1.0941E-08 4 -4.6346E-08 5 -1.2892E-07
6 -5.1197E-08 7 -3.0447E-09 8 -1.7222E-07 9 -1.0941E-08

      AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21485507E+03
1 1.0382E-01 2 -1.3204E-02 3 -4.5182E-09 4 -2.3322E-08 5 -6.3960E-08
6 -2.5321E-08 7 -1.2595E-09 8 -8.6022E-08 9 -4.5182E-09

      AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21125817E+03
1 2.2098E-01 2 -1.6258E-02 3 2.8162E-08 4 1.0311E-07 5 2.9036E-07
6 1.1561E-07 7 7.8286E-09 8 3.8564E-07 9 2.8162E-08

      AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 1.20407216E+03
1 4.5537E-01 2 -1.3579E-02 3 1.3273E-07 4 5.1504E-07 5 1.4430E-06
6 5.7394E-07 7 3.6912E-08 8 1.9211E-06 9 1.3273E-07

      AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 1.18986806E+03
1 9.2416E-01 2 -1.6949E-02 3 4.6065E-07 4 1.8214E-06 5 5.0950E-06
6 2.0258E-06 7 1.2812E-07 8 6.7882E-06 9 4.6065E-07

      AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 1.16200370E+03
1 1.8618E+00 2 -1.5078E-02 3 1.6952E-06 4 6.7857E-06 5 1.8963E-05
6 7.5379E-06 7 4.7155E-07 8 2.5277E-05 9 1.6952E-06

      AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 1.10849097E+03
1 3.7370E+00 2 -1.9708E-02 3 9.3539E-06 4 3.7816E-05 5 1.0559E-04
6 4.1965E-05 7 2.6021E-06 8 1.4080E-04 9 9.3539E-06

      AT THE 19 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00775499E+03
1 7.4874E+00 2 -2.1018E-02 3 1.4589E-04 4 5.9330E-04 5 1.6558E-03
6 6.5802E-04 7 4.0587E-05 8 2.2085E-03 9 1.4589E-04

      AT THE 20 TH ITERATION WE HAVE THE SUM OF SQUARES 8.16221974E+03
1 1.4912E+01 2 -2.9983E-02 3 -5.3449E-02 4 -2.1737E-01 5 -6.0665E-01
6 -2.4108E-01 7 -1.4869E-02 8 -8.0915E-01 9 -5.3449E-02

      AT THE 21 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00776233E+03
1 7.4874E+00 2 -2.1018E-02 3 2.4589E-04 4 5.9330E-04 5 1.6558E-03
6 6.5802E-04 7 4.0587E-05 8 2.2085E-03 9 1.4589E-04

      AT THE 22 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00760953E+03
1 7.4874E+00 2 -2.1018E-02 3 1.4587E-04 4 6.9325E-04 5 1.6558E-03
6 6.5802E-04 7 4.0587E-05 8 2.2085E-03 9 1.4589E-04

      AT THE 23 TH ITERATION WE HAVE THE SUM OF SQUARES 5.37458461E+04
1 7.9709E+00 2 -2.1202E-02 3 -8.3664E-01 4 -1.3063E-02 5 2.1132E+00
6 8.3977E-01 7 5.1795E-02 8 2.8185E+00 9 1.8618E-01

      AT THE 24 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00731643E+03
1 7.4874E+00 2 -2.1018E-02 3 1.4587E-04 4 6.9325E-04 5 1.6189E-03
6 7.5095E-04 7 4.0587E-05 8 2.2085E-03 9 1.4589E-04

      AT THE 25 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00731896E+03
1 7.4874E+00 2 -2.1018E-02 3 1.4587E-04 4 6.9325E-04 5 1.6167E-03
6 7.5011E-04 7 1.4056E-04 8 2.2085E-03 9 1.4589E-04

      AT THE 26 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00740720E+03
1 7.4874E+00 2 -2.1018E-02 3 1.4587E-04 4 6.9325E-04 5 1.5466E-03
6 7.2221E-04 7 3.8815E-05 8 2.2713E-03 9 1.4589E-04

      AT THE 27 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00724193E+03
1 7.4874E+00 2 -2.1018E-02 3 1.4587E-04 4 6.9325E-04 5 1.6159E-03
6 7.4976E-04 7 4.0514E-05 8 2.2045E-03 9 2.4576E-04

      AT THE 28 TH ITERATION WE HAVE THE SUM OF SQUARES 1.00724084E+03
1 7.4874E+00 2 -2.1118E-02 3 1.4587E-04 4 6.9326E-04 5 1.6159E-03
6 7.4976E-04 7 4.0514E-05 8 2.2045E-03 9 2.4576E-04

      AT THE 29 TH ITERATION WE HAVE THE SUM OF SQUARES 1.02228494E+03
1 7.5976E+00 2 -2.1775E-02 3 -5.1899E-01 4 2.1521E-03 5 1.7525E+00
6 -1.3907E-02 7 3.2734E-02 8 -4.0773E-01 9 -2.7131E-03

      AT THE 30 TH ITERATION WE HAVE THE SUM OF SQUARES 9.66652738E+02
1 7.5811E+00 2 -2.1393E-02 3 -2.2591E-01 4 2.3950E-03 5 9.0461E-01
6 8.8018E-03 7 7.9705E-03 8 6.3018E-02 9 2.1688E-03

*** ERROR RETURN FROM VA05A BECAUSE THERE HAVE BEEN 30 CALLS OF CALFUN

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 30 iterations
1 7.5811E+00 2 -2.1393E-02 3 -2.2591E-01 4 2.3950E-03 5 9.0461E-01
6 8.8018E-03 7 7.9705E-03 8 6.3018E-02 9 2.1688E-03

1 -2.5544E-01 2 -2.5544E-01 3 -3.1986E-02 4 -8.5339E-01 5 2.0549E-01
6 -5.9148E-02 7 1.8058E+01 8 -4.0344E-01 9 -4.0344E-01 10 -5.9329E-01
11 -2.0616E-01 12 -3.4541E-01 13 -7.3061E-02 14 -1.0511E+00 15 -1.0500E-01
16 3.1003E-01 17 3.1003E-01 18 -1.1874E+00 19 2.0697E+00 20 -1.1874E+00
21 2.0697E+00 22 -8.1248E-01 23 -1.9632E-02 24 -8.9161E-01 25 -4.2488E-02
26 -1.0436E+00 27 -9.6936E-02 28 -5.1174E-01 29 -1.5142E-01 30 2.4690E-02
31 1.0789E-01 32 2.7869E-01 33 4.7657E-01 34 6.3703E-01 35 6.9478E-01
36 5.8780E-01 37 5.9338E-01 38 3.0849E-01 39 3.8873E+00 40 6.9277E+00
41 9.0811E+00 42 1.0370E+01 43 1.0795E+01 44 1.0358E+01 45 9.0551E+00
46 6.8897E+00 47 3.8593E+00

```

THE SUM OF SQUARES IS 9.66652738E+02

PARROT: cont 30

```

Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A
Optimization continuing with same Jacobian

```

```

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 9.43485758E+02
1 7.6968E+00 2 -2.1638E-02 3 -4.8221E-01 4 7.7842E-04 5 1.7687E+00
6 7.5617E-03 7 2.2881E-02 8 2.9350E-01 9 1.8569E-03

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 9.30336226E+02
1 7.7639E+00 2 -2.1715E-02 3 -6.2024E-01 4 1.7583E-03 5 2.1317E+00

```

```
6 7.5156E-03 7 3.3863E-02 8 5.4721E-01 9 1.8047E-03
    AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 9.16903462E+02
1 7.8347E+00 2 -2.1751E-02 3 -7.5036E-01 4 7.2982E-04 5 2.4596E+00
6 9.1820E-03 7 4.5349E-02 8 8.4746E-01 9 2.2690E-03
    AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 8.93581181E+02
1 7.9780E+00 2 -2.1891E-02 3 -1.0080E+00 4 1.8143E-03 5 3.0033E+00
6 8.4573E-03 7 7.1805E-02 8 1.5517E+00 9 1.7568E-03
    AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 8.53239791E+02
1 8.2088E+00 2 -2.1735E-02 3 -1.4152E+00 4 1.1001E-03 5 3.7670E+00
6 1.5268E-02 7 1.1767E-01 8 2.7607E+00 9 4.0889E-03
    AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 7.86459840E+02
1 8.6673E+00 2 -2.2136E-02 3 -2.2168E+00 4 2.3884E-03 5 5.1004E+00
6 1.2632E-02 7 2.1480E-01 8 5.2956E+00 9 1.9285E-03
    AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 6.68969456E+02
1 9.5560E+00 2 -2.2861E-02 3 -3.7621E+00 4 3.2833E-03 5 7.4184E+00
6 8.3631E-03 7 4.1199E-01 8 1.0386E+01 9 -2.2439E-03
    AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 6.68971779E+02
1 9.5561E+00 2 -2.2861E-02 3 -3.7621E+00 4 3.2804E-03 5 7.4184E+00
6 8.3627E-03 7 4.1199E-01 8 1.0386E+01 9 -2.2446E-03
    AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 6.68999590E+02
1 9.5560E+00 2 -2.2861E-02 3 -3.7620E+00 4 3.2832E-03 5 7.4184E+00
6 8.3245E-03 7 4.1199E-01 8 1.0386E+01 9 -2.2429E-03
    AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 6.68860074E+02
1 9.5560E+00 2 -2.2861E-02 3 -3.7621E+00 4 3.3832E-03 5 7.4184E+00
6 8.3637E-03 7 4.1199E-01 8 1.0386E+01 9 -2.2439E-03
    AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.68814113E+02
1 9.5560E+00 2 -2.2861E-02 3 -3.7621E+00 4 3.3825E-03 5 7.4183E+00
6 8.4376E-03 7 4.1199E-01 8 1.0386E+01 9 -2.2403E-03
    AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 2.89588363E+02
1 1.3699E+01 2 -2.4865E-02 3 -1.0760E+01 4 8.5872E-03 5 1.2856E+01
6 2.8597E-02 7 1.5034E+00 8 1.6180E+01 9 1.1306E-03
    AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.96364585E+01
1 2.0265E+01 2 -2.8583E-02 3 -2.1815E+01 4 1.5863E-02 5 2.2957E+01
6 2.2983E-02 7 3.1713E+00 8 2.2843E+01 9 -3.1815E-04
    AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 8.23700139E+00
1 2.0270E+01 2 -2.8969E-02 3 -2.1814E+01 4 1.5427E-02 5 2.4210E+01
6 1.8667E-03 7 3.1247E+00 8 2.3040E+01 9 -5.3110E-03
    AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 8.25350817E+00
1 2.0270E+01 2 -2.8969E-02 3 -2.1814E+01 4 1.5427E-02 5 2.4210E+01
6 1.8774E-03 7 3.1248E+00 8 2.3040E+01 9 -5.3114E-03
    AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 6.32549851E+00
1 2.0269E+01 2 -2.9021E-02 3 -2.1814E+01 4 1.5360E-02 5 2.4197E+01
6 6.1884E-04 7 3.1217E+00 8 2.1781E+01 9 -4.6709E-03
    AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 7.22748666E-02
1 2.0271E+01 2 -2.9196E-02 3 -2.1814E+01 4 1.5173E-02 5 2.4551E+01
6 -8.3601E-03 7 3.1052E+00 8 2.1513E+01 9 -6.5711E-03
    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 16 iterations
1 2.0271E+01 2 -2.9196E-02 3 -2.1814E+01 4 1.5173E-02 5 2.4551E+01
6 -8.3601E-03 7 3.1052E+00 8 2.1513E+01 9 -6.5711E-03
1 9.0541E-03 2 9.0541E-03 3 1.6507E-03 4 3.9659E-02 5 1.3155E-01
6 -1.4048E-01 7 4.0557E-03 8 9.7381E-03 9 9.7381E-03 10 2.8607E-02
11 5.0468E-03 12 3.2465E-02 13 1.2091E-03 14 8.9739E-03 15 6.1630E-04
16 -1.3139E-02 17 -1.3139E-02 18 4.3757E-02 19 -4.7282E-02 20 4.3757E-02
21 -4.7282E-02 22 9.7822E-03 23 1.8330E-03 24 1.3162E-02 25 3.9872E-04
26 3.6580E-03 27 3.2706E-03 28 2.7765E-02 29 5.2828E-03 30 -1.3088E-02
31 -2.9450E-02 32 2.1775E-03 33 4.8022E-02 34 7.3106E-02 35 4.2363E-02
36 -7.8107E-02 37 1.7624E-02 38 -5.3138E-02 39 1.5649E-03 40 1.9671E-02
41 1.4318E-02 42 7.5065E-03 43 1.2359E-03 44 -4.4935E-03 45 -1.1682E-02
46 -1.8329E-02 47 -2.6435E-02
```

THE SUM OF SQUARES IS 7.22748666E-02
PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:29:26

*** OPTIMIZATION ERROR. TOO MANY ITERATIONS ***
NUMBER OF ITERATIONS: 17

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02705647E+04	0.00000000E+00	1.00000000E+03	1.60476352E+00
V2	-2.91962913E+01	0.00000000E+00	1.00000000E+03	1.00836523E-02
V11	-2.18135281E+04	0.00000000E+00	1.00000000E+03	8.65578776E-01
V12	1.51732852E+01	0.00000000E+00	1.00000000E+03	1.53481390E-03
V15	2.45514393E+04	0.00000000E+00	1.00000000E+03	1.44268144E+01
V16	-8.36014326E+00	0.00000000E+00	1.00000000E+03	5.72672914E-02
V17	3.10524501E+03	0.00000000E+00	1.00000000E+03	4.52085011E+00

```
V19      2.15132434E+04      0.00000000E+00      1.00000000E+03      9.72985872E+01
V20     -6.57113290E+00      0.00000000E+00      1.00000000E+03      6.27204239E-02
```

```
NUMBER OF OPTIMIZING VARIABLES :    9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM  1.22023362E+03 TO  7.22748666E-02
DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.90197017E-03
```

```
Number of alternate equilibria                10
```

```
$ =====  BLOCK NUMBER  1
```

```
DEFINED CONSTANTS
```

```
DX=2E-2, P0=101325, DH=500, DT=10
```

```
DEFINED FUNCTIONS AND VARIABLES%
```

```
HTR=HM(LIQUID)-HM(A2B)
```

```
1 Alternate equilibrium calc                0.04
2 Alternate equilibrium calc                0.19
2 HTR=3727                                3729.          5.00E+02  2.028      4.0557E-03
3 Alternate equilibrium calc                0.03
4 Alternate equilibrium calc                0.03
5 Alternate equilibrium calc                0.07
6 Alternate equilibrium calc                0.06
20 Alternate equilibrium calc               0.01
21 Alternate equilibrium calc               0.01
22 Alternate equilibrium calc               0.00
23 Alternate equilibrium calc               0.03
100 ACR(B)=0.94                          0.9396          2.85E-02 -3.7289E-04 -1.3088E-02
101 ACR(B)=0.84                          0.8392          2.82E-02 -8.3139E-04 -2.9450E-02
102 ACR(B)=0.74                          0.7401          2.81E-02  6.1205E-05  2.1775E-03
103 ACR(B)=0.64                          0.6414          2.81E-02  1.3504E-03  4.8022E-02
104 ACR(B)=0.54                          0.5421          2.83E-02  2.0667E-03  7.3106E-02
105 ACR(B)=0.44                          0.4412          2.86E-02  1.2102E-03  4.2363E-02
106 ACR(B)=0.34                          0.3377          2.90E-02 -2.2668E-03 -7.8107E-02
107 ACR(B)=0.23                          0.2305          2.97E-02  5.2261E-04  1.7624E-02
108 ACR(B)=0.12                          0.1184          3.05E-02 -1.6199E-03 -5.3138E-02
110 HMR(LIQUID)=-1964                    -1963.          5.00E+02  0.7825      1.5649E-03
111 HMR(LIQUID)=-3500                    -3490.          5.00E+02  9.835       1.9671E-02
112 HMR(LIQUID)=-4588                    -4581.          5.00E+02  7.159       1.4318E-02
113 HMR(LIQUID)=-5239                    -5235.          5.00E+02  3.753       7.5065E-03
114 HMR(LIQUID)=-5454                    -5453.          5.00E+02  0.6180      1.2359E-03
115 HMR(LIQUID)=-5233                    -5235.          5.00E+02 -2.247       -4.4935E-03
116 HMR(LIQUID)=-4575                    -4581.          5.00E+02 -5.841      -1.1682E-02
117 HMR(LIQUID)=-3481                    -3490.          5.00E+02 -9.165      -1.8329E-02
118 HMR(LIQUID)=-1950                    -1963.          5.00E+02 -13.22     -2.6435E-02
```

```
PARROT:
```

```
PARROT:Hit RETURN to continue
```

```
PARROT: @@ The liquid data fits reasonably. Simplify its parameters.
```

```
PARROT: l-p-d liq
```

```
Property type /ALL/: s-f-v 11-14
```

```
S-F-V is not a valid property type
```

```
11-14 is not a valid property type
```

```
Property type: @@ Rescale the start values of the parameters to current values
```

```
@@ is not a valid property type
```

```
RESCALE is not a valid property type
```

```
THE is not a valid property type
```

```
START is not a valid property type
```

```
VALUES is not a valid property type
```

```
OF is not a valid property type
```

```
THE is not a valid property type
```

```
PARAMETERS is not a valid property type
```

```
TO is not a valid property type
```

```
CURRENT is not a valid property type
```

```
VALUES is not a valid property type
```

```
Property type: resc
```

```
RESC is not a valid property type
```

```
Property type: l-a-v
```

```
L-A-V is not a valid property type
```

```
Property type:
```

```
LIQUID:L (A,B)1.0
```

```
- This phase is a liquid
```

```
==== [A] ====
G(LIQUID,A;0)                500 +14000-10*T;                2000 N
```

```
==== [B] ====
G(LIQUID,B;0)                500 +18000-12*T;                2000 N
```

```
==== [A, B] ====
L(LIQUID,A,B;0)              500 +V11+V12*T;                2000 N
L(LIQUID,A,B;1)              500 +V13+V14*T;                2000 N
```

```
PARROT:Hit RETURN to continue
```

```
PARROT: mac tcex36cpd
```

```
PARROT: set-echo
```

```
NO SUCH COMMAND, USE HELP
```

```
PARROT: @@ Calculate the phase diagram
```

```
PARROT: @@ This TCM should be run in PARROT
```

```
PARROT: go p-3
```

```
POLY:
```

```
POLY: @@ In PARROT, the global minimization is turned off automatically.
```

```
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
```

```
POLY: @@ message will be given.
```

```
POLY:
```

```
POLY: advanced-option global yes,,
```

```
Settings for global minimization:
```

```
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
```

```
Do not go back to PARROT but exit from POLY after your POLY calculations.
```

```
POLY:
```

```
POLY: def-com,,,
```

```
POLY: s-a-v 1 w(b) 0 1,,,
```

```
The condition W(B)=.1234 created
```

```
POLY: s-a-v 2 t 300 1700,,,
```

```
The condition T=942.2 created
```

```
POLY: s-c t=500
```

```
POLY: l-c
```

```
W(B)=0.1234, T=500
```

```

DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated      628 grid points in      0.021 s
Found the set of lowest grid points in      0.005 s
Calculated POLY solution      0.045 s, total time      0.071 s
POLY: save tcex36 y
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..      2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
Calculated..      14 equilibria

Phase region boundary 3 at: 6.840E-01 7.259E+02
  ** A2B
  BCC#1
  ** BCC#2

Phase region boundary 4 at: 3.606E-01 7.259E+02
  ** A2B
  BCC#1
Calculated..      14 equilibria

Phase region boundary 5 at: 3.757E-01 1.181E+03
  ** LIQUID
  ** A2B
  BCC#1

Phase region boundary 6 at: 2.876E-01 1.181E+03
  ** LIQUID
  BCC#1
Calculated      24 equilibria

Phase region boundary 7 at: 4.909E-01 1.181E+03
  ** LIQUID
  A2B
Calculated..      27 equilibria

Phase region boundary 8 at: 6.483E-01 1.032E+03
  ** LIQUID
  A2B
  ** BCC#1

Phase region boundary 9 at: 7.679E-01 1.032E+03
  A2B
  ** BCC#1
Calculated..      10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.296E-01 1.032E+03
  LIQUID
  ** BCC#1
Calculated..      7 equilibria

Phase region boundary 11 at: 8.738E-01 1.185E+03
  LIQUID
  ** BCC#1
  ** FCC

```


Phase region boundary 12 at: 8.778E-01 1.185E+03
 LIQUID
 ** FCC
 Calculated 31 equilibria

Phase region boundary 13 at: 9.364E-01 1.185E+03
 BCC#1
 ** FCC
 Calculated 20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.627E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 26 at: 3.627E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.627E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 7.938E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 29 at: 7.938E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 7.938E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 31 at: 2.394E-01 1.230E+03

```

** LIQUID
  BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  2.394E-01  1.230E+03
** LIQUID
  BCC#1
Calculated          26 equilibria

Phase region boundary 33 at:  8.874E-01  1.230E+03
** LIQUID
  FCC
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  8.874E-01  1.230E+03
** LIQUID
  FCC
Calculated          29 equilibria

Phase region boundary 35 at:  6.352E-03  1.397E+03
  LIQUID
** BCC#1
Calculated          11 equilibria

Phase region boundary 36 at:  6.352E-03  1.397E+03
  LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  2.276E-01  1.241E+03
  LIQUID
** BCC#1
Calculated          23 equilibria

Phase region boundary 38 at:  2.276E-01  1.241E+03
  LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:  6.122E-01  1.208E+03
  LIQUID
** A2B
Calculated.          12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:  6.122E-01  1.208E+03
  LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

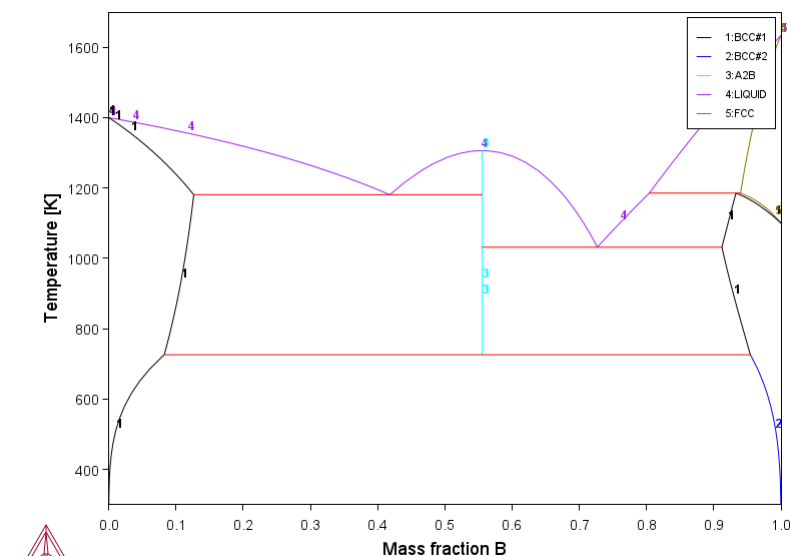
Phase region boundary 41 at:  9.928E-01  1.613E+03
  LIQUID
** FCC
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.928E-01  1.613E+03
  LIQUID
** FCC
Calculated          12 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping          5 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

```

Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 30
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

	AT THE	0	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.22748666E-02
1	2.0271E+01	2	-2.9196E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	1	ST	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.22740664E-02
1	2.0271E+01	2	-2.9196E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	2	ND	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.21425667E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	3	RD	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.21438736E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1813E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	4	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	9.55857871E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5273E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	5	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.21498915E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4552E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	6	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.90562820E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.2601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	7	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.21442403E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1053E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	8	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.21430820E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5711E-03				
	AT THE	9	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.31679213E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5173E-02	5	2.4551E+01		
6	-8.3601E-03	7	3.1052E+00	8	2.1513E+01	9	-6.4711E-03				
	AT THE	10	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.89231193E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5137E-02	5	2.4551E+01		
6	-8.4486E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5809E-03				
	AT THE	11	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.65070041E-02
1	2.0271E+01	2	-2.9096E-02	3	-2.1814E+01	4	1.5171E-02	5	2.4551E+01		
6	-8.4622E-03	7	3.1052E+00	8	2.1513E+01	9	-6.5829E-03				
	AT THE	12	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.46333297E-02
1	2.0271E+01	2	-2.9097E-02	3	-2.1814E+01	4	1.5143E-02	5	2.4551E+01		
6	-8.5305E-03	7	3.1053E+00	8	2.1513E+01	9	-6.5917E-03				
	AT THE	13	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.32446690E-02
1	2.0271E+01	2	-2.9097E-02	3	-2.1814E+01	4	1.5169E-02	5	2.4551E+01		
6	-8.5404E-03	7	3.1053E+00	8	2.1513E+01	9	-6.5933E-03				
	AT THE	14	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.22205116E-02
1	2.0271E+01	2	-2.9098E-02	3	-2.1814E+01	4	1.5149E-02	5	2.4550E+01		
6	-8.5885E-03	7	3.1053E+00	8	2.1512E+01	9	-6.6003E-03				
	AT THE	15	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.14799744E-02
1	2.0271E+01	2	-2.9099E-02	3	-2.1814E+01	4	1.5168E-02	5	2.4550E+01		
6	-8.5956E-03	7	3.1054E+00	8	2.1511E+01	9	-6.6007E-03				
	AT THE	16	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.09645818E-02
1	2.0271E+01	2	-2.9100E-02	3	-2.1814E+01	4	1.5154E-02	5	2.4549E+01		
6	-8.6249E-03	7	3.1054E+00	8	2.1508E+01	9	-6.6042E-03				
	AT THE	17	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.05952285E-02
1	2.0271E+01	2	-2.9100E-02	3	-2.1814E+01	4	1.5167E-02	5	2.4548E+01		
6	-8.6308E-03	7	3.1054E+00	8	2.1504E+01	9	-6.6024E-03				
	AT THE	18	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.03226901E-02
1	2.0271E+01	2	-2.9102E-02	3	-2.1814E+01	4	1.5157E-02	5	2.4548E+01		
6	-8.6487E-03	7	3.1055E+00	8	2.1499E+01	9	-6.6021E-03				
	AT THE	19	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.03330257E-02
1	2.0271E+01	2	-2.9102E-02	3	-2.1814E+01	4	1.5157E-02	5	2.4548E+01		
6	-8.6483E-03	7	3.1055E+00	8	2.1499E+01	9	-6.6021E-03				
	AT THE	20	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.05951509E-02
1	2.0271E+01	2	-2.9002E-02	3	-2.1814E+01	4	1.5157E-02	5	2.4548E+01		
6	-8.6483E-03	7	3.1055E+00	8	2.1499E+01	9	-6.6021E-03				
	AT THE	21	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.03241995E-02
1	2.0271E+01	2	-2.9102E-02	3	-2.1813E+01	4	1.5157E-02	5	2.4548E+01		
6	-8.6486E-03	7	3.1055E+00	8	2.1499E+01	9	-6.6021E-03				
	AT THE	22	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	6.01465871E-02
1	2.0271E+01	2	-2.9102E-02	3	-2.1814E+01	4	1.5169E-02	5	2.4551E+01		
6	-8.6582E-03	7	3.1053E+00	8	2.1493E+01	9	-6.5979E-03				
	AT THE	23	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	5.99898496E-02
1	2.0271E+01	2	-2.9103E-02	3	-2.1814E+01	4	1.5162E-02	5	2.4549E+01		
6	-8.6638E-03	7	3.1054E+00	8	2.1500E+01	9	-6.6049E-03				
	AT THE	24	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	5.98589653E-02
1	2.0271E+01	2	-2.9104E-02	3	-2.1814E+01	4	1.5170E-02	5	2.4549E+01		
6	-8.6758E-03	7	3.1055E+00	8	2.1508E+01	9	-6.6138E-03				
	AT THE	25	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	5.98623708E-02
1	2.0271E+01	2	-2.9104E-02	3	-2.1814E+01	4	1.5170E-02	5	2.4549E+01		
6	-8.6750E-03	7	3.1056E+00	8	2.1508E+01	9	-6.6138E-03				
	AT THE	26	TH	ITERATION	WE	HAVE	THE	SUM	OF	SQUARES	7.89603961E-02
1	2.0271E+01	2	-2.9104E-02	3	-2.1814E+01	4	1.5260E-02	5	2.4549E+01		
6	-8.6944E-03	7	3.1055E+00	8	2.1508E+01	9	-6.6139E-03				

AT THE 27 TH ITERATION WE HAVE THE SUM OF SQUARES 6.03853160E-02
1 2.0271E+01 2 -2.9104E-02 3 -2.1814E+01 4 1.5168E-02 5 2.4549E+01
6 -8.6864E-03 7 3.1055E+00 8 2.1508E+01 9 -6.5144E-03

AT THE 28 TH ITERATION WE HAVE THE SUM OF SQUARES 6.02472625E-02
1 2.0271E+01 2 -2.9103E-02 3 -2.1814E+01 4 1.5186E-02 5 2.4549E+01
6 -8.7455E-03 7 3.1055E+00 8 2.1508E+01 9 -6.6205E-03

AT THE 29 TH ITERATION WE HAVE THE SUM OF SQUARES 5.97166905E-02
1 2.0271E+01 2 -2.9104E-02 3 -2.1814E+01 4 1.5164E-02 5 2.4550E+01
6 -8.6811E-03 7 3.1054E+00 8 2.1517E+01 9 -6.6214E-03

AT THE 30 TH ITERATION WE HAVE THE SUM OF SQUARES 6.24882116E-02
1 2.0271E+01 2 -2.9105E-02 3 -2.1814E+01 4 1.5123E-02 5 2.4550E+01
6 -8.7492E-03 7 3.1054E+00 8 2.1517E+01 9 -6.6301E-03

*** ERROR RETURN FROM VA05A BECAUSE THERE HAVE BEEN 30 CALLS OF CALFUN

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 30 iterations
1 2.0271E+01 2 -2.9104E-02 3 -2.1814E+01 4 1.5164E-02 5 2.4550E+01
6 -8.6811E-03 7 3.1054E+00 8 2.1517E+01 9 -6.6214E-03

1 1.3024E-02 2 1.3024E-02 3 1.5821E-03 4 5.8702E-03 5 1.2900E-01
6 -1.4189E-01 7 3.8577E-03 8 1.3734E-02 9 1.3734E-02 10 4.3428E-03
11 3.6993E-03 12 5.3295E-03 13 4.2025E-04 14 5.2002E-03 15 6.6795E-04
16 2.6066E-03 17 2.6066E-03 18 1.3278E-02 19 -1.1759E-02 20 1.3278E-02
21 -1.1759E-02 22 5.7215E-03 23 1.8456E-03 24 9.2200E-03 25 4.2279E-04
26 -1.3183E-04 27 3.3216E-03 28 2.5762E-03 29 4.1378E-03 30 -1.3472E-02
31 -3.0833E-02 32 -5.9027E-04 33 4.3750E-02 34 6.7496E-02 35 3.5866E-02
36 -8.4768E-02 37 1.1816E-02 38 -5.6834E-02 39 1.5681E-03 40 1.9677E-02
41 1.4325E-02 42 7.5148E-03 43 1.2446E-03 44 -4.4852E-03 45 -1.1675E-02
46 -1.8323E-02 47 -2.6432E-02

THE SUM OF SQUARES IS 5.97166905E-02

PARROT: resc

PARROT: opt 30

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 5.97166905E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 5.97124187E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 5.97077077E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 5.97249824E-02
1 1.0001E+00 2 1.0001E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 5.97094892E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 5.97485501E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 5.96963872E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 5.96971064E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 5.97027101E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 5.96938687E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0001E+00

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 5.92368122E-02
1 1.0002E+00 2 1.0003E+00 3 9.9971E-01 4 1.0001E+00 5 9.9801E-01
6 1.0007E+00 7 9.9996E-01 8 9.9969E-01 9 1.0002E+00

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 5.90785934E-02
1 1.0002E+00 2 1.0005E+00 3 9.9998E-01 4 9.9999E-01 5 9.9783E-01
6 1.0004E+00 7 1.0002E+00 8 1.0003E+00 9 1.0022E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 5.89989883E-02
1 1.0001E+00 2 1.0010E+00 3 9.9986E-01 4 9.9994E-01 5 9.9710E-01
6 9.9993E-01 7 1.0007E+00 8 1.0014E+00 9 1.0062E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 5.89286559E-02
1 1.0002E+00 2 1.0015E+00 3 9.9996E-01 4 9.9991E-01 5 9.9663E-01
6 9.9868E-01 7 1.0016E+00 8 1.0041E+00 9 1.0141E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88541235E-02
1 1.0002E+00 2 1.0027E+00 3 9.9995E-01 4 9.9995E-01 5 9.9566E-01
6 9.9617E-01 7 1.0035E+00 8 1.0095E+00 9 1.0300E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 14 iterations
1 1.0002E+00 2 1.0027E+00 3 9.9995E-01 4 9.9995E-01 5 9.9566E-01
6 9.9617E-01 7 1.0035E+00 8 1.0095E+00 9 1.0300E+00

1 1.0077E-02 2 1.0077E-02 3 1.5693E-03 4 6.0837E-04 5 1.3098E-01
6 -1.4090E-01 7 1.1816E-03 8 1.0805E-02 9 1.0805E-02 10 -1.0207E-03
11 3.2348E-03 12 2.9233E-04 13 1.9135E-04 14 2.7222E-03 15 6.0209E-04
16 3.5206E-03 17 3.5206E-03 18 1.7996E-03 19 -7.6096E-04 20 1.7996E-03
21 -7.6096E-04 22 4.3873E-04 23 1.7938E-03 24 4.9512E-03 25 3.5710E-04
26 -2.7482E-03 27 3.2547E-03 28 -2.6672E-03 29 3.7644E-03 30 -1.3473E-02
31 -3.0837E-02 32 -5.9818E-04 33 4.3738E-02 34 6.7480E-02 35 3.5847E-02
36 -8.4787E-02 37 1.1800E-02 38 -5.6845E-02 39 1.7612E-03 40 2.0020E-02
41 1.4776E-02 42 8.0298E-03 43 1.7810E-03 44 -3.9702E-03 45 -1.1224E-02

46 -1.7980E-02 47 -2.6239E-02

THE SUM OF SQUARES IS 5.88541235E-02

PARROT: @@ No change in the parameters, check the diagram again

PARROT: mac tcex36cpd

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

POLY:

POLY: @@ In PARROT, the global minimization is turned off automatically.

POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY: @@ message will be given.

POLY:

POLY: advanced-option global yes,,

Settings for global minimization:

*** WARNING *** Global equilibrium calculation may create new composition sets and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY:

POLY: def-com,,,,

POLY: s-a-v 1 w(b) 0 1,,,,

The condition W(B)=.1234 created

POLY: s-a-v 2 t 300 1700,,,,

The condition T=942.2 created

POLY: s-c t=500

POLY: l-c

W(B)=0.1234, T=500

DEGREES OF FREEDOM 2

POLY: c-e

Creating condition P=1E5

Creating condition N=1

Using global minimization procedure

Calculated 628 grid points in 0.005 s

Found the set of lowest grid points in 0.000 s

Calculated POLY solution 0.006 s, total time 0.011 s

POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy

the results from the previous STEP or MAP commands.

POLY: map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02

BCC#1

** BCC#2

Calculated.. 2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02

BCC#1

** BCC#2

Calculated. 14 equilibria

Phase region boundary 3 at: 6.814E-01 7.290E+02

** A2B

BCC#1

** BCC#2

Phase region boundary 4 at: 3.629E-01 7.290E+02

** A2B

BCC#1

Calculated. 14 equilibria

Phase region boundary 5 at: 3.784E-01 1.181E+03

```

** LIQUID
** A2B
  BCC#1
Phase region boundary 6 at: 2.921E-01 1.181E+03
** LIQUID
  BCC#1
Calculated 27 equilibria
Phase region boundary 7 at: 4.919E-01 1.181E+03
** LIQUID
  A2B
Calculated. 32 equilibria
Phase region boundary 8 at: 6.472E-01 1.036E+03
** LIQUID
  A2B
** BCC#1
Phase region boundary 9 at: 7.632E-01 1.036E+03
  A2B
** BCC#1
Calculated. 10 equilibria
Terminating at known equilibrium
Phase region boundary 10 at: 8.247E-01 1.036E+03
  LIQUID
** BCC#1
Calculated. 8 equilibria
Phase region boundary 11 at: 8.760E-01 1.205E+03
  LIQUID
** BCC#1
** FCC
Phase region boundary 12 at: 8.814E-01 1.205E+03
  LIQUID
** FCC
Calculated 35 equilibria
Phase region boundary 13 at: 9.361E-01 1.205E+03
  BCC#1
** FCC
Calculated 21 equilibria
Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC#1
** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium
Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 16 at: 7.140E-01 3.100E+02
  BCC#1
** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium
Phase region boundary 17 at: 7.140E-01 3.100E+02
  BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 18 at: 7.140E-01 3.100E+02
  BCC#1
** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium
Phase region boundary 19 at: 7.140E-01 3.100E+02
  BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 20 at: 7.140E-01 3.100E+02
  BCC#1
** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium
Phase region boundary 21 at: 7.140E-01 3.100E+02
  BCC#1
  BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 22 at: 7.140E-01 3.100E+02
  BCC#1
  BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium
Phase region boundary 23 at: 7.140E-01 3.100E+02
  BCC#1
  BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 24 at: 7.140E-01 3.100E+02
  BCC#1
  BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 25 at: 3.650E-01 7.700E+02
** A2B
   BCC#1
Calculated.                  10 equilibria

Phase region boundary 26 at: 3.650E-01 7.700E+02
** A2B
   BCC#1
Calculated.                  3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.650E-01 7.700E+02
** A2B
   BCC#1
Calculated.                 13 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.907E-01 7.700E+02
** A2B
   BCC#1
Calculated.                 10 equilibria

Phase region boundary 29 at: 7.907E-01 7.700E+02
** A2B
   BCC#1
Calculated.                  3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.907E-01 7.700E+02
** A2B
   BCC#1
Calculated.                  9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.438E-01 1.230E+03
** LIQUID
   BCC#1
Calculated.                  4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.438E-01 1.230E+03
** LIQUID
   BCC#1
Calculated.                 26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03
** LIQUID
   FCC
Calculated.                  2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
** LIQUID
   FCC
Calculated.                 29 equilibria

Phase region boundary 35 at: 6.409E-03 1.397E+03
   LIQUID
** BCC#2
Calculated.                 13 equilibria

Phase region boundary 36 at: 6.409E-03 1.397E+03
   LIQUID
** BCC#2
Calculated.                 13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.297E-01 1.243E+03
   LIQUID
** BCC#1
Calculated.                 23 equilibria

Phase region boundary 38 at: 2.297E-01 1.243E+03
   LIQUID
** BCC#1
Calculated.                  4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.204E+03
   LIQUID
** A2B
Calculated.                 12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.204E+03
   LIQUID
** A2B
Calculated.                  7 equilibria
Terminating at known equilibrium

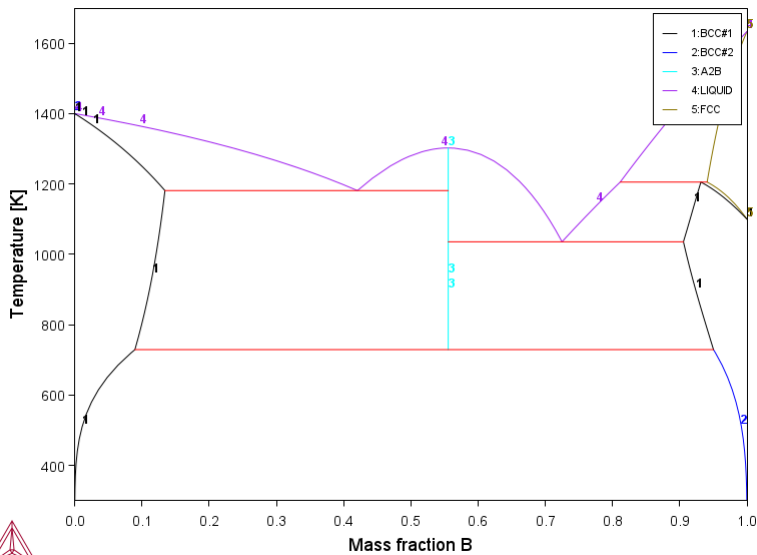
Phase region boundary 41 at: 9.927E-01 1.613E+03
   LIQUID
** FCC
Calculated.                 19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
   LIQUID
** FCC
Calculated.                 10 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping          1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
POST: plot

```



POST:
 POST: set-inter
 POST:Hit RETURN to continue
 POST: ba
 POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
 PARROT: @@ Turn off alternate mode and try to calculate all equilibria
 PARROT: s-alt Y
 Alternate calculation is on
 PARROT: ed
 ED_EXP: read 1
 ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	4	1.	1181.2		LIQUID A2B BCC
2	AINV	2	1.	1302.3		LIQUID A2B
3	AINV	3	1.	1035.7		LIQUID A2B BCC
4	AINV	3	1.	1205.4		LIQUID BCC FCC
5	AINV	4	1.	729.0		A2B BCC BCC#2
6	AINV	3	1.	726.0		BCC BCC#2
10	ALF	< unused >		1594.0		LIQUID FCC
11	ALF	< unused >		1548.0		LIQUID FCC
12	ALF	< unused >		1499.0		LIQUID FCC
13	ALF	< unused >		1438.0		LIQUID FCC
20	ATIE	3	1.	1413.0		LIQUID FCC
21	ATIE	3	1.	1337.0		LIQUID FCC
22	ATIE	3	1.	1213.0		LIQUID FCC
23	ATIE	3	1.	1100.0		LIQUID BCC
100	AA	2	1.	1573.0		LIQUID
101	AA	2	1.	1573.0		LIQUID
102	AA	2	1.	1573.0		LIQUID
103	AA	2	1.	1573.0		LIQUID
104	AA	2	1.	1573.0		LIQUID
105	AA	2	1.	1573.0		LIQUID
106	AA	2	1.	1573.0		LIQUID
107	AA	2	1.	1573.0		LIQUID
108	AA	2	1.	1573.0		LIQUID
110	AH	2	1.	1773.0		LIQUID
111	AH	2	1.	1773.0		LIQUID
112	AH	2	1.	1773.0		LIQUID
113	AH	2	1.	1773.0		LIQUID
114	AH	2	1.	1773.0		LIQUID
115	AH	2	1.	1773.0		LIQUID
116	AH	2	1.	1773.0		LIQUID
117	AH	2	1.	1773.0		LIQUID
118	AH	2	1.	1773.0		LIQUID

ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
 ED_EXP: @@ any liquid parameters and restore those with label ALF
 ED_EXP: s-we 0 100-118
 ED_EXP: s-we 1 alf
 Changed weight on 4 equilibria.
 ED_EXP: s-e 1
 Equilibrium number 1, label AINV
 ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	2	1.	1181.2		LIQUID A2B BCC
2	AINV	2	1.	1302.3		LIQUID A2B
3	AINV	2	1.	1035.7		LIQUID A2B BCC
4	AINV	2	1.	1205.4		LIQUID BCC FCC
5	AINV	2	1.	729.0		A2B BCC BCC#2
6	AINV	2	1.	726.0		BCC BCC#2
10	ALF	6	1.	1594.0		LIQUID FCC
11	ALF	6	1.	1548.0		LIQUID FCC
12	ALF	7	1.	1499.0		LIQUID FCC
13	ALF	7	1.	1438.0		LIQUID FCC
20	ATIE	2	1.	1413.0		LIQUID FCC
21	ATIE	2	1.	1337.0		LIQUID FCC
22	ATIE	2	1.	1213.0		LIQUID FCC
23	ATIE	2	1.	1100.0		LIQUID BCC
100	AA	< unused >		1573.0		LIQUID
101	AA	< unused >		1573.0		LIQUID
102	AA	< unused >		1573.0		LIQUID
103	AA	< unused >		1573.0		LIQUID
104	AA	< unused >		1573.0		LIQUID
105	AA	< unused >		1573.0		LIQUID
106	AA	< unused >		1573.0		LIQUID
107	AA	< unused >		1573.0		LIQUID
108	AA	< unused >		1573.0		LIQUID
110	AH	< unused >		1773.0		LIQUID
111	AH	< unused >		1773.0		LIQUID


```
112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID
```

ED_EXP: save

ED_EXP: @@ Save changes

ED_EXP: ba

PARROT: opt 0

Use 29 experiments, maximum is 2000

Use 740 real workspace, maximum is 50000

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:30:15
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0
```

== OPTIMIZING CONDITIONS ==

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02756027E+04	2.02708732E+04	2.02708732E+04	7.92262612E-02
V2	-2.91817289E+01	-2.91044045E+01	-2.91044045E+01	3.44288780E-01
V11	-2.18124379E+04	-2.18135107E+04	-2.18135107E+04	3.96930274E-02
V12	1.51628519E+01	1.51635617E+01	1.51635617E+01	5.86409179E-02
V15	2.44432174E+04	2.45497588E+04	2.45497588E+04	6.05871516E-01
V16	-8.64785520E+00	-8.68107698E+00	-8.68107698E+00	2.02570116E+00
V17	3.11633728E+03	3.10543242E+03	3.10543242E+03	1.46283110E+00
V19	2.17221802E+04	2.15167018E+04	2.15167018E+04	4.73035740E+00
V20	-6.81979565E+00	-6.62138477E+00	-6.62138477E+00	1.19131169E+01

```
NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 5.97166905E-02 TO 1.87896483E+01
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 9.39482416E-01
```

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1181.	10.	-11.79	-1.179
1 W(LIQUID,B)=0.408	0.4205	2.00E-02	1.2542E-02	0.6271
1 W(BCC#1,B)=0.13	0.1342	2.00E-02	4.1628E-03	0.2081
2 T=1341	1302.	10.	-38.65	-3.865
2 HTR=3727	3728.	5.00E+02	0.5907	1.1814E-03
3 T=1049	1036.	10.	-13.26	-1.326
3 W(LIQUID,A)=0.27	0.2752	2.00E-02	5.1543E-03	0.2577
3 W(BCC#1,A)=9.3E-2	9.4532E-02	2.00E-02	1.5318E-03	7.6589E-02
4 T=1203	1205.	10.	2.439	0.2439
4 W(LIQUID,A)=0.19	0.1885	2.00E-02	-1.4539E-03	-7.2697E-02
4 W(BCC#1,A)=6.9E-2	6.8528E-02	2.00E-02	-4.7216E-04	-2.3608E-02
4 W(FCC,A)=6E-2	5.9293E-02	2.00E-02	-7.0690E-04	-3.5345E-02
5 T=726	729.0	10.	3.038	0.3038
5 X(BCC#1,B)=3.7E-2	3.7832E-02	2.00E-02	8.3176E-04	4.1588E-02
5 X(BCC#2,A)=0.114	0.1158	2.00E-02	1.7985E-03	8.9926E-02
6 X(BCC#1,B)=3.7E-2	3.6971E-02	2.00E-02	-2.8811E-05	-1.4405E-03
6 X(BCC#2,A)=0.114	0.1137	2.00E-02	-3.1937E-04	-1.5968E-02
10 W(LIQUID,A)=2E-2	1.9300E-02	2.00E-02	-6.9950E-04	-3.4975E-02
11 W(LIQUID,A)=4.2E-2	4.1338E-02	2.00E-02	-6.6193E-04	-3.3096E-02
12 W(LIQUID,A)=6.5E-2	6.4209E-02	2.00E-02	-7.9131E-04	-3.9566E-02
13 W(LIQUID,A)=9.3E-2	9.1819E-02	2.00E-02	-1.1805E-03	-5.9025E-02
20 W(LIQUID,A)=0.104	0.1029	2.00E-02	-1.1401E-03	-5.7007E-02
20 W(FCC,A)=3.8E-2	3.7516E-02	2.00E-02	-4.8352E-04	-2.4176E-02
21 W(LIQUID,A)=0.136	0.1354	2.00E-02	-5.5206E-04	-2.7603E-02
21 W(FCC,A)=4.7E-2	4.6453E-02	2.00E-02	-5.4654E-04	-2.7327E-02
22 W(LIQUID,A)=0.187	0.1856	2.00E-02	-1.3986E-03	-6.9932E-02
22 W(FCC,A)=5.9E-2	5.8624E-02	2.00E-02	-3.7571E-04	-1.8786E-02
23 W(LIQUID,A)=0.245	0.2436	2.00E-02	-1.4262E-03	-7.1312E-02
23 W(BCC#1,A)=8.5E-2	8.4617E-02	2.00E-02	-3.8328E-04	-1.9164E-02

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ When we optimize zero times we sometimes find an error for

PARROT: @@ equilibrium 4. It can be on the wrong side, at high A instead

PARROT: @@ of high B. Try to correct that in the Edit module.

PARROT: ed

ED_EXP: read 1

ED_EXP: s-e 4

Equilibrium number 4 , label AINV

ED_EXP: s-a-s

T /1205.438651/: 1200

Automatic start values for phase constituents? /N/: N

Phase LIQUID

Major constituent(s) /*/: b

Phase BCC

```

Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:
P=101325
FIXED PHASES
LIQUID=1 BCC#1=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1205.44 K ( 932.29 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30232E+02
Total Gibbs energy -9.85005E+03, Enthalpy 1.98466E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
A                6.5892E-01  1.0119E-01  3.8745E-01 -9.5031E+03 SER
B                2.3411E+00  8.9881E-01  8.5819E-01 -1.5327E+03 SER

FCC              Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5916E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40707E-01 A 5.92931E-02

BCC#1            Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5339E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31472E-01 A 6.85278E-02

LIQUID           Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.8977E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.11454E-01 A 1.88546E-01
EXPERIMENT T=1203:DT $1205.44:10 NO=1
EXPERIMENT W(LIQUID,A)=0.19:DX $0.188546:2E-2 NO=2
EXPERIMENT W(BCC#1,A)=6.9E-2:DX $6.85278E-2:2E-2 NO=3
EXPERIMENT W(FCC,A)=6E-2:DX $5.92931E-2:2E-2 NO=4
ED_EXP: ba
PARROT: @@ The error is still there, calculate the phase diagram.
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0.003 s
Found the set of lowest grid points in 0.000 s
Calculated POLY solution 0.003 s, total time 0.006 s
POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11

```

```

Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
  Calculated. 14 equilibria

Phase region boundary 3 at: 6.814E-01 7.290E+02
  ** A2B
  BCC#1
  ** BCC#2

Phase region boundary 4 at: 3.629E-01 7.290E+02
  ** A2B
  BCC#1
  Calculated. 14 equilibria

Phase region boundary 5 at: 3.784E-01 1.181E+03
  ** LIQUID
  ** A2B
  BCC#1

Phase region boundary 6 at: 2.921E-01 1.181E+03
  ** LIQUID
  BCC#1
  Calculated 27 equilibria

Phase region boundary 7 at: 4.919E-01 1.181E+03
  ** LIQUID
  A2B
  Calculated. 32 equilibria

Phase region boundary 8 at: 6.472E-01 1.036E+03
  ** LIQUID
  A2B
  ** BCC#1

Phase region boundary 9 at: 7.632E-01 1.036E+03
  A2B
  ** BCC#1
  Calculated. 10 equilibria
  Terminating at known equilibrium

Phase region boundary 10 at: 8.247E-01 1.036E+03
  LIQUID
  ** BCC#1
  Calculated. 8 equilibria

Phase region boundary 11 at: 8.760E-01 1.205E+03
  LIQUID
  ** BCC#1
  ** FCC

Phase region boundary 12 at: 8.814E-01 1.205E+03
  LIQUID
  ** FCC
  Calculated 35 equilibria

Phase region boundary 13 at: 9.361E-01 1.205E+03
  BCC#1
  ** FCC
  Calculated 21 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated. 13 equilibria
  Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at known equilibrium
  Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated. 13 equilibria
  Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at known equilibrium
  Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated. 13 equilibria

```

Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.650E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 26 at: 3.650E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.650E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 7.907E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 29 at: 7.907E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 7.907E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 31 at: 2.438E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated.. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 32 at: 2.438E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated 26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated.. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated 29 equilibria

Phase region boundary 35 at: 6.409E-03 1.397E+03
 LIQUID
 ** BCC#2
 Calculated 13 equilibria

Phase region boundary 36 at: 6.409E-03 1.397E+03
 LIQUID
 ** BCC#2
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 37 at: 2.297E-01 1.243E+03
 LIQUID
 ** BCC#1
 Calculated 23 equilibria

Phase region boundary 38 at: 2.297E-01 1.243E+03
 LIQUID
 ** BCC#1

```

Calculated.                4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.204E+03
LIQUID
** A2B
Calculated.                12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.204E+03
LIQUID
** A2B
Calculated.                7 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated.                19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated                10 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

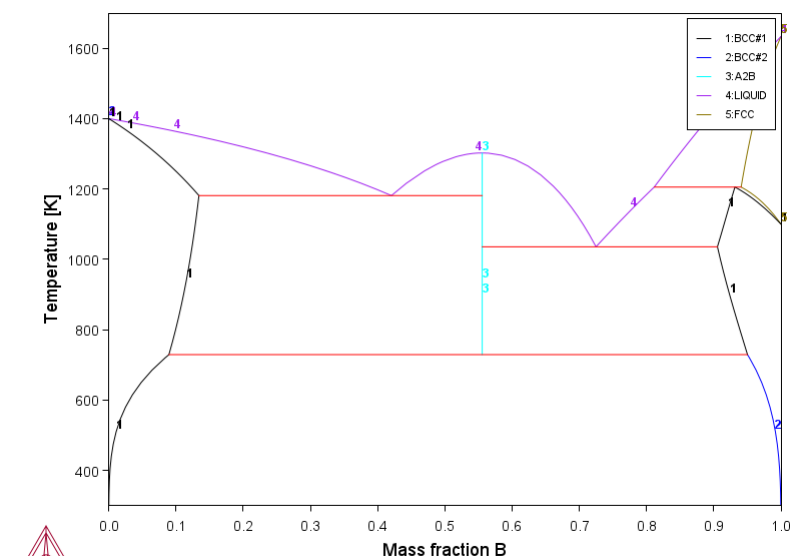
Setting automatic diagram axes

```

```

POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST:Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
POLY: ba

```

```

PARROT VERSION 5.3

Global minimization used as test only
PARROT: ed
ED_EXP: read 1
ED_EXP: s-we 0 4
ED_EXP: save
ED_EXP: ba
PARROT: opt 0
Use      25 experiments, maximum is      2000
Use      664 real workspace, maximum is    50000
PARROT: l-r C SCREEN

```

```

=====
OUTPUT FROM P A R R O T.  DATE 2025. 5.12   9:30:39

```

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

```

```

== OPTIMIZING CONDITIONS ==

```

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

```

== OPTIMIZING VARIABLES ==

```

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02756027E+04	2.02708732E+04	2.02708732E+04	7.92262612E-02
V2	-2.91817289E+01	-2.91044045E+01	-2.91044045E+01	3.44288780E-01
V11	-2.18124379E+04	-2.18135107E+04	-2.18135107E+04	3.96930274E-02
V12	1.51628519E+01	1.51635617E+01	1.51635617E+01	5.86409179E-02
V15	2.44432174E+04	2.45497588E+04	2.45497588E+04	6.05871516E-01
V16	-8.64785520E+00	-8.68107698E+00	-8.68107698E+00	2.02570116E+00
V17	3.11633728E+03	3.10543242E+03	3.10543242E+03	1.46283110E+00
V19	2.17221802E+04	2.15167018E+04	2.15167018E+04	4.73035740E+00
V20	-6.81979565E+00	-6.62138477E+00	-6.62138477E+00	1.19131169E+01

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 5.97166905E-02 TO 1.87230867E+01
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 1.17019292E+00

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1	T=1193	1181.	10.	-11.79	-1.179
1	W(LIQUID,B)=0.408	0.4205	2.00E-02	1.2542E-02	0.6271
1	W(BCC#1,B)=0.13	0.1342	2.00E-02	4.1628E-03	0.2081
2	T=1341	1302.	10.	-38.65	-3.865
2	HTR=3727	3728.	5.00E+02	0.5907	1.1814E-03
3	T=1049	1036.	10.	-13.26	-1.326
3	W(LIQUID,A)=0.27	0.2752	2.00E-02	5.1543E-03	0.2577
3	W(BCC#1,A)=9.3E-2	9.4532E-02	2.00E-02	1.5318E-03	7.6589E-02
5	T=726	729.0	10.	3.038	0.3038
5	X(BCC#1,B)=3.7E-2	3.7832E-02	2.00E-02	8.3176E-04	4.1588E-02
5	X(BCC#2,A)=0.114	0.1158	2.00E-02	1.7985E-03	8.9926E-02
6	X(BCC#1,B)=3.7E-2	3.6971E-02	2.00E-02	-2.8811E-05	-1.4405E-03
6	X(BCC#2,A)=0.114	0.1137	2.00E-02	-3.1937E-04	-1.5968E-02
10	W(LIQUID,A)=2E-2	1.9300E-02	2.00E-02	-6.9950E-04	-3.4975E-02
11	W(LIQUID,A)=4.2E-2	4.1338E-02	2.00E-02	-6.6193E-04	-3.3096E-02
12	W(LIQUID,A)=6.5E-2	6.4209E-02	2.00E-02	-7.9131E-04	-3.9566E-02
13	W(LIQUID,A)=9.3E-2	9.1819E-02	2.00E-02	-1.1805E-03	-5.9025E-02
20	W(LIQUID,A)=0.104	0.1029	2.00E-02	-1.1401E-03	-5.7007E-02
20	W(FCC,A)=3.8E-2	3.7516E-02	2.00E-02	-4.8352E-04	-2.4176E-02
21	W(LIQUID,A)=0.136	0.1354	2.00E-02	-5.5206E-04	-2.7603E-02
21	W(FCC,A)=4.7E-2	4.6453E-02	2.00E-02	-5.4654E-04	-2.7327E-02
22	W(LIQUID,A)=0.187	0.1856	2.00E-02	-1.3986E-03	-6.9932E-02
22	W(FCC,A)=5.9E-2	5.8624E-02	2.00E-02	-3.7571E-04	-1.8786E-02
23	W(LIQUID,A)=0.245	0.2436	2.00E-02	-1.4262E-03	-7.1312E-02
23	W(BCC#1,A)=8.5E-2	8.4617E-02	2.00E-02	-3.8328E-04	-1.9164E-02

PARROT:

PARROT:Hit RETURN to continue

PARROT: opt 30

Use 25 experiments, maximum is 2000
Use 664 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.87230867E+01					
1	1.0002E+00	2	1.0027E+00	3	9.9995E-01
6	9.9617E-01	7	1.0035E+00	8	1.0095E+00
AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.89605496E+01					
1	1.0003E+00	2	1.0027E+00	3	9.9995E-01
6	9.9617E-01	7	1.0035E+00	8	1.0095E+00
AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.83014084E+01					
1	1.0002E+00	2	1.0028E+00	3	9.9995E-01
6	9.9617E-01	7	1.0035E+00	8	1.0095E+00
AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.84820357E+01					
1	1.0002E+00	2	1.0028E+00	3	1.0001E+00
6	9.9617E-01	7	1.0035E+00	8	1.0095E+00
AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.81458597E+01					
1	1.0002E+00	2	1.0028E+00	3	9.9995E-01
6	9.9617E-01	7	1.0035E+00	8	1.0095E+00
AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.81533207E+01					
1	1.0002E+00	2	1.0028E+00	3	9.9995E-01
6	9.9617E-01	7	1.0035E+00	8	1.0095E+00
AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.81428975E+01					
1	1.0002E+00	2	1.0028E+00	3	9.9995E-01
6	9.9627E-01	7	1.0035E+00	8	1.0095E+00
AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.81424468E+01					
1	1.0002E+00	2	1.0028E+00	3	9.9995E-01
6	9.9627E-01	7	1.0036E+00	8	1.0095E+00
AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.81428498E+01					
1	1.0002E+00	2	1.0028E+00	3	9.9995E-01
6	9.9627E-01	7	1.0036E+00	8	1.0096E+00
AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 1.81422814E+01					
1	1.0002E+00	2	1.0028E+00	3	9.9995E-01
6	9.9627E-01	7	1.0036E+00	8	1.0095E+00
AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 2.71648791E-01					
1	9.9731E-01	2	1.0080E+00	3	9.9770E-01
6	9.9631E-01	7	1.0036E+00	8	1.0095E+00
AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 2.08936350E-01					
1	9.9807E-01	2	1.0079E+00	3	9.9771E-01
6	9.9186E-01	7	1.0026E+00	8	1.0117E+00
AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 1.23948085E-01					
1	9.9923E-01	2	1.0083E+00	3	9.9754E-01
6	9.8389E-01	7	1.0007E+00	8	1.0163E+00
AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 2.03113894E-02					
1	1.0012E+00	2	1.0080E+00	3	9.9854E-01
6	9.6202E-01	7	9.9565E-01	8	1.0233E+00

```
THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 13 iterations
1 1.0012E+00 2 1.0080E+00 3 9.9854E-01 4 1.0086E+00 5 9.8597E-01
6 9.6202E-01 7 9.9565E-01 8 1.0233E+00 9 1.0532E+00

1 -3.8357E-02 2 -1.1870E-02 3 6.3482E-03 4 -3.6856E-02 5 2.3203E-03
6 1.2698E-02 7 1.3270E-02 8 1.3631E-02 9 -1.1056E-01 10 1.1138E-03
11 -4.5495E-02 12 1.6608E-02 13 -7.5434E-03 14 -2.3309E-02 15 -1.0341E-02
16 -7.3602E-03 17 -1.7787E-02 18 -1.2819E-02 19 7.2318E-03 20 2.3231E-02
21 3.8604E-03 22 -1.4571E-02 23 4.2034E-03 24 -1.9320E-03 25 1.0875E-02
```

```
THE SUM OF SQUARES IS 2.03113894E-02
PARROT: cont 30
```

It is safe to CONTINUE only after TOO MANY ITERATIONS
and no change in variables and experiments ...
Now anything can happen ...

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:30:39
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 14
```

== OPTIMIZING CONDITIONS ==

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02943853E+04	2.02708732E+04	2.02708732E+04	1.04350637E-01
V2	-2.93382450E+01	-2.91044045E+01	-2.91044045E+01	9.59564257E-02
V11	-2.17817013E+04	-2.18135107E+04	-2.18135107E+04	2.05054030E-01
V12	1.52939540E+01	1.51635617E+01	1.51635617E+01	3.41065979E-01
V15	2.42053235E+04	2.45497588E+04	2.45497588E+04	1.49305440E-01
V16	-8.35136726E+00	-8.68107698E+00	-8.68107698E+00	5.14756063E-01
V17	3.09193286E+03	3.10543242E+03	3.10543242E+03	2.62894908E-01
V19	2.20175540E+04	2.15167018E+04	2.15167018E+04	7.15844113E-01
V20	-6.97387622E+00	-6.62138477E+00	-6.62138477E+00	1.86930402E+00

```
NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.87230867E+01 TO 2.03113894E-02
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 1.26946184E-03
```

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1193.	10.	-0.3836	-3.8357E-02
1 W(LIQUID,B)=0.408	0.4078	2.00E-02	-2.3741E-04	-1.1870E-02
1 W(BCC#1,B)=0.13	0.1301	2.00E-02	1.2696E-04	6.3482E-03
2 T=1341	1341.	10.	-0.3686	-3.6856E-02
2 HTR=3727	3728.	5.00E+02	1.160	2.3203E-03
3 T=1049	1049.	10.	0.1270	1.2698E-02
3 W(LIQUID,A)=0.27	0.2703	2.00E-02	2.6540E-04	1.3270E-02
3 W(BCC#1,A)=9.3E-2	9.3273E-02	2.00E-02	2.7261E-04	1.3631E-02
5 T=726	724.9	10.	-1.106	-0.1106
5 X(BCC#1,B)=3.7E-2	3.7022E-02	2.00E-02	2.2275E-05	1.1138E-03
5 X(BCC#2,A)=0.114	0.1131	2.00E-02	-9.0990E-04	-4.5495E-02
6 X(BCC#1,B)=3.7E-2	3.7332E-02	2.00E-02	3.3215E-04	1.6608E-02
6 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.5087E-04	-7.5434E-03
10 W(LIQUID,A)=2E-2	1.9534E-02	2.00E-02	-4.6617E-04	-2.3309E-02
11 W(LIQUID,A)=4.2E-2	4.1793E-02	2.00E-02	-2.0682E-04	-1.0341E-02
12 W(LIQUID,A)=6.5E-2	6.4853E-02	2.00E-02	-1.4720E-04	-7.3602E-03
13 W(LIQUID,A)=9.3E-2	9.2644E-02	2.00E-02	-3.5574E-04	-1.7787E-02
20 W(LIQUID,A)=0.104	0.1037	2.00E-02	-2.5638E-04	-1.2819E-02
20 W(FCC,A)=3.8E-2	3.8145E-02	2.00E-02	1.4464E-04	7.2318E-03
21 W(LIQUID,A)=0.136	0.1365	2.00E-02	4.6461E-04	2.3231E-02
21 W(FCC,A)=4.7E-2	4.7077E-02	2.00E-02	7.7209E-05	3.8604E-03
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.9142E-04	-1.4571E-02
22 W(FCC,A)=5.9E-2	5.9084E-02	2.00E-02	8.4067E-05	4.2034E-03
23 W(LIQUID,A)=0.245	0.2450	2.00E-02	-3.8639E-05	-1.9320E-03
23 W(BCC#1,A)=8.5E-2	8.5217E-02	2.00E-02	2.1749E-04	1.0875E-02

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Optimization converged, try to add equilibrium 4 again

PARROT: ed

ED_EXP: read 1

ED_EXP: s-e 4

Equilibrium number 4 , label AINV

ED_EXP: s-a-s

T 71205.438651/: 1200

Automatic start values for phase constituents? /N/: N

Phase LIQUID

Major constituent(s) /b/: b

Phase BCC

Major constituent(s) /b/: b

```

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:
P=101325
FIXED PHASES
LIQUID=1 BCC#1=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1204.49 K ( 931.34 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30105E+02
Total Gibbs energy -9.78529E+03, Enthalpy 1.98664E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
A                6.6315E-01  1.0194E-01  3.9330E-01 -9.3456E+03 SER
B                2.3368E+00  8.9806E-01  8.5787E-01 -1.5353E+03 SER

FCC              Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.5883E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40182E-01 A 5.98178E-02

BCC#1            Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.5313E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31041E-01 A 6.89587E-02

LIQUID           Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 3.8909E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.09977E-01 A 1.90023E-01
SET_WEIGHT 0,,,
EXPERIMENT T=1203:DT
EXPERIMENT W(LIQUID,A)=0.19:DX
EXPERIMENT W(BCC#1,A)=6.9E-2:DX
EXPERIMENT W(FCC,A)=6E-2:DX
ED_EXP: ba
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0.003 s
Found the set of lowest grid points in 0.000 s
Calculated POLY solution 0.003 s, total time 0.006 s
POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11

```



```

Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
  Calculated. 14 equilibria

Phase region boundary 3 at: 6.822E-01 7.249E+02
  ** A2B
  BCC#1
  ** BCC#2

Phase region boundary 4 at: 3.623E-01 7.249E+02
  ** A2B
  BCC#1
  Calculated. 15 equilibria

Phase region boundary 5 at: 3.770E-01 1.193E+03
  ** LIQUID
  ** A2B
  BCC#1

Phase region boundary 6 at: 2.827E-01 1.193E+03
  ** LIQUID
  BCC#1
  Calculated 30 equilibria

Phase region boundary 7 at: 4.863E-01 1.193E+03
  ** LIQUID
  A2B
  Calculated. 28 equilibria

Phase region boundary 8 at: 6.501E-01 1.049E+03
  ** LIQUID
  A2B
  ** BCC#1

Phase region boundary 9 at: 7.641E-01 1.049E+03
  A2B
  ** BCC#1
  Calculated. 11 equilibria
  Terminating at known equilibrium

Phase region boundary 10 at: 8.275E-01 1.049E+03
  LIQUID
  ** BCC#1
  Calculated. 8 equilibria

Phase region boundary 11 at: 8.751E-01 1.204E+03
  LIQUID
  ** BCC#1
  ** FCC

Phase region boundary 12 at: 8.804E-01 1.204E+03
  LIQUID
  ** FCC
  Calculated 32 equilibria

Phase region boundary 13 at: 9.356E-01 1.204E+03
  BCC#1
  ** FCC
  Calculated 21 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated. 13 equilibria
  Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at known equilibrium
  Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated. 13 equilibria
  Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at known equilibrium
  Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
  Calculated. 13 equilibria

```

Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.644E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 26 at: 3.644E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.644E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 14 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 7.913E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 29 at: 7.913E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 7.913E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated.. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 31 at: 2.449E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated.. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 32 at: 2.449E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated 26 equilibria

Phase region boundary 33 at: 8.860E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated.. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 34 at: 8.860E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated 29 equilibria

Phase region boundary 35 at: 6.416E-03 1.397E+03
 LIQUID
 ** BCC#1
 Calculated 8 equilibria

Phase region boundary 36 at: 6.416E-03 1.397E+03
 LIQUID
 ** BCC#1
 Calculated.. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 37 at: 2.299E-01 1.244E+03
 LIQUID
 ** BCC#1
 Calculated 18 equilibria

Phase region boundary 38 at: 2.299E-01 1.244E+03
 LIQUID
 ** BCC#1

Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.240E+03
LIQUID
** A2B

Calculated. 14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03
LIQUID
** A2B

Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC

Calculated. 19 equilibria
Terminating at known equilibrium

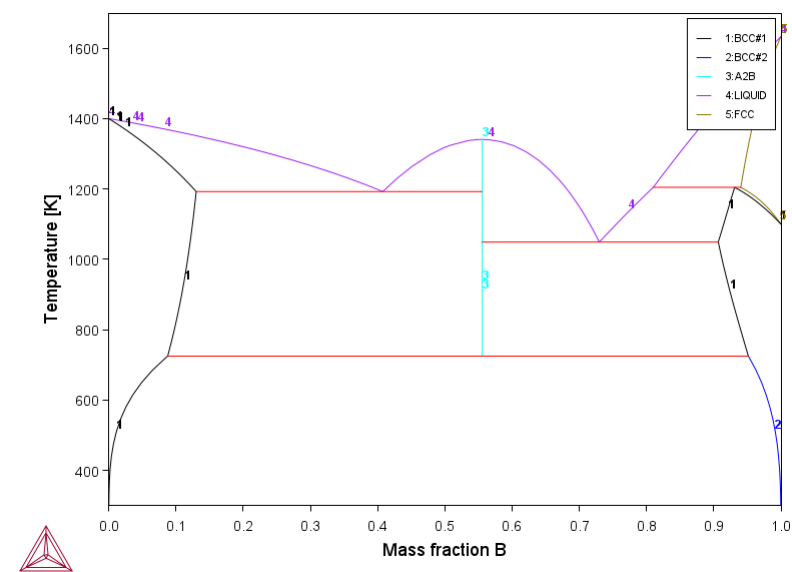
Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC

Calculated 12 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping 2 seconds

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
POST: plot



POST: set-inter
POST:Hit RETURN to continue
POST: @@ Sometimes a very strange shape of the fcc phase here and no
POST: @@ equilibrium between liq, fcc and bcc at high B content.
POST: ba
POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:31: 3

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 14

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02943853E+04	2.02708732E+04	2.02708732E+04	1.04350637E-01
V2	-2.93382450E+01	-2.91044045E+01	-2.91044045E+01	9.59564257E-02
V11	-2.17817013E+04	-2.18135107E+04	-2.18135107E+04	2.05054030E-01
V12	1.52939540E+01	1.51635617E+01	1.51635617E+01	3.41065979E-01
V15	2.42053235E+04	2.45497588E+04	2.45497588E+04	1.49305440E-01
V16	-8.35136726E+00	-8.68107698E+00	-8.68107698E+00	5.14756063E-01

```
V17      3.09193286E+03      3.10543242E+03      3.10543242E+03      2.62894908E-01
V19      2.20175540E+04      2.15167018E+04      2.15167018E+04      7.15844113E-01
V20     -6.97387622E+00     -6.62138477E+00     -6.62138477E+00      1.86930402E+00
```

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.87230867E+01 TO 2.03113894E-02
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 1.26946184E-03

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

```
1 T=1193      1193.      10.      -0.3836      -3.8357E-02
1 W(LIQUID,B)=0.408      0.4078      2.00E-02      -2.3741E-04      -1.1870E-02
1 W(BCC#1,B)=0.13      0.1301      2.00E-02      1.2696E-04      6.3482E-03
2 T=1341      1341.      10.      -0.3686      -3.6856E-02
2 HTR=3727      3728.      5.00E+02      1.160      2.3203E-03
3 T=1049      1049.      10.      0.1270      1.2698E-02
3 W(LIQUID,A)=0.27      0.2703      2.00E-02      2.6540E-04      1.3270E-02
3 W(BCC#1,A)=9.3E-2      9.3273E-02      2.00E-02      2.7261E-04      1.3631E-02
5 T=726      724.9      10.      -1.106      -0.1106
5 X(BCC#1,B)=3.7E-2      3.7022E-02      2.00E-02      2.2275E-05      1.1138E-03
5 X(BCC#2,A)=0.114      0.1131      2.00E-02      -9.0990E-04      -4.5495E-02
6 X(BCC#1,B)=3.7E-2      3.7332E-02      2.00E-02      3.3215E-04      1.6608E-02
6 X(BCC#2,A)=0.114      0.1138      2.00E-02      -1.5087E-04      -7.5434E-03
10 W(LIQUID,A)=2E-2      1.9534E-02      2.00E-02      -4.6617E-04      -2.3309E-02
11 W(LIQUID,A)=4.2E-2      4.1793E-02      2.00E-02      -2.0682E-04      -1.0341E-02
12 W(LIQUID,A)=6.5E-2      6.4853E-02      2.00E-02      -1.4720E-04      -7.3602E-03
13 W(LIQUID,A)=9.3E-2      9.2644E-02      2.00E-02      -3.5574E-04      -1.7787E-02
20 W(LIQUID,A)=0.104      0.1037      2.00E-02      -2.5638E-04      -1.2819E-02
20 W(FCC,A)=3.8E-2      3.8145E-02      2.00E-02      1.4464E-04      7.2318E-03
21 W(LIQUID,A)=0.136      0.1365      2.00E-02      4.6461E-04      2.3231E-02
21 W(FCC,A)=4.7E-2      4.7077E-02      2.00E-02      7.7209E-05      3.8604E-03
22 W(LIQUID,A)=0.187      0.1867      2.00E-02      -2.9142E-04      -1.4571E-02
22 W(FCC,A)=5.9E-2      5.9084E-02      2.00E-02      8.4067E-05      4.2034E-03
23 W(LIQUID,A)=0.245      0.2450      2.00E-02      -3.8639E-05      -1.9320E-03
23 W(BCC#1,A)=8.5E-2      8.5217E-02      2.00E-02      2.1749E-04      1.0875E-02
```

PARROT:

PARROT: @@ Note that all other experiments are well fitted.

PARROT: @@ Try to improve by optimizing a little more...

PARROT: resc

PARROT: opt 30

Use 25 experiments, maximum is 2000

Use 664 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```
AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 2.03113894E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 2.09433436E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 2.13822277E-02
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 2.22484123E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.93075860E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.98930651E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.91984750E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.91871477E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.92004543E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0001E+00 9 1.0000E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 1.91824224E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 1.76093969E-02
1 1.0002E+00 2 9.9996E-01 3 9.9993E-01 4 1.0002E+00 5 9.9994E-01
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 1.62254706E-02
1 1.0002E+00 2 1.0000E+00 3 9.9991E-01 4 1.0002E+00 5 9.9991E-01
6 1.0000E+00 7 1.0001E+00 8 1.0001E+00 9 1.0002E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 1.49619224E-02
1 1.0003E+00 2 1.0000E+00 3 9.9987E-01 4 1.0003E+00 5 9.9982E-01
6 9.9982E-01 7 1.0000E+00 8 1.0002E+00 9 1.0005E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 1.35517636E-02
1 1.0003E+00 2 1.0000E+00 3 9.9985E-01 4 1.0003E+00 5 9.9971E-01
6 9.9938E-01 7 9.9993E-01 8 1.0005E+00 9 1.0011E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 1.17454569E-02
1 1.0005E+00 2 1.0001E+00 3 9.9983E-01 4 1.0004E+00 5 9.9947E-01
6 9.9849E-01 7 9.9972E-01 8 1.0010E+00 9 1.0022E+00

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 9.25431213E-03
1 1.0007E+00 2 1.0001E+00 3 9.9983E-01 4 1.0006E+00 5 9.9902E-01
```

```

6  9.9671E-01  7  9.9930E-01  8  1.0022E+00  9  1.0044E+00

      AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 6.17558783E-03
1  1.0011E+00  2  1.0002E+00  3  9.9983E-01  4  1.0010E+00  5  9.9811E-01
6  9.9311E-01  7  9.9845E-01  8  1.0044E+00  9  1.0089E+00

      AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 4.81236826E-03
1  1.0015E+00  2  1.0003E+00  3  9.9985E-01  4  1.0014E+00  5  9.9691E-01
6  9.8836E-01  7  9.9733E-01  8  1.0073E+00  9  1.0147E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 17 iterations
1  1.0015E+00  2  1.0003E+00  3  9.9985E-01  4  1.0014E+00  5  9.9691E-01
6  9.8836E-01  7  9.9733E-01  8  1.0073E+00  9  1.0147E+00

1 -3.1807E-02  2 -1.3182E-02  3 -4.4012E-03  4  1.7574E-03  5 -1.5990E-02
6  1.5796E-02  7  1.4975E-02  8  3.8285E-03  9 -3.8311E-03 10  2.0959E-02
11 -9.7954E-03 12  2.1498E-02 13 -8.4810E-03 14 -2.0919E-02 15 -6.1139E-03
16 -2.0488E-03 17 -1.2086E-02 18 -7.2061E-03 19  1.0744E-02 20  2.7883E-02
21  4.8109E-03 22 -1.3149E-02 23 -2.6929E-03 24 -1.7123E-03 25 -7.3070E-06

```

THE SUM OF SQUARES IS 4.81236826E-03
PARROT: l-r C SCREEN

```

=====
OUTPUT FROM  P A R R O T.  DATE 2025. 5.12    9:31: 3

```

*** SUCCESSFUL OPTIMIZATION. ***
 NUMBER OF ITERATIONS: 18

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03239810E+04	2.02943853E+04	2.02943853E+04	1.07559802E-01
V2	-2.93471952E+01	-2.93382450E+01	-2.93382450E+01	9.88133978E-02
V11	-2.17785061E+04	-2.17817013E+04	-2.17817013E+04	2.11797817E-01
V12	1.53148537E+01	1.52939540E+01	1.52939540E+01	3.48100762E-01
V15	2.41304970E+04	2.42053235E+04	2.42053235E+04	1.52390625E-01
V16	-8.25418969E+00	-8.35136726E+00	-8.35136726E+00	5.41250685E-01
V17	3.08367945E+03	3.09193286E+03	3.09193286E+03	2.65305952E-01
V19	2.21788112E+04	2.20175540E+04	2.20175540E+04	7.24036379E-01
V20	-7.07623325E+00	-6.97387622E+00	-6.97387622E+00	1.86011386E+00

NUMBER OF OPTIMIZING VARIABLES : 9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM 2.03113894E-02 TO 4.81236826E-03
 DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.00773016E-04

\$ ===== BLOCK NUMBER 1

```

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)

```

1 T=1193	1193.	10.	-0.3181	-3.1807E-02
1 W(LIQUID,B)=0.408	0.4077	2.00E-02	-2.6364E-04	-1.3182E-02
1 W(BCC#1,B)=0.13	0.1299	2.00E-02	-8.8024E-05	-4.4012E-03
2 T=1341	1341.	10.	1.7574E-02	1.7574E-03
2 HTR=3727	3719.	5.00E+02	-7.995	-1.5990E-02
3 T=1049	1049.	10.	0.1580	1.5796E-02
3 W(LIQUID,A)=0.27	0.2703	2.00E-02	2.9950E-04	1.4975E-02
3 W(BCC#1,A)=9.3E-2	9.3077E-02	2.00E-02	7.6569E-05	3.8285E-03
5 T=726	726.0	10.	-3.8311E-02	-3.8311E-03
5 X(BCC#1,B)=3.7E-2	3.7419E-02	2.00E-02	4.1918E-04	2.0959E-02
5 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.9591E-04	-9.7954E-03
6 X(BCC#1,B)=3.7E-2	3.7430E-02	2.00E-02	4.2995E-04	2.1498E-02
6 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.6962E-04	-8.4810E-03
10 W(LIQUID,A)=2E-2	1.9582E-02	2.00E-02	-4.1839E-04	-2.0919E-02
11 W(LIQUID,A)=4.2E-2	4.1878E-02	2.00E-02	-1.2228E-04	-6.1139E-03
12 W(LIQUID,A)=6.5E-2	6.4959E-02	2.00E-02	-4.0975E-05	-2.0488E-03
13 W(LIQUID,A)=9.3E-2	9.2758E-02	2.00E-02	-2.4173E-04	-1.2086E-02
20 W(LIQUID,A)=0.104	0.1039	2.00E-02	-1.4412E-04	-7.2061E-03
20 W(FCC,A)=3.8E-2	3.8215E-02	2.00E-02	2.1487E-04	1.0744E-02
21 W(LIQUID,A)=0.136	0.1366	2.00E-02	5.5767E-04	2.7883E-02
21 W(FCC,A)=4.7E-2	4.7096E-02	2.00E-02	9.6218E-05	4.8109E-03
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.6298E-04	-1.3149E-02
22 W(FCC,A)=5.9E-2	5.8946E-02	2.00E-02	-5.3858E-05	-2.6929E-03
23 W(LIQUID,A)=0.245	0.2450	2.00E-02	-3.4246E-05	-1.7123E-03
23 W(BCC#1,A)=8.5E-2	8.5000E-02	2.00E-02	-1.4614E-07	-7.3070E-06

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3

POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.

```

POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0.002 s
Found the set of lowest grid points in 0.001 s
Calculated POLY solution 0.003 s, total time 0.006 s
POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
BCC#1
** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.821E-01 7.260E+02
** A2B
BCC#1
** BCC#2

Phase region boundary 4 at: 3.626E-01 7.260E+02
** A2B
BCC#1
Calculated. 15 equilibria

Phase region boundary 5 at: 3.769E-01 1.193E+03
** LIQUID
** A2B
BCC#1

Phase region boundary 6 at: 2.826E-01 1.193E+03
** LIQUID
BCC#1
Calculated 27 equilibria

Phase region boundary 7 at: 4.863E-01 1.193E+03
** LIQUID
A2B
Calculated. 33 equilibria

```

Phase region boundary 8 at: 6.500E-01 1.049E+03
 ** LIQUID
 A2B
 ** BCC#1

Phase region boundary 9 at: 7.642E-01 1.049E+03
 A2B
 ** BCC#1
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 10 at: 8.276E-01 1.049E+03
 LIQUID
 ** BCC#1
 Calculated. 8 equilibria

Phase region boundary 11 at: 8.751E-01 1.204E+03
 LIQUID
 ** BCC#1
 ** FCC

Phase region boundary 12 at: 8.804E-01 1.204E+03
 LIQUID
 ** FCC
 Calculated 33 equilibria

Phase region boundary 13 at: 9.358E-01 1.204E+03
 BCC#1
 ** FCC
 Calculated 20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1

```

Calculated.                14  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.912E-01  7.700E+02
** A2B
   BCC#1
Calculated                10  equilibria

Phase region boundary  29 at:   7.912E-01  7.700E+02
** A2B
   BCC#1
Calculated.                3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.912E-01  7.700E+02
** A2B
   BCC#1
Calculated.                9  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.448E-01  1.230E+03
** LIQUID
   BCC#1
Calculated.                4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.448E-01  1.230E+03
** LIQUID
   BCC#1
Calculated                26  equilibria

Phase region boundary  33 at:   8.860E-01  1.230E+03
** LIQUID
   FCC
Calculated.                2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.860E-01  1.230E+03
** LIQUID
   FCC
Calculated                29  equilibria

Phase region boundary  35 at:   6.414E-03  1.397E+03
   LIQUID
** BCC#1
Calculated                11  equilibria

Phase region boundary  36 at:   6.414E-03  1.397E+03
   LIQUID
** BCC#1
Calculated.                13  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.298E-01  1.244E+03
   LIQUID
** BCC#1
Calculated                19  equilibria

Phase region boundary  38 at:   2.298E-01  1.244E+03
   LIQUID
** BCC#1
Calculated.                4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.240E+03
   LIQUID
** A2B
Calculated.                14  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.240E+03
   LIQUID
** A2B
Calculated.                8  equilibria
Terminating at known equilibrium

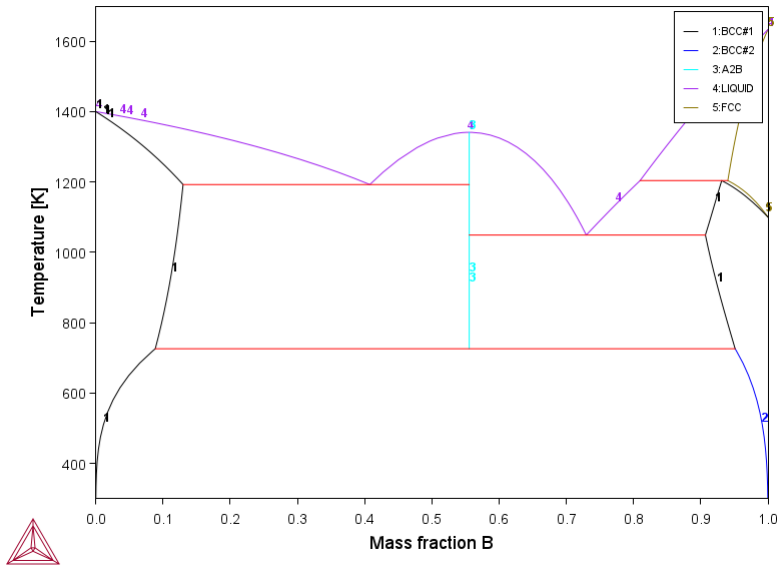
Phase region boundary  41 at:   9.927E-01  1.613E+03
   LIQUID
** FCC
Calculated.                19  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:   9.927E-01  1.613E+03
   LIQUID
** FCC
Calculated                10  equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping                1  seconds
POLY: post
      POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
POST: plot

```

POST:
 POST: set-inter
 POST: Hit RETURN to continue
 POST: ba
 POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
 PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid
 PARROT: @@ at high B. Restore equilibrium 4 on the POP file
 PARROT: ed
 ED_EXP: read 1
 ED_EXP: s-e 4
 Equilibrium number 4 , label AINV
 ED_EXP: s-we 1
 Equilibria (range) or label(s) /PRESENT/: PRESENT
 ED_EXP: s-a-s
 T /1205.438651/: 1200
 Automatic start values for phase constituents? /N/: N

Phase LIQUID
 Major constituent(s) /b/: b

Phase BCC
 Major constituent(s) /b/: b

Phase FCC
 Major constituent(s) /b/: b

ED_EXP:
 c-e
 Testing result with global minimization
 13 ITS, CPU TIME USED 0 SECONDS
 ED_EXP: l-e

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS
 Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:
 P=101325
 FIXED PHASES
 LIQUID=1 BCC#1=1 FCC=1
 DEGREES OF FREEDOM 0

Temperature 1203.85 K (930.70 C), Pressure 1.013250E+05
 Number of moles of components 3.00000E+00, Mass in grams 1.30108E+02
 Total Gibbs energy -9.75161E+03, Enthalpy 1.98660E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
A	6.6308E-01	1.0193E-01	3.9435E-01	-9.3138E+03	SER
B	2.3369E+00	8.9807E-01	8.5824E-01	-1.5301E+03	SER

FCC Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 4.5889E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 9.40282E-01 A 5.97184E-02

BCC#1 Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 4.5321E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 9.31176E-01 A 6.88244E-02

LIQUID Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 3.8897E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 8.09707E-01 A 1.90293E-01
 EXPERIMENT T=1203:DT \$1203.85:10 NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX \$0.190293:2E-2 NO=2
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX \$6.88244E-2:2E-2 NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX \$5.97184E-2:2E-2 NO=4

ED_EXP: @@ Now equilibrium 4 is on the high B side

ED_EXP: save

ED_EXP: ba

PARROT: resc

PARROT: opt 0

Use 29 experiments, maximum is 2000
 Use 740 real workspace, maximum is 50000

PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:31:26

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03239810E+04	2.03239810E+04	2.03239810E+04	0.00000000E+00
V2	-2.93471952E+01	-2.93471952E+01	-2.93471952E+01	0.00000000E+00
V11	-2.17785061E+04	-2.17785061E+04	-2.17785061E+04	0.00000000E+00
V12	1.53148537E+01	1.53148537E+01	1.53148537E+01	0.00000000E+00
V15	2.41304970E+04	2.41304970E+04	2.41304970E+04	0.00000000E+00
V16	-8.25418969E+00	-8.25418969E+00	-8.25418969E+00	0.00000000E+00
V17	3.08367945E+03	3.08367945E+03	3.08367945E+03	0.00000000E+00
V19	2.21788112E+04	2.21788112E+04	2.21788112E+04	0.00000000E+00
V20	-7.07623325E+00	-7.07623325E+00	-7.07623325E+00	0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.25795062E-02
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 6.28975310E-04

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1193.	10.	-0.3181	-3.1807E-02
1 W(LIQUID,B)=0.408	0.4077	2.00E-02	-2.6364E-04	-1.3182E-02
1 W(BCC#1,B)=0.13	0.1299	2.00E-02	-8.8024E-05	-4.4012E-03
2 T=1341	1341.	10.	1.7574E-02	1.7574E-03
2 HTR=3727	3719.	5.00E+02	-7.995	-1.5990E-02
3 T=1049	1049.	10.	0.1580	1.5796E-02
3 W(LIQUID,A)=0.27	0.2703	2.00E-02	2.9950E-04	1.4975E-02
3 W(BCC#1,A)=9.3E-2	9.3077E-02	2.00E-02	7.6569E-05	3.8285E-03
4 T=1203	1204.	10.	0.8531	8.5307E-02
4 W(LIQUID,A)=0.19	0.1903	2.00E-02	2.9300E-04	1.4650E-02
4 W(BCC#1,A)=6.9E-2	6.8824E-02	2.00E-02	-1.7559E-04	-8.7793E-03
4 W(FCC,A)=6E-2	5.9718E-02	2.00E-02	-2.8155E-04	-1.4078E-02
5 T=726	726.0	10.	-3.8311E-02	-3.8311E-03
5 X(BCC#1,B)=3.7E-2	3.7419E-02	2.00E-02	4.1918E-04	2.0959E-02
5 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.9591E-04	-9.7954E-03
6 X(BCC#1,B)=3.7E-2	3.7430E-02	2.00E-02	4.2995E-04	2.1498E-02
6 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.6962E-04	-8.4810E-03
10 W(LIQUID,A)=2E-2	1.9582E-02	2.00E-02	-4.1839E-04	-2.0919E-02
11 W(LIQUID,A)=4.2E-2	4.1878E-02	2.00E-02	-1.2228E-04	-6.1139E-03
12 W(LIQUID,A)=6.5E-2	6.4959E-02	2.00E-02	-4.0975E-05	-2.0488E-03
13 W(LIQUID,A)=9.3E-2	9.2758E-02	2.00E-02	-2.4173E-04	-1.2086E-02
20 W(LIQUID,A)=0.104	0.1039	2.00E-02	-1.4412E-04	-7.2061E-03
20 W(FCC,A)=3.8E-2	3.8215E-02	2.00E-02	2.1487E-04	1.0744E-02
21 W(LIQUID,A)=0.136	0.1366	2.00E-02	5.5767E-04	2.7883E-02
21 W(FCC,A)=4.7E-2	4.7096E-02	2.00E-02	9.6218E-05	4.8109E-03
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.6298E-04	-1.3149E-02
22 W(FCC,A)=5.9E-2	5.8946E-02	2.00E-02	-5.3858E-05	-2.6929E-03
23 W(LIQUID,A)=0.245	0.2450	2.00E-02	-3.4246E-05	-1.7123E-03
23 W(BCC#1,A)=8.5E-2	8.5000E-02	2.00E-02	-1.4614E-07	-7.3070E-06

PARROT:

PARROT:Hit RETURN to continue

PARROT: opt 30

Use 29 experiments, maximum is 2000

Use 740 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.25795062E-02				
1	1.0000E+00	2	1.0000E+00	3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6	1.0000E+00	7	1.0000E+00	8 1.0000E+00 9 1.0000E+00
AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.34147293E-02				
1	1.0001E+00	2	1.0000E+00	3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6	1.0000E+00	7	1.0000E+00	8 1.0000E+00 9 1.0000E+00
AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.53070237E-02				
1	1.0000E+00	2	1.0001E+00	3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6	1.0000E+00	7	1.0000E+00	8 1.0000E+00 9 1.0000E+00
AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.28163845E-02				
1	1.0000E+00	2	1.0000E+00	3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6	1.0000E+00	7	1.0000E+00	8 1.0000E+00 9 1.0000E+00
AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.31841444E-02				
1	1.0000E+00	2	1.0000E+00	3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6	1.0000E+00	7	1.0000E+00	8 1.0000E+00 9 1.0000E+00
AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.07470885E-02				
1	1.0000E+00	2	1.0000E+00	3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6	1.0000E+00	7	1.0000E+00	8 1.0000E+00 9 1.0000E+00
AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.14583924E-02				
1	1.0000E+00	2	1.0000E+00	3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6	1.0001E+00	7	1.0000E+00	8 1.0000E+00 9 1.0000E+00
AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.08970106E-02				
1	1.0000E+00	2	1.0000E+00	3 1.0000E+00 4 1.0000E+00 5 1.0001E+00

```

6 1.0000E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21772375E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 1.02510217E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0001E+00

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.86772661E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 9.9998E-01 5 1.0003E+00
6 9.9991E-01 7 9.9998E-01 8 9.9982E-01 9 1.0002E+00

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 6.72903834E-03
1 1.0000E+00 2 1.0001E+00 3 9.9991E-01 4 9.9983E-01 5 1.0003E+00
6 1.0000E+00 7 9.9992E-01 8 9.9986E-01 9 1.0004E+00

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.56407049E-03
1 1.0001E+00 2 1.0001E+00 3 9.9971E-01 4 9.9953E-01 5 1.0003E+00
6 1.0002E+00 7 9.9982E-01 8 9.9994E-01 9 1.0008E+00

      AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 6.34191917E-03
1 1.0003E+00 2 1.0003E+00 3 9.9932E-01 4 9.9890E-01 5 1.0004E+00
6 1.0006E+00 7 9.9959E-01 8 1.0001E+00 9 1.0017E+00

      AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 6.08448353E-03
1 1.0007E+00 2 1.0006E+00 3 9.9854E-01 4 9.9765E-01 5 1.0004E+00
6 1.0014E+00 7 9.9915E-01 8 1.0005E+00 9 1.0034E+00

      AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 5.98271438E-03
1 1.0011E+00 2 1.0010E+00 3 9.9762E-01 4 9.9614E-01 5 1.0005E+00
6 1.0024E+00 7 9.9862E-01 8 1.0009E+00 9 1.0054E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 15 iterations
1 1.0011E+00 2 1.0010E+00 3 9.9762E-01 4 9.9614E-01 5 1.0005E+00
6 1.0024E+00 7 9.9862E-01 8 1.0009E+00 9 1.0054E+00

1 -3.4110E-02 2 -1.6134E-02 3 -4.8975E-03 4 2.9026E-03 5 -7.2601E-03
6 1.1782E-02 7 1.1607E-02 8 3.8732E-03 9 7.2223E-03 10 2.9066E-02
11 -5.8157E-03 12 -5.4689E-03 13 -2.8366E-03 14 2.3683E-02 15 -9.7508E-03
16 2.4082E-02 17 -8.7767E-03 18 -2.1085E-02 19 -6.5178E-03 20 -2.7321E-03
21 -1.3089E-02 22 -8.3119E-03 23 1.2191E-02 24 2.6627E-02 25 7.4289E-03
26 -1.3946E-02 27 2.4127E-03 28 -7.2775E-03 29 -1.5805E-03

      THE SUM OF SQUARES IS 5.98271438E-03
PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:31:27

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 16

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR. VALUE START VALUE SCALING FACTOR REL.STAND.DEV
V1 2.03454598E+04 2.03239810E+04 2.03239810E+04 1.02423466E-01
V2 -2.93769553E+01 -2.93471952E+01 -2.93471952E+01 9.37762247E-02
V11 -2.17266456E+04 -2.17785061E+04 -2.17785061E+04 2.00749380E-01
V12 1.52556729E+01 1.53148537E+01 1.53148537E+01 3.29240608E-01
V15 2.41427097E+04 2.41304970E+04 2.41304970E+04 1.34940930E-01
V16 -8.27427337E+00 -8.25418969E+00 -8.25418969E+00 4.84822531E-01
V17 3.07943197E+03 3.08367945E+03 3.08367945E+03 2.31440510E-01
V19 2.21987951E+04 2.21788112E+04 2.21788112E+04 5.66912120E-01
V20 -7.11454006E+00 -7.07623325E+00 -7.07623325E+00 1.53559103E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.25795062E-02 TO 5.98271438E-03
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99135719E-04

$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1193. 10. -0.3411 -3.4110E-02
1 W(LIQUID,B)=0.408 0.4077 2.00E-02 -3.2269E-04 -1.6134E-02
1 W(BCC#1,B)=0.13 0.1299 2.00E-02 -9.7950E-05 -4.8975E-03
2 T=1341 1341. 10. 2.9026E-02 2.9026E-03
2 HTR=3727 3723. 5.00E+02 -3.630 -7.2601E-03
3 T=1049 1049. 10. 0.1178 1.1782E-02
3 W(LIQUID,A)=0.27 0.2702 2.00E-02 2.3214E-04 1.1607E-02
3 W(BCC#1,A)=9.3E-2 9.3077E-02 2.00E-02 7.7465E-05 3.8732E-03
4 T=1203 1203. 10. 7.2223E-02 7.2223E-03
4 W(LIQUID,A)=0.19 0.1906 2.00E-02 5.8132E-04 2.9066E-02
4 W(BCC#1,A)=6.9E-2 6.8884E-02 2.00E-02 -1.1631E-04 -5.8157E-03
4 W(ECC,A)=6E-2 5.9891E-02 2.00E-02 -1.0938E-04 -5.4689E-03
5 T=726 726.0 10. -2.8366E-02 -2.8366E-03
5 X(BCC#1,B)=3.7E-2 3.7474E-02 2.00E-02 4.7365E-04 2.3683E-02
5 X(BCC#2,A)=0.114 0.1138 2.00E-02 -1.9502E-04 -9.7508E-03
6 X(BCC#1,B)=3.7E-2 3.7482E-02 2.00E-02 4.8164E-04 2.4082E-02

```

```
6 X(BCC#2,A)=0.114      0.1138      2.00E-02 -1.7553E-04 -8.7767E-03
10 W(LIQUID,A)=2E-2      1.9578E-02  2.00E-02 -4.2170E-04 -2.1085E-02
11 W(LIQUID,A)=4.2E-2    1.1870E-02  2.00E-02 -1.3036E-04 -6.5178E-03
12 W(LIQUID,A)=6.5E-2    6.4945E-02  2.00E-02 -5.4643E-05 -2.7321E-03
13 W(LIQUID,A)=9.3E-2    9.2738E-02  2.00E-02 -2.6178E-04 -1.3089E-02
20 W(LIQUID,A)=0.104     0.1038      2.00E-02 -1.6624E-04 -8.3119E-03
20 W(FCC,A)=3.8E-2       3.8244E-02  2.00E-02  2.4382E-04  1.2191E-02
21 W(LIQUID,A)=0.136     0.1365      2.00E-02  5.3254E-04  2.6627E-02
21 W(FCC,A)=4.7E-2       4.7149E-02  2.00E-02  1.4858E-04  7.4289E-03
22 W(LIQUID,A)=0.187     0.1867      2.00E-02 -2.7893E-04 -1.3946E-02
22 W(FCC,A)=5.9E-2       5.9048E-02  2.00E-02  4.8254E-05  2.4127E-03
23 W(LIQUID,A)=0.245     0.2449      2.00E-02 -1.4555E-04 -7.2775E-03
23 W(BCC#1,A)=8.5E-2     8.4968E-02  2.00E-02 -3.1610E-05 -1.5805E-03
```

```
PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03454598E+04	2.03239810E+04	2.03239810E+04	1.02423466E-01
V2	-2.93769553E+01	-2.93471952E+01	-2.93471952E+01	9.37762247E-02
V11	-2.17266456E+04	-2.17785061E+04	-2.17785061E+04	2.00749380E-01
V12	1.52556729E+01	1.53148537E+01	1.53148537E+01	3.29240608E-01
V15	2.41427097E+04	2.41304970E+04	2.41304970E+04	1.34940930E-01
V16	-8.27427337E+00	-8.25418969E+00	-8.25418969E+00	4.84822531E-01
V17	3.07943197E+03	3.08367945E+03	3.08367945E+03	2.31440510E-01
V19	2.21987951E+04	2.21788112E+04	2.21788112E+04	5.66912120E-01
V20	-7.11454006E+00	-7.07623325E+00	-7.07623325E+00	1.53559103E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.25795062E-02 TO 5.98271438E-03
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99135719E-04

PARROT: s-o-v 11-12

PARROT: ed

ED_EXP: read 1

ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	2	1.	1192.7		LIQUID A2B BCC
2	AINV	2	1.	1341.0		LIQUID A2B
3	AINV	2	1.	1049.1		LIQUID A2B BCC
4	AINV	2	1.	1203.1		LIQUID BCC FCC
5	AINV	2	1.	726.0		A2B BCC BCC#2
6	AINV	2	1.	726.0		BCC BCC#2
10	ALF	2	1.	1594.0		LIQUID FCC
11	ALF	2	1.	1548.0		LIQUID FCC
12	ALF	2	1.	1499.0		LIQUID FCC
13	ALF	2	1.	1438.0		LIQUID FCC
20	ATIE	2	1.	1413.0		LIQUID FCC
21	ATIE	2	1.	1337.0		LIQUID FCC
22	ATIE	2	1.	1213.0		LIQUID FCC
23	ATIE	2	1.	1100.0		LIQUID BCC
100	AA	< unused >		1573.0		LIQUID
101	AA	< unused >		1573.0		LIQUID
102	AA	< unused >		1573.0		LIQUID
103	AA	< unused >		1573.0		LIQUID
104	AA	< unused >		1573.0		LIQUID
105	AA	< unused >		1573.0		LIQUID
106	AA	< unused >		1573.0		LIQUID
107	AA	< unused >		1573.0		LIQUID
108	AA	< unused >		1573.0		LIQUID
110	AH	< unused >		1773.0		LIQUID
111	AH	< unused >		1773.0		LIQUID
112	AH	< unused >		1773.0		LIQUID
113	AH	< unused >		1773.0		LIQUID
114	AH	< unused >		1773.0		LIQUID
115	AH	< unused >		1773.0		LIQUID
116	AH	< unused >		1773.0		LIQUID
117	AH	< unused >		1773.0		LIQUID
118	AH	< unused >		1773.0		LIQUID

ED_EXP: s-we 1 100-118

ED_EXP: s-e 1

Equilibrium number 1 , label AINV

ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	2	1.	1192.7		LIQUID A2B BCC
2	AINV	2	1.	1341.0		LIQUID A2B
3	AINV	2	1.	1049.1		LIQUID A2B BCC
4	AINV	2	1.	1203.1		LIQUID BCC FCC
5	AINV	2	1.	726.0		A2B BCC BCC#2
6	AINV	2	1.	726.0		BCC BCC#2
10	ALF	2	1.	1594.0		LIQUID FCC
11	ALF	2	1.	1548.0		LIQUID FCC
12	ALF	2	1.	1499.0		LIQUID FCC
13	ALF	2	1.	1438.0		LIQUID FCC
20	ATIE	2	1.	1413.0		LIQUID FCC
21	ATIE	2	1.	1337.0		LIQUID FCC
22	ATIE	2	1.	1213.0		LIQUID FCC
23	ATIE	2	1.	1100.0		LIQUID BCC
100	AA	2	1.	1573.0		LIQUID
101	AA	2	1.	1573.0		LIQUID
102	AA	2	1.	1573.0		LIQUID
103	AA	2	1.	1573.0		LIQUID
104	AA	2	1.	1573.0		LIQUID
105	AA	2	1.	1573.0		LIQUID
106	AA	2	1.	1573.0		LIQUID
107	AA	2	1.	1573.0		LIQUID
108	AA	2	1.	1573.0		LIQUID
110	AH	2	1.	1773.0		LIQUID
111	AH	2	1.	1773.0		LIQUID
112	AH	2	1.	1773.0		LIQUID
113	AH	2	1.	1773.0		LIQUID
114	AH	2	1.	1773.0		LIQUID
115	AH	2	1.	1773.0		LIQUID
116	AH	2	1.	1773.0		LIQUID
117	AH	2	1.	1773.0		LIQUID
118	AH	2	1.	1773.0		LIQUID

```
ED_EXP: save
ED_EXP: ba
PARROT: opt 30
Use      47 experiments, maximum is      2000
Use    1082 real workspace, maximum is    50000
The following output is provided by subroutine VA05A

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      8.33565700E-02
1  1.0011E+00      2  1.0010E+00      3  1.0000E+00      4  1.0000E+00      5  1.0005E+00
6  1.0024E+00      7  9.9862E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      8.41932586E-02
1  1.0012E+00      2  1.0010E+00      3  1.0000E+00      4  1.0000E+00      5  1.0005E+00
6  1.0024E+00      7  9.9862E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      8.60712416E-02
1  1.0011E+00      2  1.0011E+00      3  1.0000E+00      4  1.0000E+00      5  1.0005E+00
6  1.0024E+00      7  9.9862E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      8.25031405E-02
1  1.0011E+00      2  1.0010E+00      3  1.0001E+00      4  1.0000E+00      5  1.0005E+00
6  1.0024E+00      7  9.9862E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      8.29651624E-02
1  1.0011E+00      2  1.0010E+00      3  1.0001E+00      4  1.0001E+00      5  1.0005E+00
6  1.0024E+00      7  9.9862E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      8.28355238E-02
1  1.0011E+00      2  1.0010E+00      3  1.0001E+00      4  1.0000E+00      5  1.0006E+00
6  1.0024E+00      7  9.9862E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      8.24865273E-02
1  1.0011E+00      2  1.0010E+00      3  1.0001E+00      4  1.0000E+00      5  1.0005E+00
6  1.0025E+00      7  9.9862E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      8.24928250E-02
1  1.0011E+00      2  1.0010E+00      3  1.0001E+00      4  1.0000E+00      5  1.0005E+00
6  1.0025E+00      7  9.9872E-01      8  1.0009E+00      9  1.0054E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      8.26740949E-02
1  1.0011E+00      2  1.0010E+00      3  1.0001E+00      4  1.0000E+00      5  1.0005E+00
6  1.0025E+00      7  9.9862E-01      8  1.0010E+00      9  1.0054E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      8.24679525E-02
1  1.0011E+00      2  1.0010E+00      3  1.0001E+00      4  1.0000E+00      5  1.0005E+00
6  1.0025E+00      7  9.9862E-01      8  1.0009E+00      9  1.0055E+00

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      8.18220368E-02
1  1.0010E+00      2  1.0011E+00      3  1.0001E+00      4  9.9998E-01      5  1.0005E+00
6  1.0026E+00      7  9.9864E-01      8  1.0009E+00      9  1.0055E+00

      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      8.12655996E-02
1  1.0011E+00      2  1.0011E+00      3  1.0002E+00      4  9.9994E-01      5  1.0005E+00
6  1.0027E+00      7  9.9865E-01      8  1.0008E+00      9  1.0054E+00

      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      8.05804376E-02
1  1.0010E+00      2  1.0011E+00      3  1.0002E+00      4  9.9991E-01      5  1.0005E+00
6  1.0028E+00      7  9.9868E-01      8  1.0008E+00      9  1.0053E+00

      AT THE     13 TH ITERATION WE HAVE THE SUM OF SQUARES      7.96875956E-02
1  1.0011E+00      2  1.0011E+00      3  1.0002E+00      4  9.9982E-01      5  1.0006E+00
6  1.0031E+00      7  9.9874E-01      8  1.0006E+00      9  1.0051E+00

      AT THE     14 TH ITERATION WE HAVE THE SUM OF SQUARES      7.83106824E-02
1  1.0011E+00      2  1.0012E+00      3  1.0002E+00      4  9.9969E-01      5  1.0007E+00
6  1.0037E+00      7  9.9886E-01      8  1.0003E+00      9  1.0048E+00

      AT THE     15 TH ITERATION WE HAVE THE SUM OF SQUARES      7.61191432E-02
1  1.0012E+00      2  1.0014E+00      3  1.0002E+00      4  9.9942E-01      5  1.0009E+00
6  1.0049E+00      7  9.9911E-01      8  9.9967E-01      9  1.0040E+00

      AT THE     16 TH ITERATION WE HAVE THE SUM OF SQUARES      7.26639907E-02
1  1.0014E+00      2  1.0017E+00      3  1.0003E+00      4  9.9891E-01      5  1.0014E+00
6  1.0073E+00      7  9.9962E-01      8  9.9843E-01      9  1.0026E+00

      AT THE     17 TH ITERATION WE HAVE THE SUM OF SQUARES      6.84352095E-02
1  1.0019E+00      2  1.0023E+00      3  1.0003E+00      4  9.9788E-01      5  1.0023E+00
6  1.0121E+00      7  1.0006E+00      8  9.9596E-01      9  9.9973E-01

      AT THE     18 TH ITERATION WE HAVE THE SUM OF SQUARES      6.73854818E-02
1  1.0022E+00      2  1.0028E+00      3  1.0003E+00      4  9.9703E-01      5  1.0030E+00
6  1.0160E+00      7  1.0014E+00      8  9.9410E-01      9  9.9781E-01

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      18 iterations
1  1.0022E+00      2  1.0028E+00      3  1.0003E+00      4  9.9703E-01      5  1.0030E+00
6  1.0160E+00      7  1.0014E+00      8  9.9410E-01      9  9.9781E-01

1 -5.7840E-02      2 -9.3600E-03      3  1.4182E-02      4  2.0795E-02      5 -2.5749E-02
6 -5.2102E-02      7  1.9270E-02      8  2.6821E-02      9  1.3107E-02     10  2.7155E-02
11  8.7712E-03     12  1.3244E-02     13 -4.8660E-02     14  2.1787E-02     15  4.7259E-03
16  2.8667E-02     17  2.1548E-02     18 -2.2040E-02     19 -8.2405E-03     20 -4.9758E-03
21 -1.5646E-02     22 -1.0901E-02     23  1.5212E-02     24  2.4270E-02     25  1.4695E-02
26 -1.4884E-02     27  2.0284E-02     28 -1.2749E-02     29  1.5398E-02     30 -9.5907E-03
31 -1.6831E-02     32  2.7436E-02     33  8.7019E-02     34  1.2434E-01     35  1.0168E-01
36 -1.7318E-02     37  7.0579E-02     38 -1.9476E-02     39  1.6076E-02     40  4.5469E-02
41  4.8178E-02     42  4.6204E-02     43  4.1546E-02     44  3.4204E-02     45  2.2178E-02
46  7.4692E-03     47 -1.1924E-02

      THE SUM OF SQUARES IS      6.73854818E-02
PARROT: l-r C SCREEN

=====
OUTPUT FROM  P A R R O T.  DATE 2025. 5.12      9:31:27

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 19

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
```

```
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03690179E+04	2.03239810E+04	2.03239810E+04	2.99183016E-02
V2	-2.94289024E+01	-2.93471952E+01	-2.93471952E+01	2.27346718E-02
V11	-2.17329087E+04	-2.17266456E+04	-2.17266456E+04	3.48585314E-02
V12	1.52104360E+01	1.52556729E+01	1.52556729E+01	5.50983526E-02
V15	2.42024575E+04	2.41304970E+04	2.41304970E+04	8.32034883E-02
V16	-8.38635739E+00	-8.25418969E+00	-8.25418969E+00	2.56517959E-01
V17	3.08808414E+03	3.08367945E+03	3.08367945E+03	2.30211247E-01
V19	2.20479620E+04	2.21788112E+04	2.21788112E+04	4.85933520E-01
V20	-7.06072568E+00	-7.07623325E+00	-7.07623325E+00	1.21890045E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.33565700E-02 TO 6.73854818E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77330215E-03

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1192.	10.	-0.5784	-5.7840E-02
1 W(LIQUID,B)=0.408	0.4078	2.00E-02	-1.8720E-04	-9.3600E-03
1 W(BCC#1,B)=0.13	0.1303	2.00E-02	2.8363E-04	1.4182E-02
2 T=1341	1341.	10.	0.2079	2.0795E-02
2 HTR=3727	3714.	5.00E+02	-12.87	-2.5749E-02
3 T=1049	1048.	10.	-0.5210	-5.2102E-02
3 W(LIQUID,A)=0.27	0.2704	2.00E-02	3.8540E-04	1.9270E-02
3 W(BCC#1,A)=9.3E-2	9.3536E-02	2.00E-02	5.3643E-04	2.6821E-02
4 T=1203	1203.	10.	0.1311	1.3107E-02
4 W(LIQUID,A)=0.19	0.1905	2.00E-02	5.4310E-04	2.7155E-02
4 W(BCC#1,A)=6.9E-2	6.9175E-02	2.00E-02	1.7542E-04	8.7712E-03
4 W(FCC,A)=6E-2	6.0265E-02	2.00E-02	2.6489E-04	1.3244E-02
5 T=726	725.5	10.	-0.4866	-4.8660E-02
5 X(BCC#1,B)=3.7E-2	3.7436E-02	2.00E-02	4.3575E-04	2.1787E-02
5 X(BCC#2,A)=0.114	0.1141	2.00E-02	9.4518E-05	4.7259E-03
6 X(BCC#1,B)=3.7E-2	3.7573E-02	2.00E-02	5.7335E-04	2.8667E-02
6 X(BCC#2,A)=0.114	0.1144	2.00E-02	4.3095E-04	2.1548E-02
10 W(LIQUID,A)=2E-2	1.9559E-02	2.00E-02	-4.4080E-04	-2.2040E-02
11 W(LIQUID,A)=4.2E-2	4.1835E-02	2.00E-02	-1.6481E-04	-8.2405E-03
12 W(LIQUID,A)=6.5E-2	6.4900E-02	2.00E-02	-9.9516E-05	-4.9758E-03
13 W(LIQUID,A)=9.3E-2	9.2687E-02	2.00E-02	-3.1292E-04	-1.5646E-02
20 W(LIQUID,A)=0.104	0.1038	2.00E-02	-2.1802E-04	-1.0901E-02
20 W(FCC,A)=3.8E-2	3.8304E-02	2.00E-02	3.0425E-04	1.5212E-02
21 W(LIQUID,A)=0.136	0.1365	2.00E-02	4.8540E-04	2.4270E-02
21 W(FCC,A)=4.7E-2	4.7294E-02	2.00E-02	2.9390E-04	1.4695E-02
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.9768E-04	-1.4884E-02
22 W(FCC,A)=5.9E-2	5.9406E-02	2.00E-02	4.0567E-04	2.0284E-02
23 W(LIQUID,A)=0.245	0.2447	2.00E-02	-2.5499E-04	-1.2749E-02
23 W(BCC#1,A)=8.5E-2	8.5308E-02	2.00E-02	3.0796E-04	1.5398E-02
100 ACR(B)=0.94	0.9397	2.85E-02	-2.7298E-04	-9.5907E-03
101 ACR(B)=0.84	0.8395	2.82E-02	-4.7442E-04	-1.6831E-02
102 ACR(B)=0.74	0.7408	2.81E-02	7.6972E-04	2.7436E-02
103 ACR(B)=0.64	0.6424	2.81E-02	2.4423E-03	8.7019E-02
104 ACR(B)=0.54	0.5435	2.82E-02	3.5095E-03	0.1243
105 ACR(B)=0.44	0.4429	2.85E-02	2.9022E-03	0.1017
106 ACR(B)=0.34	0.3395	2.90E-02	-5.0270E-04	-1.7318E-02
107 ACR(B)=0.23	0.2321	2.97E-02	2.0966E-03	7.0579E-02
108 ACR(B)=0.12	0.1194	3.06E-02	-5.9597E-04	-1.9476E-02
110 HMR(LIQUID)=-1964	-1956.	5.00E+02	8.038	1.6076E-02
111 HMR(LIQUID)=-3500	-3477.	5.00E+02	22.73	4.5469E-02
112 HMR(LIQUID)=-4588	-4564.	5.00E+02	24.09	4.8178E-02
113 HMR(LIQUID)=-5239	-5216.	5.00E+02	23.10	4.6204E-02
114 HMR(LIQUID)=-5454	-5433.	5.00E+02	20.77	4.1546E-02
115 HMR(LIQUID)=-5233	-5216.	5.00E+02	17.10	3.4204E-02
116 HMR(LIQUID)=-4575	-4564.	5.00E+02	11.09	2.2178E-02
117 HMR(LIQUID)=-3481	-3477.	5.00E+02	3.735	7.4692E-03
118 HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.962	-1.1924E-02

PARROT:

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Calculate the phase diagram one last time.

PARROT: mac tcex36cpd

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

POLY:

POLY: @@ In PARROT, the global minimization is turned off automatically.

POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY: @@ message will be given.

POLY:

POLY: advanced-option global yes,,

Settings for global minimization:

*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY:

POLY: def-com,,,

POLY: s-a-v 1 w(b) 0 1,,,

The condition W(B)=.1234 created

POLY: s-a-v 2 t 300 1700,,,

The condition T=942.2 created

POLY: s-c t=500

POLY: l-c

```

W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated      628 grid points in      0.003 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.003 s, total time      0.006 s
POLY: save tcex36 y

```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..      2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
Calculated.      14 equilibria

Phase region boundary 3 at: 6.819E-01 7.255E+02
  ** A2B
  BCC#1
  ** BCC#2

Phase region boundary 4 at: 3.626E-01 7.255E+02
  ** A2B
  BCC#1
Calculated.      15 equilibria

Phase region boundary 5 at: 3.771E-01 1.192E+03
  ** LIQUID
  ** A2B
  BCC#1

Phase region boundary 6 at: 2.828E-01 1.192E+03
  ** LIQUID
  BCC#1
Calculated      28 equilibria

Phase region boundary 7 at: 4.863E-01 1.192E+03
  ** LIQUID
  A2B
Calculated.      28 equilibria

Phase region boundary 8 at: 6.500E-01 1.048E+03
  ** LIQUID
  A2B
  ** BCC#1

Phase region boundary 9 at: 7.639E-01 1.048E+03
  A2B
  ** BCC#1
Calculated.      11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.273E-01 1.048E+03
  LIQUID
  ** BCC#1
Calculated.      8 equilibria

```

Phase region boundary 11 at: 8.748E-01 1.203E+03
 LIQUID
 ** BCC#1
 ** FCC

Phase region boundary 12 at: 8.800E-01 1.203E+03
 LIQUID
 ** FCC
 Calculated 33 equilibria

Phase region boundary 13 at: 9.353E-01 1.203E+03
 BCC#1
 ** FCC
 Calculated 20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.647E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 26 at: 3.647E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.647E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 14 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 7.910E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 29 at: 7.910E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 7.910E-01 7.700E+02


```

** A2B
  BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:  2.448E-01  1.230E+03
** LIQUID
  BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  2.448E-01  1.230E+03
** LIQUID
  BCC#1
Calculated          26 equilibria

Phase region boundary 33 at:  8.858E-01  1.230E+03
** LIQUID
  FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  8.858E-01  1.230E+03
** LIQUID
  FCC
Calculated          29 equilibria

Phase region boundary 35 at:  6.415E-03  1.397E+03
  LIQUID
** BCC#1
Calculated          13 equilibria

Phase region boundary 36 at:  6.415E-03  1.397E+03
  LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  2.299E-01  1.244E+03
  LIQUID
** BCC#1
Calculated          20 equilibria

Phase region boundary 38 at:  2.299E-01  1.244E+03
  LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:  6.122E-01  1.240E+03
  LIQUID
** A2B
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:  6.122E-01  1.240E+03
  LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

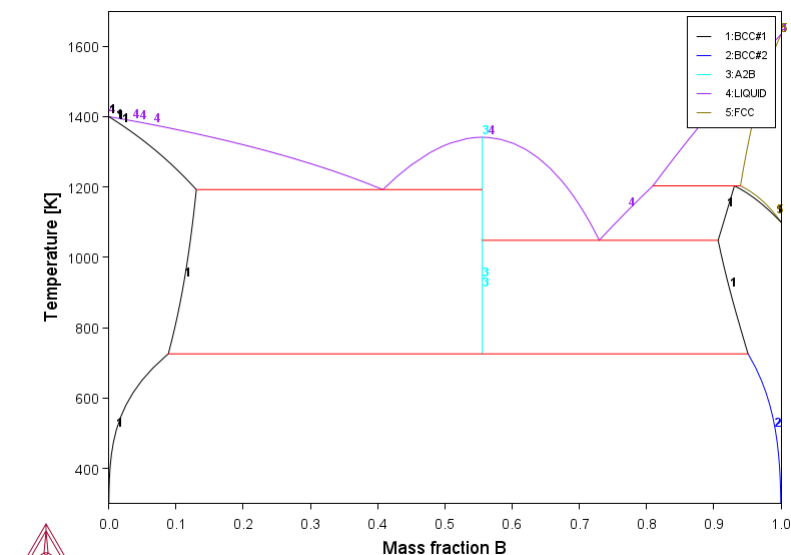
Phase region boundary 41 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated          8 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping          1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
POST: plot

```

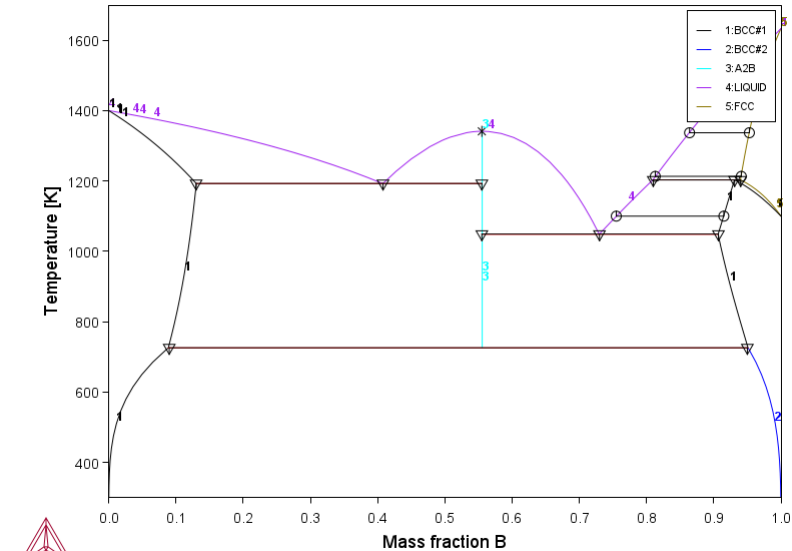


```

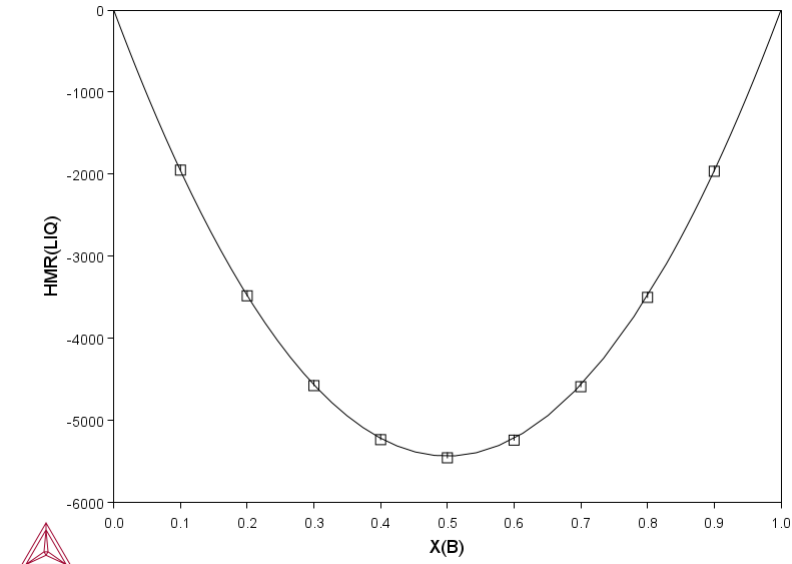
POST:
POST: set-inter

```

POST:Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
POST: plot

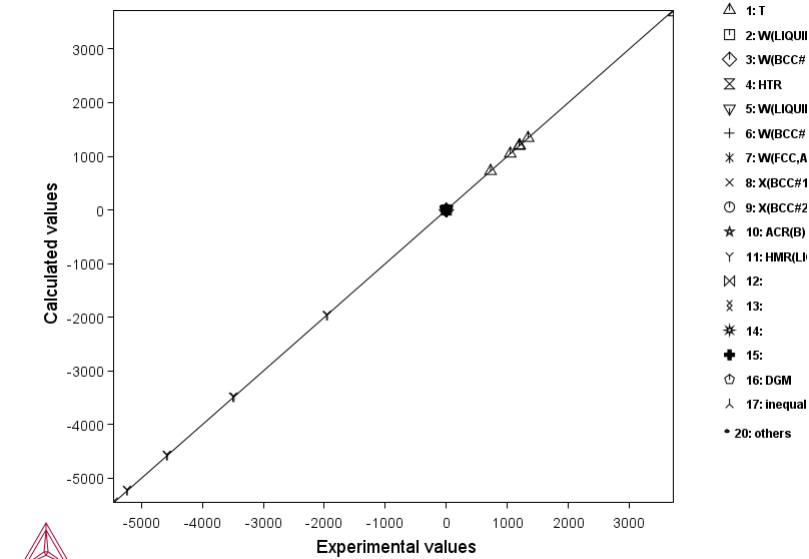


POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
POLY: read,,,
POLY:
POLY:
POLY: s-a-v 2 none
POLY: s-c t=1773
POLY: c-e
Using global minimization procedure
Calculated 628 grid points in 0.009 s
Found the set of lowest grid points in 0.000 s
Calculated POLY solution 0.004 s, total time 0.013 s
POLY: sh hmr
HMR=13116.471
POLY: l-st c
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
A ENTERED SER
B ENTERED SER
POLY: s-r-s a liq * 1e5
POLY: s-r-s b liq * 1e5
POLY: save tcex36h y
POLY: step normal
No initial equilibrium, using default
Step will start from axis value 0.123400
...OK
Phase Region from 0.123400 for:
LIQUID
Global test at 3.23400E-01 OK
Global test at 5.73400E-01 OK
Global test at 8.23400E-01 OK
Global test at 9.53400E-01 OK
Global test at 1.00000E+00 OK
Terminating at 1.00000
Calculated 51 equilibria
Phase Region from 0.123400 for:
LIQUID
Global test at 8.34000E-02 OK
Global test at 3.34000E-02 OK
Terminating at 0.25000E-11
Calculated 28 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36h.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x x(b)
POST: s-d-a y hmr(liq)
POST: a-e-d y exp36 0; 2
POST: plot

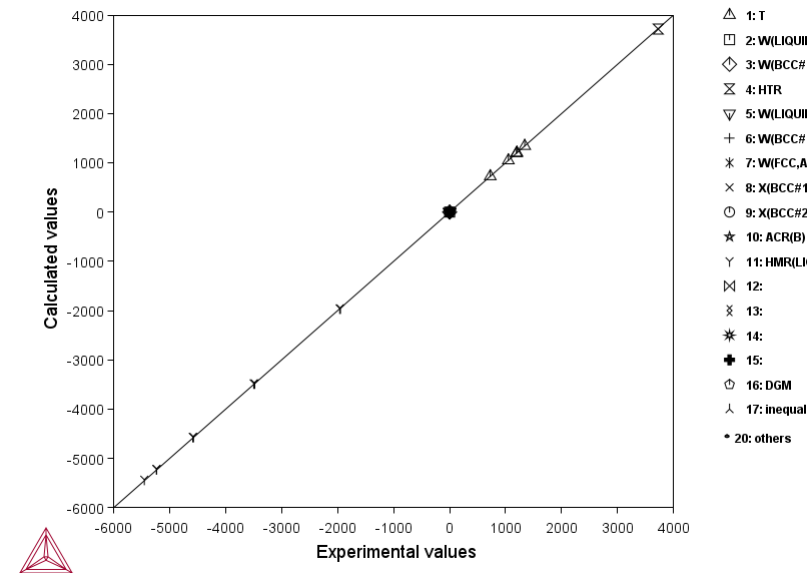


POST: Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
POLY: ba

PARROT VERSION 5.3
Global minimization used as test only
PARROT: l-result gra pexp36 1,



POST: s-s-s y n -6000 4000
POST: s-s-s x n -6000 4000
POST: plot




POST: b
PARROT: set-inter
PARROT: set-inter
PARROT:

tcex36a-tcex36b

PARROT>About

NO SUCH COMMAND, USE HELP

PARROT:PARROT:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36b.TCM.test"

PARROT: s-s-f tcex36

PARROT: @@ List parameters to be optimized, all zero initially

PARROT: l-a-v

OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03690179E+04	2.03239810E+04	2.03239810E+04	2.99183016E-02
V2	-2.94289024E+01	-2.93471952E+01	-2.93471952E+01	2.27346718E-02
V11	-2.17329087E+04	-2.17266456E+04	-2.17266456E+04	3.48585314E-02
V12	1.52104360E+01	1.52556729E+01	1.52556729E+01	5.50983526E-02
V15	2.42024575E+04	2.41304970E+04	2.41304970E+04	8.32034883E-02
V16	-8.38635739E+00	-8.25418969E+00	-8.25418969E+00	2.56517959E-01
V17	3.08808414E+03	3.08367945E+03	3.08367945E+03	2.30211247E-01
V19	2.20479620E+04	2.21788112E+04	2.21788112E+04	4.85933520E-01
V20	-7.06072568E+00	-7.07623325E+00	-7.07623325E+00	1.21890045E+00

NUMBER OF OPTIMIZING VARIABLES : 9

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 8.33565700E-02 TO 6.73854818E-02

DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77330215E-03

PARROT: @@ Set alt mode to start

PARROT: s-alt Y

PARROT: @@ Check if all equilibria can be calculated

PARROT: ed

ED_EXP: read 1

ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	*alt*	1.0	1193.0		LIQUID A2B BCC
2	AINV	*alt*	1.0	1341.0		LIQUID A2B
3	AINV	*alt*	1.0	1049.0		LIQUID A2B BCC
4	AINV	*alt*	1.0	1203.0		LIQUID BCC FCC
5	AINV	*alt*	1.0	726.0		A2B BCC BCC#2
6	AINV	*alt*	1.0	726.0		BCC BCC#2
Failed using alternate for FCC#1						
10	ALF	*alt*	1.0	1594.0		LIQUID FCC
Failed using alternate for FCC#1						
11	ALF	*alt*	1.0	1548.0		LIQUID FCC
Failed using alternate for FCC#1						
12	ALF	*alt*	1.0	1499.0		LIQUID FCC
Failed using alternate for FCC#1						
13	ALF	*alt*	1.0	1438.0		LIQUID FCC
20	ATIE	*alt*	1.0	1413.0		LIQUID FCC
21	ATIE	*alt*	1.0	1337.0		LIQUID FCC
22	ATIE	*alt*	1.0	1213.0		LIQUID FCC
23	ATIE	*alt*	1.0	1100.0		LIQUID BCC
100	AA	2	1.	1573.0		LIQUID
101	AA	2	1.	1573.0		LIQUID
102	AA	2	1.	1573.0		LIQUID
103	AA	2	1.	1573.0		LIQUID
104	AA	2	1.	1573.0		LIQUID
105	AA	2	1.	1573.0		LIQUID
106	AA	2	1.	1573.0		LIQUID
107	AA	2	1.	1573.0		LIQUID
108	AA	2	1.	1573.0		LIQUID
110	AH	2	1.	1773.0		LIQUID
111	AH	2	1.	1773.0		LIQUID
112	AH	2	1.	1773.0		LIQUID
113	AH	2	1.	1773.0		LIQUID
114	AH	2	1.	1773.0		LIQUID
115	AH	2	1.	1773.0		LIQUID
116	AH	2	1.	1773.0		LIQUID
117	AH	2	1.	1773.0		LIQUID
118	AH	2	1.	1773.0		LIQUID

Number of alternate equilibria 14

ED_EXP: @@ Equilibra with label ALF cannot use alt mode

ED_EXP: s-we 0 alf

Changed weight on 4 equilibria.

ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
118	AH	2	1.	1773.0		LIQUID

ED_EXP: save

ED_EXP: @@ Save changes of weights before leaving the editor

ED_EXP: ba

PARROT: @@ Optimize zero times as a check

PARROT: opt 0

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:34:16

*** SUCCESSFUL OPTIMIZATION. ***

NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N

MINIMUM SAVE ON FILE: Y

ERROR FOR INEQUALITIES = 1.00000000E+00

RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04

ARGUMENTS FOR SUBROUTINE VA05AD (HSL)

MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04

ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03690179E+04	2.03239810E+04	2.03239810E+04	2.99183016E-02
V2	-2.94289024E+01	-2.93471952E+01	-2.93471952E+01	2.27346718E-02
V11	-2.17329087E+04	-2.17266456E+04	-2.17266456E+04	3.48585314E-02
V12	1.52104360E+01	1.52556729E+01	1.52556729E+01	5.50983526E-02
V15	2.42024575E+04	2.41304970E+04	2.41304970E+04	8.32034883E-02
V16	-8.38635739E+00	-8.25418969E+00	-8.25418969E+00	2.56517959E-01
V17	3.08808414E+03	3.08367945E+03	3.08367945E+03	2.30211247E-01
V19	2.20479620E+04	2.21788112E+04	2.21788112E+04	4.85933520E-01
V20	-7.06072568E+00	-7.07623325E+00	-7.07623325E+00	1.21890045E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.33565700E-02 TO 8.89363143E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.34042932E-03

Number of alternate equilibria 10

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 Alternate equilibrium calc				0.00
2 Alternate equilibrium calc				0.19
2 HTR=3727	3714.	5.00E+02	-12.87	-2.5749E-02
3 Alternate equilibrium calc				0.00
4 Alternate equilibrium calc				0.00
5 Alternate equilibrium calc				0.01
6 Alternate equilibrium calc				0.01
20 Alternate equilibrium calc				0.01
21 Alternate equilibrium calc				0.00
22 Alternate equilibrium calc				0.01
23 Alternate equilibrium calc				0.00
100 ACR(B)=0.94	0.9397	2.85E-02	-2.7298E-04	-9.5907E-03
101 ACR(B)=0.84	0.8395	2.82E-02	-4.7442E-04	-1.6831E-02
102 ACR(B)=0.74	0.7408	2.81E-02	7.6972E-04	2.7436E-02
103 ACR(B)=0.64	0.6424	2.81E-02	2.4423E-03	8.7019E-02
104 ACR(B)=0.54	0.5435	2.82E-02	3.5095E-03	0.1243
105 ACR(B)=0.44	0.4429	2.85E-02	2.9022E-03	0.1017
106 ACR(B)=0.34	0.3395	2.90E-02	-5.0270E-04	-1.7318E-02
107 ACR(B)=0.23	0.2321	2.97E-02	2.0966E-03	7.0579E-02
108 ACR(B)=0.12	0.1194	3.06E-02	-5.9597E-04	-1.9476E-02
110 HMR(LIQUID)=-1964	-1956.	5.00E+02	8.038	1.6076E-02
111 HMR(LIQUID)=-3500	-3477.	5.00E+02	22.73	4.5469E-02
112 HMR(LIQUID)=-4588	-4564.	5.00E+02	24.09	4.8178E-02
113 HMR(LIQUID)=-5239	-5216.	5.00E+02	23.10	4.6204E-02
114 HMR(LIQUID)=-5454	-5433.	5.00E+02	20.77	4.1546E-02
115 HMR(LIQUID)=-5233	-5216.	5.00E+02	17.10	3.4204E-02
116 HMR(LIQUID)=-4575	-4564.	5.00E+02	11.09	2.2178E-02
117 HMR(LIQUID)=-3481	-3477.	5.00E+02	3.735	7.4692E-03
118 HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.962	-1.1924E-02

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Note only one error from alternate calculations.

PARROT: @@ This error represents the difference in chemical

PARROT: @@ potentials of the phases.

PARROT: @@ Experiments with just one phase is calculated as normal.

PARROT: @@ Next command supresses the listing of parameters.

PARROT: s-o-l 1 Y Y N n N

PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:34:16

*** SUCCESSFUL OPTIMIZATION. ***

NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03690179E+04	2.03239810E+04	2.03239810E+04	2.99183016E-02
V2	-2.94289024E+01	-2.93471952E+01	-2.93471952E+01	2.27346718E-02
V11	-2.17329087E+04	-2.17266456E+04	-2.17266456E+04	3.48585314E-02
V12	1.52104360E+01	1.52556729E+01	1.52556729E+01	5.50983526E-02
V15	2.42024575E+04	2.41304970E+04	2.41304970E+04	8.32034883E-02
V16	-8.38635739E+00	-8.25418969E+00	-8.25418969E+00	2.56517959E-01
V17	3.08808414E+03	3.08367945E+03	3.08367945E+03	2.30211247E-01
V19	2.20479620E+04	2.21788112E+04	2.21788112E+04	4.85933520E-01
V20	-7.06072568E+00	-7.07623325E+00	-7.07623325E+00	1.21890045E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.33565700E-02 TO 8.89363143E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.34042932E-03

Number of alternate equilibria 10

SYMBOL	STATUS	VALUE/FUNCTION	
FUNCTION R	298.15	8.314510000000000	; 6000 N REF0 !
2 RTLN P	20000000	+R*T*LN(1E-05*P)	
FUNCTION V1	298.15	20369.0178746185	; 6000 N REF0 !
FUNCTION V2	298.15	-29.4289023977347	; 6000 N REF0 !
FUNCTION V11	298.15	-21732.9087387769	; 6000 N REF0 !
FUNCTION V12	298.15	15.2104360334441	; 6000 N REF0 !
FUNCTION V15	298.15	24202.4574535693	; 6000 N REF0 !
FUNCTION V16	298.15	-8.38635738693246	; 6000 N REF0 !
FUNCTION V17	298.15	3088.08414285253	; 6000 N REF0 !
FUNCTION V19	298.15	22047.9619850235	; 6000 N REF0 !
FUNCTION V20	298.15	-7.06072567830689	; 6000 N REF0 !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 Alternate equilibrium calc				0.00
2 Alternate equilibrium calc				0.19
2 HTR=3727	3714.	5.00E+02	-12.87	-2.5749E-02
3 Alternate equilibrium calc				0.00
4 Alternate equilibrium calc				0.00
5 Alternate equilibrium calc				0.01
6 Alternate equilibrium calc				0.01
20 Alternate equilibrium calc				0.01
21 Alternate equilibrium calc				0.00
22 Alternate equilibrium calc				0.01
23 Alternate equilibrium calc				0.00
100 ACR(B)=0.94	0.9397	2.85E-02	-2.7298E-04	-9.5907E-03
101 ACR(B)=0.84	0.8395	2.82E-02	-4.7442E-04	-1.6831E-02
102 ACR(B)=0.74	0.7408	2.81E-02	7.6972E-04	2.7436E-02
103 ACR(B)=0.64	0.6424	2.81E-02	2.4423E-03	8.7019E-02
104 ACR(B)=0.54	0.5435	2.82E-02	3.5095E-03	0.1243
105 ACR(B)=0.44	0.4429	2.85E-02	2.9022E-03	0.1017
106 ACR(B)=0.34	0.3395	2.90E-02	-5.0270E-04	-1.7318E-02
107 ACR(B)=0.23	0.2321	2.97E-02	2.0966E-03	7.0579E-02
108 ACR(B)=0.12	0.1194	3.06E-02	-5.9597E-04	-1.9476E-02
110 HMR(LIQUID)=-1964	-1956.	5.00E+02	8.038	1.6076E-02
111 HMR(LIQUID)=-3500	-3477.	5.00E+02	22.73	4.5469E-02
112 HMR(LIQUID)=-4588	-4564.	5.00E+02	24.09	4.8178E-02
113 HMR(LIQUID)=-5239	-5216.	5.00E+02	23.10	4.6204E-02
114 HMR(LIQUID)=-5454	-5433.	5.00E+02	20.77	4.1546E-02
115 HMR(LIQUID)=-5233	-5216.	5.00E+02	17.10	3.4204E-02
116 HMR(LIQUID)=-4575	-4564.	5.00E+02	11.09	2.2178E-02
117 HMR(LIQUID)=-3481	-3477.	5.00E+02	3.735	7.4692E-03
118 HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.962	-1.1924E-02

PARROT:

PARROT: @@ Now optimize

PARROT: opt 30

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 8.89363143E-02
1 1.0022E+00 2 1.0028E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9410E-01 9 9.9781E-01

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 8.90038376E-02
1 1.0023E+00 2 1.0028E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9410E-01 9 9.9781E-01

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 8.89455540E-02
1 1.0022E+00 2 1.0029E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9410E-01 9 9.9781E-01

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 8.79612366E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9410E-01 9 9.9781E-01

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 8.85897164E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9713E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9410E-01 9 9.9781E-01

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79383628E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0160E+00 7 1.0014E+00 8 9.9410E-01 9 9.9781E-01

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79442916E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0161E+00 7 1.0014E+00 8 9.9410E-01 9 9.9781E-01

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79365891E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0160E+00 7 1.0015E+00 8 9.9410E-01 9 9.9781E-01

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79319351E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0160E+00 7 1.0015E+00 8 9.9420E-01 9 9.9781E-01

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79338846E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00

```

6 1.0160E+00 7 1.0015E+00 8 9.9420E-01 9 9.9791E-01

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.30390311E-02
1 1.0020E+00 2 1.0027E+00 3 1.0040E+00 4 9.9469E-01 5 1.0032E+00
6 1.0160E+00 7 1.0015E+00 8 9.9422E-01 9 9.9780E-01

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 5.99860835E-02
1 9.9913E-01 2 1.0021E+00 3 1.0031E+00 4 9.9346E-01 5 1.0040E+00
6 1.0181E+00 7 1.0024E+00 8 9.9352E-01 9 9.9654E-01

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 5.92638875E-02
1 9.9864E-01 2 1.0002E+00 3 1.0037E+00 4 9.9347E-01 5 1.0062E+00
6 1.0254E+00 7 1.0053E+00 8 9.9231E-01 9 9.9464E-01

      AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88513918E-02
1 9.9781E-01 2 9.9672E-01 3 1.0039E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8927E-01 9 9.8924E-01

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 13 iterations
1 9.9781E-01 2 9.9672E-01 3 1.0039E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8927E-01 9 9.8924E-01

1 7.4325E-03 2 7.4325E-03 3 1.5765E-03 4 2.3878E-03 5 1.3275E-01
6 -1.4001E-01 7 -7.2766E-04 8 8.1724E-03 9 8.1724E-03 10 -3.4800E-04
11 3.2690E-03 12 1.6870E-03 13 2.3658E-04 14 2.8649E-03 15 6.0691E-04
16 1.5561E-03 17 1.5561E-03 18 1.4159E-04 19 1.0024E-03 20 1.4159E-04
21 1.0024E-03 22 -2.0800E-03 23 1.7706E-03 24 3.3746E-03 25 3.3485E-04
26 -2.7391E-03 27 3.2562E-03 28 -1.7542E-03 29 3.8068E-03 30 -1.3488E-02
31 -3.0889E-02 32 -7.0116E-04 33 4.3579E-02 34 6.7271E-02 35 3.5606E-02
36 -8.5035E-02 37 1.1584E-02 38 -5.6982E-02 39 2.0218E-03 40 2.0483E-02
41 1.5384E-02 42 8.7249E-03 43 2.5051E-03 44 -3.2751E-03 45 -1.0616E-02
46 -1.7517E-02 47 -2.5978E-02

      THE SUM OF SQUARES IS 5.88513918E-02
PARROT: cont 30

It is safe to CONTINUE only after TOO MANY ITERATIONS
and no change in variables and experiments ...
Now anything can happen ...

PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:34:16

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 14

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR. VALUE START VALUE SCALING FACTOR REL.STAND.DEV
V1 2.02794319E+04 2.03239810E+04 2.03239810E+04 7.90191614E-02
V2 -2.92509609E+01 -2.93471952E+01 -2.93471952E+01 3.41438730E-01
V11 -2.18109899E+04 -2.17266456E+04 -2.17266456E+04 3.98516948E-02
V12 1.51615699E+01 1.52556729E+01 1.52556729E+01 5.81303279E-02
V15 2.43818947E+04 2.41304970E+04 2.41304970E+04 6.16278444E-01
V16 -8.58039023E+00 -8.25418969E+00 -8.25418969E+00 2.12994541E+00
V17 3.11711686E+03 3.08367945E+03 3.08367945E+03 1.47315321E+00
V19 2.19409070E+04 2.21788112E+04 2.21788112E+04 4.58887798E+00
V20 -7.00006043E+00 -7.07623325E+00 -7.07623325E+00 1.11463860E+01

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.89363143E-02 TO 5.88513918E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.54872084E-03

Number of alternate equilibria 10

SYMBOL STATUS VALUE/FUNCTION
FUNCTION R 298.15 8.31451000000000 ; 6000 N REF0 !
2 RTLN 20000000 +R*T*LN(1E-05*P)
FUNCTION V1 298.15 20279.4319193713 ; 6000 N REF0 !
FUNCTION V2 298.15 -29.2509608750716 ; 6000 N REF0 !
FUNCTION V11 298.15 -21810.9898544882 ; 6000 N REF0 !
FUNCTION V12 298.15 15.1615698692971 ; 6000 N REF0 !
FUNCTION V15 298.15 24381.8947426071 ; 6000 N REF0 !
FUNCTION V16 298.15 -8.58039022981766 ; 6000 N REF0 !
FUNCTION V17 298.15 3117.11686286455 ; 6000 N REF0 !
FUNCTION V19 298.15 21940.9070317692 ; 6000 N REF0 !
FUNCTION V20 298.15 -7.00006043410854 ; 6000 N REF0 !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N

```


L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 Alternate equilibrium calc 0.01
2 Alternate equilibrium calc 0.19
2 HTR=3727 3727. 5.00E+02 -0.3638 -7.2766E-04
3 Alternate equilibrium calc 0.01
4 Alternate equilibrium calc 0.00
5 Alternate equilibrium calc 0.00
6 Alternate equilibrium calc 0.00
20 Alternate equilibrium calc 0.00
21 Alternate equilibrium calc 0.00
22 Alternate equilibrium calc 0.00
23 Alternate equilibrium calc 0.00
100 ACR(B)=0.94 0.9396 2.85E-02 -3.8431E-04 -1.3488E-02
101 ACR(B)=0.84 0.8391 2.82E-02 -8.7217E-04 -3.0889E-02
102 ACR(B)=0.74 0.7400 2.81E-02 -1.9712E-05 -7.0116E-04
103 ACR(B)=0.64 0.6412 2.81E-02 1.2257E-03 4.3579E-02
104 ACR(B)=0.54 0.5419 2.83E-02 1.9021E-03 6.7271E-02
105 ACR(B)=0.44 0.4410 2.86E-02 1.0172E-03 3.5606E-02
106 ACR(B)=0.34 0.3375 2.90E-02 -2.4678E-03 -8.5035E-02
107 ACR(B)=0.23 0.2303 2.96E-02 3.4343E-04 1.1584E-02
108 ACR(B)=0.12 0.1183 3.05E-02 -1.7363E-03 -5.6982E-02
110 HMR(LIQUID)=-1964 -1963. 5.00E+02 1.011 2.0218E-03
111 HMR(LIQUID)=-3500 -3490. 5.00E+02 10.24 2.0483E-02
112 HMR(LIQUID)=-4588 -4580. 5.00E+02 7.692 1.5384E-02
113 HMR(LIQUID)=-5239 -5235. 5.00E+02 4.362 8.7249E-03
114 HMR(LIQUID)=-5454 -5453. 5.00E+02 1.253 2.5051E-03
115 HMR(LIQUID)=-5233 -5235. 5.00E+02 -1.638 -3.2751E-03
116 HMR(LIQUID)=-4575 -4580. 5.00E+02 -5.308 -1.0616E-02
117 HMR(LIQUID)=-3481 -3490. 5.00E+02 -8.758 -1.7517E-02
118 HMR(LIQUID)=-1950 -1963. 5.00E+02 -12.99 -2.5978E-02

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ The liquid data fits reasonably. Simplify its parameters.
PARROT: l-p-d liq
Property type /ALL/: s-f-v 11-14
S-F-V is not a valid property type
11-14 is not a valid property type
Property type: @@ Rescale the start values of the parameters to current values
@@ is not a valid property type
RESCALE is not a valid property type
THE is not a valid property type
START is not a valid property type
VALUES is not a valid property type
OF is not a valid property type
THE is not a valid property type
PARAMETERS is not a valid property type
TO is not a valid property type
CURRENT is not a valid property type
VALUES is not a valid property type
Property type: resc
RESC is not a valid property type
Property type: l-a-v
L-A-V is not a valid property type
Property type:
LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

PARROT:Hit RETURN to continue
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0.002 s
Found the set of lowest grid points in 0.000 s

Calculated POLY solution 0.003 s, total time 0.005 s
POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map

Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
BCC#1
** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.816E-01 7.270E+02
** A2B
BCC#1
** BCC#2

Phase region boundary 4 at: 3.626E-01 7.270E+02
** A2B
BCC#1
Calculated. 15 equilibria

Phase region boundary 5 at: 3.779E-01 1.184E+03
** LIQUID
** A2B
BCC#1

Phase region boundary 6 at: 2.893E-01 1.184E+03
** LIQUID
BCC#1
Calculated 29 equilibria

Phase region boundary 7 at: 4.903E-01 1.184E+03
** LIQUID
A2B
Calculated. 33 equilibria

Phase region boundary 8 at: 6.480E-01 1.038E+03
** LIQUID
A2B
** BCC#1

Phase region boundary 9 at: 7.636E-01 1.038E+03
A2B
** BCC#1
Calculated. 10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.257E-01 1.038E+03
LIQUID
** BCC#1
Calculated. 8 equilibria

Phase region boundary 11 at: 8.759E-01 1.204E+03
LIQUID
** BCC#1
** FCC

Phase region boundary 12 at: 8.812E-01 1.204E+03
LIQUID

```

** FCC
Calculated                29 equilibria

Phase region boundary 13 at:  9.361E-01  1.204E+03
  BCC#1
** FCC
Calculated                24 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
  BCC#1
  BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
  BCC#1
  BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
  BCC#1
  BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  7.140E-01  3.100E+02
  BCC#1
  BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  3.646E-01  7.700E+02
  A2B
  BCC#1
Calculated                10 equilibria

Phase region boundary 26 at:  3.646E-01  7.700E+02
  A2B
  BCC#1
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at:  3.646E-01  7.700E+02
  A2B
  BCC#1
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:  7.909E-01  7.700E+02
  A2B
  BCC#1
Calculated                10 equilibria

Phase region boundary 29 at:  7.909E-01  7.700E+02
  A2B
  BCC#1
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:  7.909E-01  7.700E+02
  A2B
  BCC#1
Calculated.                9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:  2.436E-01  1.230E+03
  LIQUID
  BCC#1

```

```

Calculated.                4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.436E-01 1.230E+03
** LIQUID
   BCC#1
Calculated                26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03
** LIQUID
   FCC
Calculated.                2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
** LIQUID
   FCC
Calculated                29 equilibria

Phase region boundary 35 at: 6.405E-03 1.397E+03
   LIQUID
** BCC#1
Calculated                9 equilibria

Phase region boundary 36 at: 6.405E-03 1.397E+03
   LIQUID
** BCC#1
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.296E-01 1.243E+03
   LIQUID
** BCC#1
Calculated                20 equilibria

Phase region boundary 38 at: 2.296E-01 1.243E+03
   LIQUID
** BCC#1
Calculated.                4 equilibria
Terminating at known equilibrium

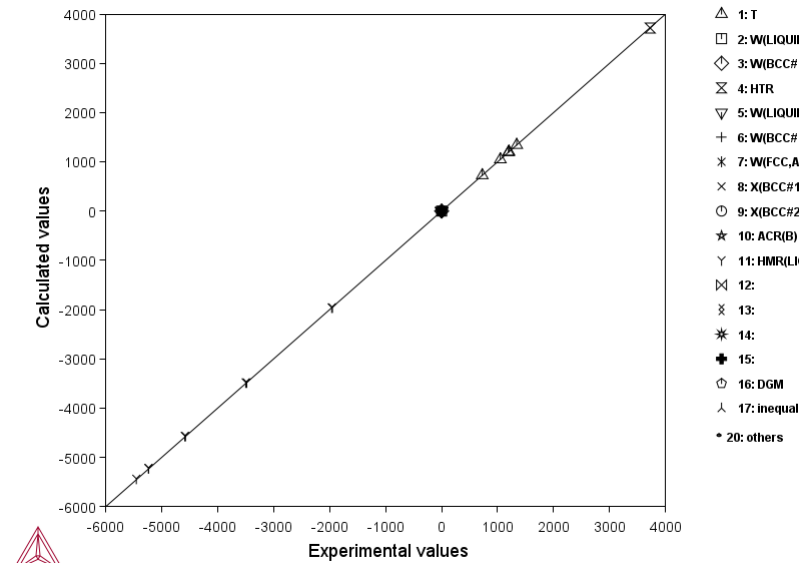
Phase region boundary 39 at: 6.122E-01 1.213E+03
   LIQUID
** A2B
Calculated.                12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.213E+03
   LIQUID
** A2B
Calculated.                8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
   LIQUID
** FCC
Calculated.                19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
   LIQUID
** FCC
Calculated                14 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping                1 seconds
POLY: post
POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

```

PARROT VERSION 5.3

```

Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 30
Alternate calculation is on
Use      47 experiments, maximum is      2000
Use     1082 real workspace, maximum is    50000

```

The following output is provided by subroutine VA05A

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88513918E-02
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0104E+00
6  1.0395E+00    7  1.0108E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      5.88554335E-02
1  9.9791E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0104E+00
6  1.0395E+00    7  1.0108E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      5.88532486E-02
1  9.9781E-01    2  9.9682E-01    3  1.0039E+00    4  9.9383E-01    5  1.0104E+00
6  1.0395E+00    7  1.0108E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      5.88529323E-02
1  9.9781E-01    2  9.9672E-01    3  1.0040E+00    4  9.9383E-01    5  1.0104E+00
6  1.0395E+00    7  1.0108E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88588765E-02
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9393E-01    5  1.0104E+00
6  1.0395E+00    7  1.0108E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88509980E-02
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0105E+00
6  1.0395E+00    7  1.0108E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88507646E-02
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0105E+00
6  1.0396E+00    7  1.0108E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88505918E-02
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0105E+00
6  1.0396E+00    7  1.0109E+00    8  9.8927E-01    9  9.8924E-01

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88511951E-02
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0105E+00
6  1.0396E+00    7  1.0109E+00    8  9.8937E-01    9  9.8924E-01

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88504179E-02
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0105E+00
6  1.0396E+00    7  1.0109E+00    8  9.8927E-01    9  9.8934E-01

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      9 iterations
1  9.9781E-01    2  9.9672E-01    3  1.0039E+00    4  9.9383E-01    5  1.0105E+00
6  1.0396E+00    7  1.0109E+00    8  9.8927E-01    9  9.8934E-01

1  7.4325E-03    2  7.4325E-03    3  1.5772E-03    4  2.5374E-03    5  1.3275E-01
6 -1.4001E-01    7 -7.2766E-04    8  8.1724E-03    9  8.1724E-03   10 -2.3973E-04
11 3.2732E-03   12 1.7798E-03   13 2.3826E-04   14 2.8016E-03   15 6.0530E-04
16 1.4494E-03   17 1.4494E-03   18 3.5504E-04   19 6.8562E-04   20 3.5504E-04
21 6.8562E-04   22 -2.1505E-03   23 1.7700E-03   24 3.3071E-03   25 3.3383E-04
26 -2.8027E-03   27 3.2547E-03   28 -1.6513E-03   29 3.8100E-03   30 -1.3488E-02
31 -3.0889E-02   32 -7.0116E-04   33 4.3579E-02   34 6.7271E-02   35 3.5606E-02
36 -8.5035E-02   37 1.1584E-02   38 -5.6982E-02   39 2.0218E-03   40 2.0483E-02
41 1.5384E-02   42 8.7249E-03   43 2.5051E-03   44 -3.2751E-03   45 -1.0616E-02
46 -1.7517E-02   47 -2.5978E-02

      THE SUM OF SQUARES IS      5.88504179E-02
```

PARROT: resc

PARROT: opt 30

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88504179E-02
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      5.88543988E-02
1  1.0001E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      5.88523184E-02
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      5.88520435E-02
1  1.0000E+00    2  1.0000E+00    3  1.0001E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88578038E-02
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88509909E-02
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0001E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88502728E-02
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88500972E-02
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0000E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88506086E-02
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0001E+00    9  1.0000E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      5.88499598E-02
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      9 iterations
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

1  7.4325E-03    2  7.4325E-03    3  1.5772E-03    4  2.4672E-03    5  1.3275E-01
6 -1.4001E-01    7 -7.2766E-04    8  8.1724E-03    9  8.1724E-03   10 -3.0928E-04
11 3.2656E-03   12 1.6981E-03   13 2.3393E-04   14 2.7390E-03   15 6.0370E-04
16 1.4676E-03   17 1.4676E-03   18 2.5191E-04   19 7.3748E-04   20 2.5191E-04
21 7.3748E-04   22 -2.2202E-03   23 1.7693E-03   24 3.2404E-03   25 3.3281E-04
```

```

26 -2.8656E-03 27 3.2531E-03 28 -1.7248E-03 29 3.8036E-03 30 -1.3488E-02
31 -3.0889E-02 32 -7.0116E-04 33 4.3579E-02 34 6.7271E-02 35 3.5606E-02
36 -8.5035E-02 37 1.1584E-02 38 -5.6982E-02 39 2.0218E-03 40 2.0483E-02
41 1.5384E-02 42 8.7249E-03 43 2.5051E-03 44 -3.2751E-03 45 -1.0616E-02
46 -1.7517E-02 47 -2.5978E-02

```

THE SUM OF SQUARES IS 5.88499598E-02

PARROT: @@ No change in the parameters, check the diagram again

PARROT: mac tcex36cpd

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

POLY:

POLY: @@ In PARROT, the global minimization is turned off automatically.

POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY: @@ message will be given.

POLY:

POLY: advanced-option global yes,,

Settings for global minimization:

*** WARNING *** Global equilibrium calculation may create new composition sets and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY:

POLY: def-com,,,

POLY: s-a-v 1 w(b) 0 1,,,

The condition W(B)=.1234 created

POLY: s-a-v 2 t 300 1700,,,

The condition T=942.2 created

POLY: s-c t=500

POLY: l-c

W(B)=0.1234, T=500

DEGREES OF FREEDOM 2

POLY: c-e

Creating condition P=1E5

Creating condition N=1

Using global minimization procedure

Calculated 628 grid points in 0.003 s

Found the set of lowest grid points in 0.000 s

Calculated POLY solution 0.004 s, total time 0.007 s

POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

POLY: map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02

BCC#1

** BCC#2

Calculated.. 2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02

BCC#1

** BCC#2

Calculated.. 14 equilibria

Phase region boundary 3 at: 6.816E-01 7.270E+02

** A2B

BCC#1

** BCC#2

Phase region boundary 4 at: 3.625E-01 7.270E+02

** A2B

```

    BCC#1
Calculated.                15 equilibria

Phase region boundary  5 at:  3.779E-01  1.184E+03
** LIQUID
** A2B
    BCC#1

Phase region boundary  6 at:  2.893E-01  1.184E+03
** LIQUID
    BCC#1
Calculated.                28 equilibria

Phase region boundary  7 at:  4.903E-01  1.184E+03
** LIQUID
    A2B
Calculated.                33 equilibria

Phase region boundary  8 at:  6.480E-01  1.038E+03
** LIQUID
    A2B
** BCC#1

Phase region boundary  9 at:  7.636E-01  1.038E+03
    A2B
** BCC#1
Calculated.                10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.257E-01  1.038E+03
    LIQUID
** BCC#1
Calculated.                8 equilibria

Phase region boundary 11 at:  8.758E-01  1.204E+03
    LIQUID
** BCC#1
** FCC

Phase region boundary 12 at:  8.811E-01  1.204E+03
    LIQUID
** FCC
Calculated                31 equilibria

Phase region boundary 13 at:  9.361E-01  1.204E+03
    BCC#1
** FCC
Calculated                21 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
    BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  7.140E-01  3.100E+02
    BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
    BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
    BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
    BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
    BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
    BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
** BCC#1
    BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
** BCC#1
    BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
** BCC#1
    BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  7.140E-01  3.100E+02
** BCC#1

```

```

    BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
** A2B
    BCC#1
Calculated.                10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
** A2B
    BCC#1
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
** A2B
    BCC#1
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02
** A2B
    BCC#1
Calculated.                10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02
** A2B
    BCC#1
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02
** A2B
    BCC#1
Calculated.                9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.436E-01 1.230E+03
** LIQUID
    BCC#1
Calculated.                4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.436E-01 1.230E+03
** LIQUID
    BCC#1
Calculated.                26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03
** LIQUID
    FCC
Calculated.                2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
** LIQUID
    FCC
Calculated.                29 equilibria

Phase region boundary 35 at: 6.405E-03 1.397E+03
    LIQUID
** BCC#1
Calculated.                10 equilibria

Phase region boundary 36 at: 6.405E-03 1.397E+03
    LIQUID
** BCC#1
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.296E-01 1.243E+03
    LIQUID
** BCC#1
Calculated.                23 equilibria

Phase region boundary 38 at: 2.296E-01 1.243E+03
    LIQUID
** BCC#1
Calculated.                4 equilibria
Terminating at known equilibrium

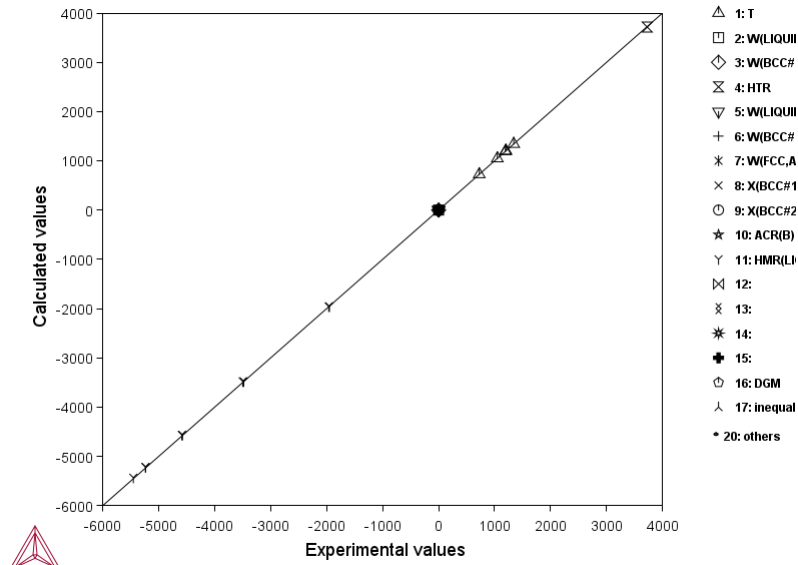
Phase region boundary 39 at: 6.122E-01 1.213E+03
    LIQUID
** A2B
Calculated.                12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.213E+03
    LIQUID
** A2B
Calculated.                8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
    LIQUID
** FCC
Calculated.                19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
    LIQUID
** FCC
Calculated.                14 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping                1 seconds
POLY: post
POST: s-l d
POST: plot

```

POST:
 POST: set-inter
 POST: Hit RETURN to continue
 POST: ba
 POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
 PARROT: @@ Turn off alternate mode and try to calculate all equilibria
 PARROT: s-alt Y
 Alternate calculation is on
 PARROT: ed
 ED_EXP: read 1
 ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	4	1.	1184.0		LIQUID A2B BCC
2	AINV	2	1.	1312.5		LIQUID A2B
3	AINV	3	1.	1038.5		LIQUID A2B BCC
4	AINV	3	1.	1204.4		LIQUID BCC FCC
5	AINV	3	1.	727.0		A2B BCC BCC#2
6	AINV	2	1.	726.0		BCC BCC#2
10	ALF	< unused >		1594.0		LIQUID FCC
11	ALF	< unused >		1548.0		LIQUID FCC
12	ALF	< unused >		1499.0		LIQUID FCC
13	ALF	< unused >		1438.0		LIQUID FCC
20	ATIE	3	1.	1413.0		LIQUID FCC
21	ATIE	3	1.	1337.0		LIQUID FCC
22	ATIE	3	1.	1213.0		LIQUID FCC
23	ATIE	3	1.	1100.0		LIQUID BCC
100	AA	2	1.	1573.0		LIQUID
101	AA	2	1.	1573.0		LIQUID
102	AA	2	1.	1573.0		LIQUID
103	AA	2	1.	1573.0		LIQUID
104	AA	2	1.	1573.0		LIQUID
105	AA	2	1.	1573.0		LIQUID
106	AA	2	1.	1573.0		LIQUID
107	AA	2	1.	1573.0		LIQUID
108	AA	2	1.	1573.0		LIQUID
110	AH	2	1.	1773.0		LIQUID
111	AH	2	1.	1773.0		LIQUID
112	AH	2	1.	1773.0		LIQUID
113	AH	2	1.	1773.0		LIQUID
114	AH	2	1.	1773.0		LIQUID
115	AH	2	1.	1773.0		LIQUID
116	AH	2	1.	1773.0		LIQUID
117	AH	2	1.	1773.0		LIQUID
118	AH	2	1.	1773.0		LIQUID

ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
 ED_EXP: @@ any liquid parameters and restore those with label ALF
 ED_EXP: s-we 0 100-118
 ED_EXP: s-we 1 alf
 Changed weight on 4 equilibria.
 ED_EXP: s-e 1
 Equilibrium number 1, label AINV
 ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	2	1.	1184.0		LIQUID A2B BCC
2	AINV	2	1.	1312.5		LIQUID A2B
3	AINV	2	1.	1038.5		LIQUID A2B BCC
4	AINV	2	1.	1204.4		LIQUID BCC FCC
5	AINV	2	1.	727.0		A2B BCC BCC#2
6	AINV	2	1.	726.0		BCC BCC#2
10	ALF	3	1.	1594.0		LIQUID FCC
11	ALF	3	1.	1548.0		LIQUID FCC
12	ALF	3	1.	1499.0		LIQUID FCC
13	ALF	3	1.	1438.0		LIQUID FCC
20	ATIE	2	1.	1413.0		LIQUID FCC
21	ATIE	2	1.	1337.0		LIQUID FCC
22	ATIE	2	1.	1213.0		LIQUID FCC
23	ATIE	2	1.	1100.0		LIQUID BCC
100	AA	< unused >		1573.0		LIQUID
101	AA	< unused >		1573.0		LIQUID
102	AA	< unused >		1573.0		LIQUID
103	AA	< unused >		1573.0		LIQUID
104	AA	< unused >		1573.0		LIQUID
105	AA	< unused >		1573.0		LIQUID
106	AA	< unused >		1573.0		LIQUID
107	AA	< unused >		1573.0		LIQUID
108	AA	< unused >		1573.0		LIQUID
110	AH	< unused >		1773.0		LIQUID
111	AH	< unused >		1773.0		LIQUID

```
112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID
```

ED_EXP: save

ED_EXP: @@ Save changes

ED_EXP: ba

PARROT: opt 0

Use 29 experiments, maximum is 2000

Use 740 real workspace, maximum is 50000

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:35: 7
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0
```

== OPTIMIZING CONDITIONS ==

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02794319E+04	2.02794319E+04	2.02794319E+04	7.91928241E-02
V2	-2.92509609E+01	-2.92509609E+01	-2.92509609E+01	3.42563239E-01
V11	-2.18109899E+04	-2.18109899E+04	-2.18109899E+04	3.96976149E-02
V12	1.51615699E+01	1.51615699E+01	1.51615699E+01	5.86492610E-02
V15	2.43843078E+04	2.43843078E+04	2.43843078E+04	6.09982906E-01
V16	-8.58207377E+00	-8.58121565E+00	-8.58121565E+00	2.04927402E+00
V17	3.11773697E+03	3.11742523E+03	3.11742523E+03	1.45720358E+00
V19	2.19409070E+04	2.19409070E+04	2.19409070E+04	4.63891666E+00
V20	-7.00146813E+00	-7.00076806E+00	-7.00076806E+00	1.12675840E+01

```
NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 5.88504179E-02 TO 1.03752134E+01
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 5.18760669E-01
```

SYMBOL	STATUS	VALUE/FUNCTION
FUNCTION R	298.15	8.314510000000000 ; 6000 N REFO !
2 RTLNP	20000000	+R*T*LN(1E-05*P)
FUNCTION V1	298.15	20279.4319193713 ; 6000 N REFO !
FUNCTION V2	298.15	-29.2509608750716 ; 6000 N REFO !
FUNCTION V11	298.15	-21810.9898544882 ; 6000 N REFO !
FUNCTION V12	298.15	15.1615698692971 ; 6000 N REFO !
FUNCTION V15	298.15	24384.3077923055 ; 6000 N REFO !
FUNCTION V16	298.15	-8.58207377035163 ; 6000 N REFO !
FUNCTION V17	298.15	3117.73697333268 ; 6000 N REFO !
FUNCTION V19	298.15	21940.9070317692 ; 6000 N REFO !
FUNCTION V20	298.15	-7.00146813423884 ; 6000 N REFO !

LIQUID:L (A,B)1.0
- This phase is a liquid

```
==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N
```

```
==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N
```

```
==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N
```

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1184.	10.	-9.002	-0.9002
1 W(LIQUID,B)=0.408	0.4170	2.00E-02	9.0021E-03	0.4501
1 W(BCC#1,B)=0.13	0.1325	2.00E-02	2.5110E-03	0.1255
2 T=1341	1312.	10.	-28.53	-2.853
2 HTR=3727	3727.	5.00E+02	-0.3639	-7.2788E-04
3 T=1049	1038.	10.	-10.54	-1.054
3 W(LIQUID,A)=0.27	0.2738	2.00E-02	3.7579E-03	0.1879
3 W(BCC#1,A)=9.3E-2	9.3931E-02	2.00E-02	9.3108E-04	4.6554E-02
4 T=1203	1204.	10.	1.425	0.1425
4 W(LIQUID,A)=0.19	0.1889	2.00E-02	-1.0604E-03	-5.3019E-02
4 W(BCC#1,A)=6.9E-2	6.8483E-02	2.00E-02	-5.1667E-04	-2.5834E-02
4 W(FCC,A)=6E-2	5.9382E-02	2.00E-02	-6.1769E-04	-3.0884E-02
5 T=726	727.0	10.	1.009	0.1009
5 X(BCC#1,B)=3.7E-2	3.7326E-02	2.00E-02	3.2603E-04	1.6302E-02
5 X(BCC#2,A)=0.114	0.1146	2.00E-02	6.4963E-04	3.2481E-02
6 X(BCC#1,B)=3.7E-2	3.7042E-02	2.00E-02	4.1921E-05	2.0961E-03
6 X(BCC#2,A)=0.114	0.1139	2.00E-02	-5.0616E-05	-2.5308E-03
10 W(LIQUID,A)=2E-2	1.9382E-02	2.00E-02	-6.1755E-04	-3.0878E-02

11 W(LIQUID,A)=4.2E-2	4.1481E-02	2.00E-02	-5.1852E-04	-2.5926E-02
12 W(LIQUID,A)=6.5E-2	6.4385E-02	2.00E-02	-6.1455E-04	-3.0727E-02
13 W(LIQUID,A)=9.3E-2	9.2002E-02	2.00E-02	-9.9752E-04	-4.9876E-02
20 W(LIQUID,A)=0.104	0.1030	2.00E-02	-9.6352E-04	-4.8176E-02
20 W(FCC,A)=3.8E-2	3.7715E-02	2.00E-02	-2.8484E-04	-1.4242E-02
21 W(LIQUID,A)=0.136	0.1356	2.00E-02	-4.1873E-04	-2.0936E-02
21 W(FCC,A)=4.7E-2	4.6618E-02	2.00E-02	-3.8208E-04	-1.9104E-02
22 W(LIQUID,A)=0.187	0.1856	2.00E-02	-1.3888E-03	-6.9440E-02
22 W(FCC,A)=5.9E-2	5.8640E-02	2.00E-02	-3.6039E-04	-1.8019E-02
23 W(LIQUID,A)=0.245	0.2435	2.00E-02	-1.5427E-03	-7.7133E-02
23 W(BCC#1,A)=8.5E-2	8.4427E-02	2.00E-02	-5.7341E-04	-2.8670E-02

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for
PARROT: @@ equilibrium 4. It can be on the wrong side, at high A instead
PARROT: @@ of high B. Try to correct that in the Edit module.
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
      Equilibrium number          4 , label AINV
ED_EXP: s-a-s
T /1204.42469/: 1200
Automatic start values for phase constituents? /N/: N

      Phase LIQUID
Major constituent(s) /b/: b

      Phase BCC
Major constituent(s) /b/: b

      Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
      Testing result with global minimization
          13 ITS, CPU TIME USED  0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
      Output from POLY-3, equilibrium =          4, label AINV, database:

Conditions:
P=101325
FIXED PHASES
LIQUID=1 BCC#1=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1204.42 K ( 931.27 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30212E+02
Total Gibbs energy -9.82809E+03, Enthalpy 1.98600E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
A                6.5962E-01  1.0131E-01 3.8835E-01 -9.4718E+03 SER
B                2.3404E+00  8.9869E-01 8.5833E-01 -1.5298E+03 SER

FCC              Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5911E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40618E-01 A 5.93823E-02

BCC#1            Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5342E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31517E-01 A 6.84833E-02

LIQUID           Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.8959E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.11060E-01 A 1.88940E-01
EXPERIMENT T=1203:DT $1204.42:10 NO=1
EXPERIMENT W(LIQUID,A)=0.19:DX $0.18894:2E-2 NO=2
EXPERIMENT W(BCC#1,A)=6.9E-2:DX $6.84833E-2:2E-2 NO=3
EXPERIMENT W(FCC,A)=6E-2:DX $5.93823E-2:2E-2 NO=4
ED_EXP: ba
PARROT: @@ The error is still there, calculate the phase diagram.
PARROT: mac tcex36cpd
PARROT: set-echo
      NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
      Settings for global minimization:
      *** WARNING *** Global equilibrium calculation may create new composition sets
      and this may corrupt your PARROT work file (.PAR file).
      Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
      The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
      The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
      W(B)=0.1234, T=500
      DEGREES OF FREEDOM 2
POLY: c-e
      Creating condition P=1E5
      Creating condition N=1
      Using global minimization procedure
      Calculated 628 grid points in 0.002 s
      Found the set of lowest grid points in 0.001 s
      Calculated POLY solution 0.003 s, total time 0.006 s
POLY: save tcex36 y

      This file contains results from a previous STEP or MAP command.
      The SAVE command will save the current status of the program but destroy
      the results from the previous STEP or MAP commands.

POLY: map

```

Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
BCC#1
** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.816E-01 7.270E+02
** A2B
BCC#1
** BCC#2

Phase region boundary 4 at: 3.625E-01 7.270E+02
** A2B
BCC#1
Calculated. 15 equilibria

Phase region boundary 5 at: 3.779E-01 1.184E+03
** LIQUID
** A2B
BCC#1

Phase region boundary 6 at: 2.893E-01 1.184E+03
** LIQUID
BCC#1
Calculated 28 equilibria

Phase region boundary 7 at: 4.903E-01 1.184E+03
** LIQUID
A2B
Calculated. 33 equilibria

Phase region boundary 8 at: 6.480E-01 1.038E+03
** LIQUID
A2B
** BCC#1

Phase region boundary 9 at: 7.636E-01 1.038E+03
A2B
** BCC#1
Calculated. 10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.257E-01 1.038E+03
LIQUID
** BCC#1
Calculated. 8 equilibria

Phase region boundary 11 at: 8.758E-01 1.204E+03
LIQUID
** BCC#1
** FCC

Phase region boundary 12 at: 8.811E-01 1.204E+03
LIQUID
** FCC
Calculated 31 equilibria

Phase region boundary 13 at: 9.361E-01 1.204E+03
BCC#1
** FCC
Calculated 21 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 31 at: 2.436E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 32 at: 2.436E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated 26 equilibria

```

Phase region boundary 33 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated 29 equilibria

Phase region boundary 35 at: 6.405E-03 1.397E+03
LIQUID
** BCC#1
Calculated 10 equilibria

Phase region boundary 36 at: 6.405E-03 1.397E+03
LIQUID
** BCC#1
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.296E-01 1.243E+03
LIQUID
** BCC#1
Calculated 23 equilibria

Phase region boundary 38 at: 2.296E-01 1.243E+03
LIQUID
** BCC#1
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.213E+03
LIQUID
** A2B
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.213E+03
LIQUID
** A2B
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated. 19 equilibria
Terminating at known equilibrium

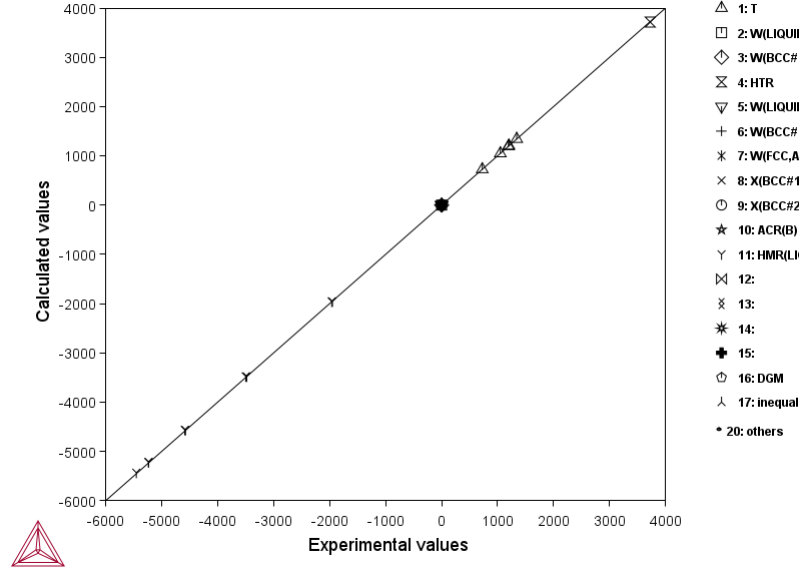
Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated 14 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping 1 seconds

```

```

POLY: post
POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST:Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
POLY: ba

```

```

PARROT VERSION 5.3

Global minimization used as test only
PARROT: ed
ED_EXP: read 1
ED_EXP: s-we 0 4
ED_EXP: save
ED_EXP: ba
PARROT: opt 0
Use 25 experiments, maximum is 2000
Use 664 real workspace, maximum is 50000
PARROT: l-r C SCREEN

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR. VALUE START VALUE SCALING FACTOR REL.STAND.DEV
V1 2.02794319E+04 2.02794319E+04 2.02794319E+04 7.91928241E-02
V2 -2.92509609E+01 -2.92509609E+01 -2.92509609E+01 3.42563239E-01
V11 -2.18109899E+04 -2.18109899E+04 -2.18109899E+04 3.96976149E-02
V12 1.51615699E+01 1.51615699E+01 1.51615699E+01 5.86492610E-02
V15 2.43843078E+04 2.43843078E+04 2.43843078E+04 6.09982906E-01
V16 -8.58207377E+00 -8.58121565E+00 -8.58121565E+00 2.04927402E+00
V17 3.11773697E+03 3.11742523E+03 3.11742523E+03 1.45720358E+00
V19 2.19409070E+04 2.19409070E+04 2.19409070E+04 4.63891666E+00
V20 -7.00146813E+00 -7.00076806E+00 -7.00076806E+00 1.12675840E+01

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 5.88504179E-02 TO 1.03504837E+01
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 6.46905234E-01

SYMBOL STATUS VALUE/FUNCTION
FUNCTION R 298.15 8.31451000000000 ; 6000 N REF0 !
2 RTLN P 20000000 +R*T*LN(1E-05*P)
FUNCTION V1 298.15 20279.4319193713 ; 6000 N REF0 !
FUNCTION V2 298.15 -29.2509608750716 ; 6000 N REF0 !
FUNCTION V11 298.15 -21810.9898544882 ; 6000 N REF0 !
FUNCTION V12 298.15 15.1615698692971 ; 6000 N REF0 !
FUNCTION V15 298.15 24384.3077923055 ; 6000 N REF0 !
FUNCTION V16 298.15 -8.58207377035163 ; 6000 N REF0 !
FUNCTION V17 298.15 3117.73697333268 ; 6000 N REF0 !
FUNCTION V19 298.15 21940.9070317692 ; 6000 N REF0 !
FUNCTION V20 298.15 -7.00146813423884 ; 6000 N REF0 !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193 1184. 10. -9.002 -0.9002
1 W(LIQUID,B)=0.408 0.4170 2.00E-02 9.0021E-03 0.4501
1 W(BCC#1,B)=0.13 0.1325 2.00E-02 2.5110E-03 0.1255
2 T=1341 1312. 10. -28.53 -2.853
2 HTR=3727 3727. 5.00E+02 -0.3639 -7.2788E-04
3 T=1049 1038. 10. -10.54 -1.054
3 W(LIQUID,A)=0.27 0.2738 2.00E-02 3.7579E-03 0.1879
3 W(BCC#1,A)=9.3E-2 9.3931E-02 2.00E-02 9.3108E-04 4.6554E-02
5 T=726 727.0 10. 1.009 0.1009
5 X(BCC#1,B)=3.7E-2 3.7326E-02 2.00E-02 3.2603E-04 1.6302E-02
5 X(BCC#2,A)=0.114 0.1146 2.00E-02 6.4963E-04 3.2481E-02
6 X(BCC#1,B)=3.7E-2 3.7042E-02 2.00E-02 4.1921E-05 2.0961E-03
6 X(BCC#2,A)=0.114 0.1139 2.00E-02 -5.0616E-05 -2.5308E-03
10 W(LIQUID,A)=2E-2 1.9382E-02 2.00E-02 -6.1755E-04 -3.0878E-02
11 W(LIQUID,A)=4.2E-2 4.1481E-02 2.00E-02 -5.1852E-04 -2.5926E-02
12 W(LIQUID,A)=6.5E-2 6.4385E-02 2.00E-02 -6.1455E-04 -3.0727E-02
13 W(LIQUID,A)=9.3E-2 9.2002E-02 2.00E-02 -9.9752E-04 -4.9876E-02
20 W(LIQUID,A)=0.104 0.1030 2.00E-02 -9.6352E-04 -4.8176E-02
20 W(FCC,A)=3.8E-2 3.7715E-02 2.00E-02 -2.8484E-04 -1.4242E-02
21 W(LIQUID,A)=0.136 0.1356 2.00E-02 -4.1873E-04 -2.0936E-02
21 W(FCC,A)=4.7E-2 4.6618E-02 2.00E-02 -3.8208E-04 -1.9104E-02
22 W(LIQUID,A)=0.187 0.1856 2.00E-02 -1.3888E-03 -6.9440E-02
22 W(FCC,A)=5.9E-2 5.8640E-02 2.00E-02 -3.6039E-04 -1.8019E-02
23 W(LIQUID,A)=0.245 0.2435 2.00E-02 -1.5427E-03 -7.7133E-02
23 W(BCC#1,A)=8.5E-2 8.4427E-02 2.00E-02 -5.7341E-04 -2.8670E-02

PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30

Use 25 experiments, maximum is 2000
Use 664 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      1.03504837E+01
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      1.05255993E+01
1  1.0001E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      1.00354042E+01
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      1.01709982E+01
1  1.0000E+00    2  1.0001E+00    3  1.0001E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      9.91831533E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      9.92532898E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0001E+00    5  1.0001E+00
6  1.0001E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      9.91565551E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0002E+00    7  1.0001E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      9.91528315E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0002E+00    7  1.0002E+00    8  1.0000E+00    9  1.0001E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      9.91563242E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0002E+00    7  1.0002E+00    8  1.0001E+00    9  1.0001E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      9.91513597E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0002E+00    7  1.0002E+00    8  1.0000E+00    9  1.0002E+00

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      2.62188124E-01
1  9.9791E-01    2  1.0039E+00    3  9.9835E-01    4  1.0015E+00    5  9.9992E-01
6  1.0002E+00    7  1.0002E+00    8  1.0000E+00    9  1.0002E+00

      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      1.84422128E-01
1  9.9876E-01    2  1.0036E+00    3  9.9813E-01    4  1.0027E+00    5  9.9858E-01
6  9.9624E-01    7  9.9908E-01    8  1.0011E+00    9  1.0013E+00

      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      9.30556795E-02
1  9.9982E-01    2  1.0039E+00    3  9.9787E-01    4  1.0041E+00    5  9.9651E-01
6  9.8851E-01    7  9.9668E-01    8  1.0039E+00    9  1.0050E+00

      AT THE     13 TH ITERATION WE HAVE THE SUM OF SQUARES      1.62059647E-02
1  1.0012E+00    2  1.0033E+00    3  9.9860E-01    4  1.0085E+00    5  9.9194E-01
6  9.7109E-01    7  9.9185E-01    8  1.0062E+00    9  1.0032E+00

      AT THE     14 TH ITERATION WE HAVE THE SUM OF SQUARES      4.83083572E-03
1  1.0020E+00    2  1.0031E+00    3  9.9903E-01    4  1.0110E+00    5  9.8937E-01
6  9.6104E-01    7  9.8922E-01    8  1.0081E+00    9  1.0035E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      14 iterations
1  1.0020E+00    2  1.0031E+00    3  9.9903E-01    4  1.0110E+00    5  9.8937E-01
6  9.6104E-01    7  9.8922E-01    8  1.0081E+00    9  1.0035E+00

1 -3.1045E-02    2 -1.2730E-02    3 -4.4920E-03    4  2.6759E-03    5 -1.7908E-02
6  1.5844E-02    7  1.5494E-02    8  3.3258E-03    9 -3.9381E-03   10  2.0912E-02
11 -9.6602E-03   12  2.1466E-02   13 -8.3094E-03   14 -2.1576E-02   15 -7.1596E-03
16 -3.1652E-03   17 -1.2932E-02   18 -7.8558E-03   19  9.4297E-03   20  2.8031E-02
21  4.0812E-03   22 -1.1349E-02   23 -1.3920E-03   24 -9.7046E-04   25 -2.6691E-04
```

```

      THE SUM OF SQUARES IS      4.83083572E-03
PARROT: cont 30
```

```

It is safe to CONTINUE only after TOO MANY ITERATIONS
and no change in variables and experiments ...
Now anything can happen ...
```

```
PARROT: l-r C SCREEN
```

```

=====
OUTPUT FROM P A R R O T.  DATE 2025. 5.12    9:35:31
```

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 15
```

```
== OPTIMIZING CONDITIONS ==
```

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

```
== OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO V00
```

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03192527E+04	2.02794319E+04	2.02794319E+04	1.03256221E-01
V2	-2.93407339E+01	-2.92509609E+01	-2.92509609E+01	9.50350186E-02
V11	-2.17899144E+04	-2.18109899E+04	-2.18109899E+04	2.03679696E-01
V12	1.53278493E+01	1.51615699E+01	1.51615699E+01	3.38209292E-01
V15	2.41251227E+04	2.43843078E+04	2.43843078E+04	1.49764170E-01
V16	-8.24687790E+00	-8.58121565E+00	-8.58121565E+00	5.17740851E-01

V17 3.08382020E+03 3.11742523E+03 3.11742523E+03 2.63521371E-01
V19 2.21176839E+04 2.19409070E+04 2.19409070E+04 6.93239037E-01
V20 -7.02506538E+00 -7.00076806E+00 -7.00076806E+00 1.73850896E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.03504837E+01 TO 4.83083572E-03
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.01927232E-04

SYMBOL	STATUS	VALUE/FUNCTION
FUNCTION R	298.15	8.314510000000000 ; 6000 N REF0 !
2 RTLN P	20000000	+R*T*LN(1E-05*P)
FUNCTION V1	298.15	20319.2526653087 ; 6000 N REF0 !
FUNCTION V2	298.15	-29.3407339185364 ; 6000 N REF0 !
FUNCTION V11	298.15	-21789.9143927222 ; 6000 N REF0 !
FUNCTION V12	298.15	15.3278493274781 ; 6000 N REF0 !
FUNCTION V15	298.15	24125.1227058560 ; 6000 N REF0 !
FUNCTION V16	298.15	-8.24687790276837 ; 6000 N REF0 !
FUNCTION V17	298.15	3083.82020183051 ; 6000 N REF0 !
FUNCTION V19	298.15	22117.6838962366 ; 6000 N REF0 !
FUNCTION V20	298.15	-7.02506538292445 ; 6000 N REF0 !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1193.	10.	-0.3105	-3.1045E-02
1 W(LIQUID,B)=0.408	0.4077	2.00E-02	-2.5459E-04	-1.2730E-02
1 W(BCC#1,B)=0.13	0.1299	2.00E-02	-8.9839E-05	-4.4920E-03
2 T=1341	1341.	10.	2.6759E-02	2.6759E-03
2 HTR=3727	3718.	5.00E+02	-8.954	-1.7908E-02
3 T=1049	1049.	10.	0.1584	1.5844E-02
3 W(LIQUID,A)=0.27	0.2703	2.00E-02	3.0989E-04	1.5494E-02
3 W(BCC#1,A)=9.3E-2	9.3067E-02	2.00E-02	6.6517E-05	3.3258E-03
5 T=726	726.0	10.	-3.9381E-02	-3.9381E-03
5 X(BCC#1,B)=3.7E-2	3.7418E-02	2.00E-02	4.1825E-04	2.0912E-02
5 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.9320E-04	-9.6602E-03
6 X(BCC#1,B)=3.7E-2	3.7429E-02	2.00E-02	4.2932E-04	2.1466E-02
6 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.6619E-04	-8.3094E-03
10 W(LIQUID,A)=2E-2	1.9568E-02	2.00E-02	-4.3151E-04	-2.1576E-02
11 W(LIQUID,A)=4.2E-2	4.1857E-02	2.00E-02	-1.4319E-04	-7.1596E-03
12 W(LIQUID,A)=6.5E-2	6.4937E-02	2.00E-02	-6.3304E-05	-3.1652E-03
13 W(LIQUID,A)=9.3E-2	9.2741E-02	2.00E-02	-2.5863E-04	-1.2932E-02
20 W(LIQUID,A)=0.104	0.1038	2.00E-02	-1.5712E-04	-7.8558E-03
20 W(FCC,A)=3.8E-2	3.8189E-02	2.00E-02	1.8859E-04	9.4297E-03
21 W(LIQUID,A)=0.136	0.1366	2.00E-02	5.6062E-04	2.8031E-02
21 W(FCC,A)=4.7E-2	4.7082E-02	2.00E-02	8.1625E-05	4.0812E-03
22 W(LIQUID,A)=0.187	0.1868	2.00E-02	-2.2697E-04	-1.1349E-02
22 W(FCC,A)=5.9E-2	5.8972E-02	2.00E-02	-2.7839E-05	-1.3920E-03
23 W(LIQUID,A)=0.245	0.2450	2.00E-02	-1.9409E-05	-9.7046E-04
23 W(BCC#1,A)=8.5E-2	8.4995E-02	2.00E-02	-5.3382E-06	-2.6691E-04

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
Equilibrium number 4 , label AINV
ED_EXP: s-a-s
T /1204.42469/: 1200
Automatic start values for phase constituents? /N/: N

Phase LIQUID
Major constituent(s) /b/: b

Phase BCC
Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b

ED_EXP:
ED_EXP: c-e
Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS

ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:
P=101325
FIXED PHASES
LIQUID=1 BCC#1=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1203.73 K (930.58 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30100E+02
Total Gibbs energy -9.74919E+03, Enthalpy 1.98559E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
A	6.6333E-01	1.0197E-01	3.9460E-01	-9.3067E+03	SER

```

B                2.3367E+00  8.9803E-01  8.5822E-01 -1.5303E+03 SER

FCC              Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.5887E+01, Volume fraction 0.0000E+00  Mass fractions:
B  9.40241E-01  A  5.97588E-02

BCC#1            Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.5320E+01, Volume fraction 0.0000E+00  Mass fractions:
B  9.31155E-01  A  6.88454E-02

LIQUID           Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 3.8893E+01, Volume fraction 0.0000E+00  Mass fractions:
B  8.09622E-01  A  1.90378E-01
SET WEIGHT 0,,,
EXPERIMENT T=1203:DT
EXPERIMENT W(LIQUID,A)=0.19:DX
EXPERIMENT W(BCC#1,A)=6.9E-2:DX
EXPERIMENT W(FCC,A)=6E-2:DX
ED EXP: ba
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated          628 grid points in          0.003 s
Found the set of lowest grid points in          0.000 s
Calculated POLY solution          0.003 s, total time          0.006 s
POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map
Version S mapping is selected
Generating start equilibrium  1
Generating start equilibrium  2
Generating start equilibrium  3
Generating start equilibrium  4
Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary  1 at:  7.140E-01  3.100E+02
      BCC#1
** BCC#2
Calculated..          2 equilibria
Terminating at axis limit.

```

Phase region boundary 2 at: 7.141E-01 3.000E+02
 BCC#1
 ** BCC#2
 Calculated. 14 equilibria

Phase region boundary 3 at: 6.821E-01 7.260E+02
 ** A2B
 BCC#1
 ** BCC#2

Phase region boundary 4 at: 3.626E-01 7.260E+02
 ** A2B
 BCC#1
 Calculated. 15 equilibria

Phase region boundary 5 at: 3.769E-01 1.193E+03
 ** LIQUID
 ** A2B
 BCC#1

Phase region boundary 6 at: 2.826E-01 1.193E+03
 ** LIQUID
 BCC#1
 Calculated 28 equilibria

Phase region boundary 7 at: 4.863E-01 1.193E+03
 ** LIQUID
 A2B
 Calculated. 33 equilibria

Phase region boundary 8 at: 6.500E-01 1.049E+03
 ** LIQUID
 A2B
 ** BCC#1

Phase region boundary 9 at: 7.642E-01 1.049E+03
 A2B
 ** BCC#1
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 10 at: 8.276E-01 1.049E+03
 LIQUID
 ** BCC#1
 Calculated. 8 equilibria

Phase region boundary 11 at: 8.750E-01 1.204E+03
 LIQUID
 ** BCC#1
 ** FCC

Phase region boundary 12 at: 8.803E-01 1.204E+03
 LIQUID
 ** FCC
 Calculated 32 equilibria

Phase region boundary 13 at: 9.357E-01 1.204E+03
 BCC#1
 ** FCC
 Calculated 23 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2

Calculated. 13 equilibria
 Terminating at known equilibrium

 Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

 Phase region boundary 25 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

 Phase region boundary 26 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

 Phase region boundary 27 at: 3.646E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 14 equilibria
 Terminating at known equilibrium

 Phase region boundary 28 at: 7.912E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

 Phase region boundary 29 at: 7.912E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

 Phase region boundary 30 at: 7.912E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 9 equilibria
 Terminating at known equilibrium

 Phase region boundary 31 at: 2.448E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated. 4 equilibria
 Terminating at known equilibrium

 Phase region boundary 32 at: 2.448E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated 26 equilibria

 Phase region boundary 33 at: 8.860E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated. 2 equilibria
 Terminating at known equilibrium

 Phase region boundary 34 at: 8.860E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated 29 equilibria

 Phase region boundary 35 at: 6.414E-03 1.397E+03
 LIQUID
 ** BCC#1
 Calculated 11 equilibria

 Phase region boundary 36 at: 6.414E-03 1.397E+03
 LIQUID
 ** BCC#1
 Calculated. 13 equilibria
 Terminating at known equilibrium

 Phase region boundary 37 at: 2.298E-01 1.244E+03
 LIQUID
 ** BCC#1
 Calculated 18 equilibria

 Phase region boundary 38 at: 2.298E-01 1.244E+03
 LIQUID
 ** BCC#1
 Calculated. 4 equilibria
 Terminating at known equilibrium

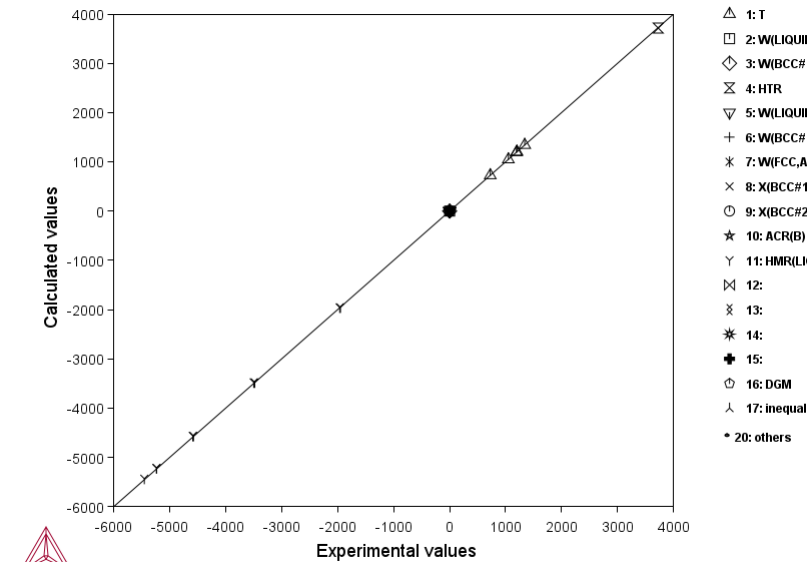
 Phase region boundary 39 at: 6.122E-01 1.240E+03
 LIQUID
 ** A2B
 Calculated. 14 equilibria
 Terminating at known equilibrium

 Phase region boundary 40 at: 6.122E-01 1.240E+03
 LIQUID
 ** A2B
 Calculated. 8 equilibria
 Terminating at known equilibrium

 Phase region boundary 41 at: 9.927E-01 1.613E+03
 LIQUID
 ** FCC
 Calculated. 19 equilibria
 Terminating at known equilibrium

 Phase region boundary 42 at: 9.927E-01 1.613E+03
 LIQUID
 ** FCC
 Calculated 9 equilibria

*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping 1 seconds
POLY: post
POST: s-l d
POST: plot



POST:
POST: set-inter
POST:Hit RETURN to continue
POST: @@ Sometimes a very strange shape of the fcc phase here and no
POST: @@ equilibrium between liq, fcc and bcc at high B content.
POST: ba
POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:35:55

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 15

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V20

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03192527E+04	2.02794319E+04	2.02794319E+04	1.03256221E-01
V2	-2.93407339E+01	-2.92509609E+01	-2.92509609E+01	9.50350186E-02
V11	-2.17899144E+04	-2.18109899E+04	-2.18109899E+04	2.03679696E-01
V12	1.53278493E+01	1.51615699E+01	1.51615699E+01	3.38209292E-01
V15	2.41251227E+04	2.43843078E+04	2.43843078E+04	1.49764170E-01
V16	-8.24687790E+00	-8.58121565E+00	-8.58121565E+00	5.17740851E-01
V17	3.08382020E+03	3.11742523E+03	3.11742523E+03	2.63521371E-01
V19	2.21176839E+04	2.19409070E+04	2.19409070E+04	6.93239037E-01
V20	-7.02506538E+00	-7.00076806E+00	-7.00076806E+00	1.73850896E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.03504837E+01 TO 4.83083572E-03
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.01927232E-04

SYMBOL	STATUS	VALUE/FUNCTION
FUNCTION R	298.15	8.314510000000000
2 RTLN P	20000000	+R*T*LN(1E-05*P)
FUNCTION V1	298.15	20319.2526653087
FUNCTION V2	298.15	-29.3407339185364
FUNCTION V11	298.15	-21789.9143927222
FUNCTION V12	298.15	15.3278493274781
FUNCTION V15	298.15	24125.1227058560
FUNCTION V16	298.15	-8.24687790276837
FUNCTION V17	298.15	3083.82020183051
FUNCTION V19	298.15	22117.6838962366
FUNCTION V20	298.15	-7.02506538292445

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====

```

G(LIQUID,A;0)                500 +14000-10*T;                2000 N

==== [B] ====
G(LIQUID,B;0)                500 +18000-12*T;                2000 N

==== [A, B] ====
L(LIQUID,A,B;0)              500 +V11+V12*T;                2000 N
L(LIQUID,A,B;1)              500 +V13+V14*T;                2000 N

```

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

```

1 T=1193                1193.                10.                -0.3105                -3.1045E-02
1 W(LIQUID,B)=0.408      0.4077                2.00E-02                -2.5459E-04                -1.2730E-02
1 W(BCC#1,B)=0.13        0.1299                2.00E-02                -8.9839E-05                -4.4920E-03
2 T=1341                1341.                10.                2.6759E-02                2.6759E-03
2 HTR=3727              3718.                5.00E+02                -8.954                    -1.7908E-02
3 T=1049                1049.                10.                0.1584                    1.5844E-02
3 W(LIQUID,A)=0.27        0.2703                2.00E-02                3.0989E-04                1.5494E-02
3 W(BCC#1,A)=9.3E-2      9.3067E-02            2.00E-02                6.6517E-05                3.3258E-03
5 T=726                 726.0                10.                -3.9381E-02                -3.9381E-03
5 X(BCC#1,B)=3.7E-2      3.7418E-02            2.00E-02                4.1825E-04                2.0912E-02
5 X(BCC#2,A)=0.114       0.1138                2.00E-02                -1.9320E-04                -9.6602E-03
6 X(BCC#1,B)=3.7E-2      3.7429E-02            2.00E-02                4.2932E-04                2.1466E-02
6 X(BCC#2,A)=0.114       0.1138                2.00E-02                -1.6619E-04                -8.3094E-03
10 W(LIQUID,A)=2E-2      1.9568E-02            2.00E-02                -4.3151E-04                -2.1576E-02
11 W(LIQUID,A)=4.2E-2    4.1857E-02            2.00E-02                -1.4319E-04                -7.1596E-03
12 W(LIQUID,A)=6.5E-2    6.4937E-02            2.00E-02                -6.3304E-05                -3.1652E-03
13 W(LIQUID,A)=9.3E-2    9.2741E-02            2.00E-02                -2.5863E-04                -1.2932E-02
20 W(LIQUID,A)=0.104     0.1038                2.00E-02                -1.5712E-04                -7.8558E-03
20 W(FCC,A)=3.8E-2       3.8189E-02            2.00E-02                1.8859E-04                9.4297E-03
21 W(LIQUID,A)=0.136     0.1366                2.00E-02                5.6062E-04                2.8031E-02
21 W(FCC,A)=4.7E-2       4.7082E-02            2.00E-02                8.1625E-05                4.0812E-03
22 W(LIQUID,A)=0.187     0.1868                2.00E-02                -2.2697E-04                -1.1349E-02
22 W(FCC,A)=5.9E-2       5.8972E-02            2.00E-02                -2.7839E-05                -1.3920E-03
23 W(LIQUID,A)=0.245     0.2450                2.00E-02                -1.9409E-05                -9.7046E-04
23 W(BCC#1,A)=8.5E-2     8.4995E-02            2.00E-02                -5.3382E-06                -2.6691E-04

```

PARROT:

PARROT: @@ Note that all other experiments are well fitted.

PARROT: @@ Try to improve by optimizing a little more...

PARROT: resc

PARROT: opt 30

Use 25 experiments, maximum is 2000

Use 664 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      4.83083572E-03
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      5.61883384E-03
1  1.0001E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      7.65790897E-03
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      5.28376043E-03
1  1.0000E+00    2  1.0000E+00    3  1.0001E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      5.25227156E-03
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      4.87673773E-03
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0001E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      4.83638927E-03
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0001E+00    7  1.0000E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      4.83105850E-03
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0001E+00    8  1.0000E+00    9  1.0000E+00

```

```

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      4.83476049E-03
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0001E+00    9  1.0000E+00

```

```

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      4.83108564E-03
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0001E+00

```

```

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      4.82945307E-03
1  1.0000E+00    2  1.0000E+00    3  9.9999E-01    4  9.9999E-01    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0000E+00    9  1.0001E+00

```

```

      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      4.82870256E-03
1  1.0000E+00    2  1.0000E+00    3  9.9998E-01    4  9.9998E-01    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0001E+00    9  1.0002E+00

```

```

      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      4.82775875E-03
1  1.0000E+00    2  1.0000E+00    3  9.9997E-01    4  9.9996E-01    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00    8  1.0001E+00    9  1.0004E+00

```

```

      AT THE     13 TH ITERATION WE HAVE THE SUM OF SQUARES      4.82617816E-03
1  1.0000E+00    2  1.0000E+00    3  9.9995E-01    4  9.9991E-01    5  1.0000E+00
6  1.0001E+00    7  1.0000E+00    8  1.0003E+00    9  1.0007E+00

```

```

      AT THE     14 TH ITERATION WE HAVE THE SUM OF SQUARES      4.82385483E-03
1  1.0000E+00    2  1.0000E+00    3  9.9990E-01    4  9.9985E-01    5  1.0000E+00
6  1.0002E+00    7  1.0000E+00    8  1.0005E+00    9  1.0013E+00

```

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 4.81986364E-03
1 1.0001E+00 2 1.0001E+00 3 9.9982E-01 4 9.9971E-01 5 1.0001E+00
6 1.0003E+00 7 1.0000E+00 8 1.0010E+00 9 1.0025E+00

AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 4.81442198E-03
1 1.0001E+00 2 1.0001E+00 3 9.9966E-01 4 9.9944E-01 5 1.0002E+00
6 1.0006E+00 7 9.9999E-01 8 1.0019E+00 9 1.0049E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 16 iterations
1 1.0001E+00 2 1.0001E+00 3 9.9966E-01 4 9.9944E-01 5 1.0002E+00
6 1.0006E+00 7 9.9999E-01 8 1.0019E+00 9 1.0049E+00

1 -3.1647E-02 2 -1.2983E-02 3 -4.4578E-03 4 1.6762E-03 5 -1.6612E-02
6 1.5808E-02 7 1.5173E-02 8 3.6678E-03 9 -3.9296E-03 10 2.0887E-02
11 -9.7709E-03 12 2.1440E-02 13 -8.4228E-03 14 -2.1134E-02 15 -6.4546E-03
16 -2.4108E-03 17 -1.2357E-02 18 -7.4116E-03 19 1.0311E-02 20 2.7942E-02
21 4.5683E-03 22 -1.2547E-02 23 -2.2732E-03 24 -1.4362E-03 25 -7.9621E-05

THE SUM OF SQUARES IS 4.81442198E-03
PARROT: 1-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:35:55

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 17

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03222961E+04	2.03192527E+04	2.03192527E+04	1.07718651E-01
V2	-2.93449014E+01	-2.93407339E+01	-2.93407339E+01	9.89624525E-02
V11	-2.17824331E+04	-2.17899144E+04	-2.17899144E+04	2.12028667E-01
V12	1.53193306E+01	1.53278493E+01	1.53278493E+01	3.47657566E-01
V15	2.41287695E+04	2.41251227E+04	2.41251227E+04	1.52846788E-01
V16	-8.25177708E+00	-8.24687790E+00	-8.24687790E+00	5.48129891E-01
V17	3.08380219E+03	3.08382020E+03	3.08382020E+03	2.65350522E-01
V19	2.21586119E+04	2.21176839E+04	2.21176839E+04	7.19986978E-01
V20	-7.05926518E+00	-7.02506538E+00	-7.02506538E+00	1.84443681E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 4.83083572E-03 TO 4.81442198E-03
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.00901374E-04

SYMBOL	STATUS	VALUE/FUNCTION	
FUNCTION R	298.15	8.31451000000000	; 6000 N REFO !
2 RTLN	20000000	+R*T*LN(1E-05*P)	
FUNCTION V1	298.15	20322.2960954001	; 6000 N REFO !
FUNCTION V2	298.15	-29.3449013535391	; 6000 N REFO !
FUNCTION V11	298.15	-21782.4331470453	; 6000 N REFO !
FUNCTION V12	298.15	15.3193306162049	; 6000 N REFO !
FUNCTION V15	298.15	24128.7695290274	; 6000 N REFO !
FUNCTION V16	298.15	-8.25177707962393	; 6000 N REFO !
FUNCTION V17	298.15	3083.80219468804	; 6000 N REFO !
FUNCTION V19	298.15	22158.6118969593	; 6000 N REFO !
FUNCTION V20	298.15	-7.05926517686829	; 6000 N REFO !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====

G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====

G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====

L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1193.	10.	-0.3165	-3.1647E-02
1 W(LIQUID,B)=0.408	0.4077	2.00E-02	-2.5966E-04	-1.2983E-02
1 W(BCC#1,B)=0.13	0.1299	2.00E-02	-8.9156E-05	-4.4578E-03
2 T=1341	1341.	10.	1.6762E-02	1.6762E-03
2 HTR=3727	3719.	5.00E+02	-8.306	-1.6612E-02
3 T=1049	1049.	10.	0.1581	1.5808E-02
3 W(LIQUID,A)=0.27	0.2703	2.00E-02	3.0346E-04	1.5173E-02
3 W(BCC#1,A)=9.3E-2	9.3073E-02	2.00E-02	7.3356E-05	3.6678E-03
5 T=726	726.0	10.	-3.9296E-02	-3.9296E-03
5 X(BCC#1,B)=3.7E-2	3.7418E-02	2.00E-02	4.1774E-04	2.0887E-02
5 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.9542E-04	-9.7709E-03
6 X(BCC#1,B)=3.7E-2	3.7429E-02	2.00E-02	4.2879E-04	2.1440E-02

6 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.6846E-04	-8.4228E-03
10 W(LIQUID,A)=2E-2	1.9577E-02	2.00E-02	-4.2268E-04	-2.1134E-02
11 W(LIQUID,A)=4.2E-2	4.1871E-02	2.00E-02	-1.2909E-04	-6.4546E-03
12 W(LIQUID,A)=6.5E-2	6.4952E-02	2.00E-02	-4.8216E-05	-2.4108E-03
13 W(LIQUID,A)=9.3E-2	9.2753E-02	2.00E-02	-2.4714E-04	-1.2357E-02
20 W(LIQUID,A)=0.104	0.1039	2.00E-02	-1.4823E-04	-7.4116E-03
20 W(FCC,A)=3.8E-2	3.8206E-02	2.00E-02	2.0622E-04	1.0311E-02
21 W(LIQUID,A)=0.136	0.1366	2.00E-02	5.5883E-04	2.7942E-02
21 W(FCC,A)=4.7E-2	4.7091E-02	2.00E-02	9.1366E-05	4.5683E-03
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.5095E-04	-1.2547E-02
22 W(FCC,A)=5.9E-2	5.8955E-02	2.00E-02	-4.5463E-05	-2.2732E-03
23 W(LIQUID,A)=0.245	0.2450	2.00E-02	-2.8725E-05	-1.4362E-03
23 W(BCC#1,A)=8.5E-2	8.4998E-02	2.00E-02	-1.5924E-06	-7.9621E-05

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0.003 s
Found the set of lowest grid points in 0.000 s
Calculated POLY solution 0.004 s, total time 0.007 s
POLY: save tcex36 y

```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

```

```

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

```

```

Phase region boundary 2 at: 7.141E-01 3.000E+02
BCC#1

```



```

** BCC#2
Calculated.                14 equilibria

Phase region boundary  3 at:  6.821E-01  7.260E+02
** A2B
  BCC#1
** BCC#2

Phase region boundary  4 at:  3.626E-01  7.260E+02
** A2B
  BCC#1
Calculated.                15 equilibria

Phase region boundary  5 at:  3.769E-01  1.193E+03
** LIQUID
** A2B
  BCC#1

Phase region boundary  6 at:  2.826E-01  1.193E+03
** LIQUID
  BCC#1
Calculated                26 equilibria

Phase region boundary  7 at:  4.863E-01  1.193E+03
** LIQUID
  A2B
Calculated.                33 equilibria

Phase region boundary  8 at:  6.500E-01  1.049E+03
** LIQUID
  A2B
** BCC#1

Phase region boundary  9 at:  7.642E-01  1.049E+03
  A2B
** BCC#1
Calculated.                11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.276E-01  1.049E+03
  LIQUID
** BCC#1
Calculated.                8 equilibria

Phase region boundary 11 at:  8.751E-01  1.204E+03
  LIQUID
** BCC#1
** FCC

Phase region boundary 12 at:  8.804E-01  1.204E+03
  LIQUID
** FCC
Calculated                32 equilibria

Phase region boundary 13 at:  9.357E-01  1.204E+03
  BCC#1
** FCC
Calculated                24 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
** BCC#1
  BCC#2
Calculated..                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
** BCC#1
  BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 23 at: 7.140E-01 3.100E+02
** BCC#1
   BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
** BCC#1
   BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
** A2B
   BCC#1
Calculated 10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
** A2B
   BCC#1
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
** A2B
   BCC#1
Calculated. 14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.912E-01 7.700E+02
** A2B
   BCC#1
Calculated 10 equilibria

Phase region boundary 29 at: 7.912E-01 7.700E+02
** A2B
   BCC#1
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.912E-01 7.700E+02
** A2B
   BCC#1
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
** LIQUID
   BCC#1
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
** LIQUID
   BCC#1
Calculated 26 equilibria

Phase region boundary 33 at: 8.860E-01 1.230E+03
** LIQUID
   FCC
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.860E-01 1.230E+03
** LIQUID
   FCC
Calculated 29 equilibria

Phase region boundary 35 at: 6.414E-03 1.397E+03
LIQUID
** BCC#1
Calculated 12 equilibria

Phase region boundary 36 at: 6.414E-03 1.397E+03
LIQUID
** BCC#1
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.298E-01 1.244E+03
LIQUID
** BCC#1
Calculated 18 equilibria

Phase region boundary 38 at: 2.298E-01 1.244E+03
LIQUID
** BCC#1
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated. 14 equilibria
Terminating at known equilibrium

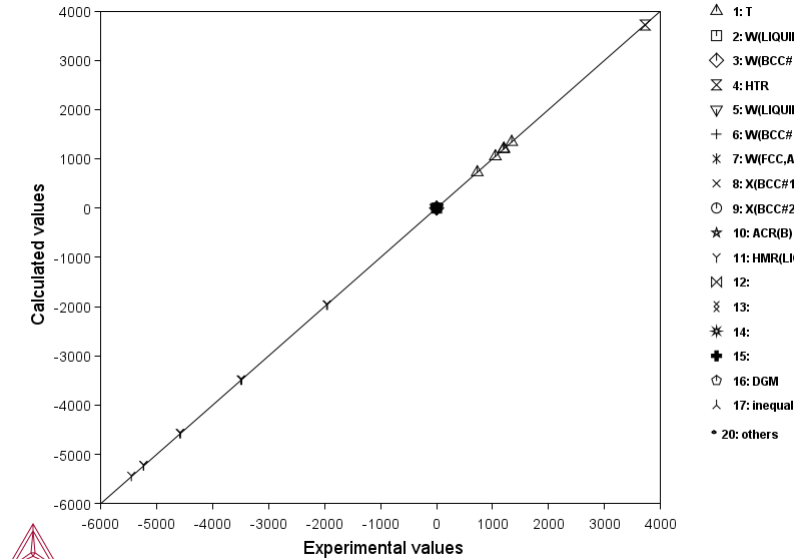
Phase region boundary 40 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated 10 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping 1 seconds

```

POLY: post
POST: s-l d
POST: plot



POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

PARROT VERSION 5.3

Global minimization used as test only

PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid

PARROT: @@ at high B. Restore equilibrium 4 on the POP file

PARROT: ed

ED_EXP: read 1

ED_EXP: s-e 4

Equilibrium number 4 , label AINV

ED_EXP: s-we 1

Equilibria (range) or label(s) /PRESENT/: PRESENT

ED_EXP: s-a-s

T /1204.42469/: 1200

Automatic start values for phase constituents? /N/: N

Phase LIQUID

Major constituent(s) /b/: b

Phase BCC

Major constituent(s) /b/: b

Phase FCC

Major constituent(s) /b/: b

ED_EXP:

ED_EXP: c-e

Testing result with global minimization

13 ITS, CPU TIME USED 0 SECONDS

ED_EXP: l-e

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:

P=101325

FIXED PHASES

LIQUID=1 BCC#1=1 FCC=1

DEGREES OF FREEDOM 0

Temperature 1203.82 K (930.67 C), Pressure 1.013250E+05

Number of moles of components 3.00000E+00, Mass in grams 1.30105E+02

Total Gibbs energy -9.75086E+03, Enthalpy 1.98626E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
A	6.6316E-01	1.0194E-01	3.9443E-01	-9.3116E+03	SER
B	2.3368E+00	8.9806E-01	8.5823E-01	-1.5302E+03	SER

FCC

Status FIXED

Driving force 0.0000E+00

Moles 1.0000E+00, Mass 4.5889E+01, Volume fraction 0.0000E+00

Mass fractions:

B 9.40269E-01 A 5.97312E-02

BCC#1

Status FIXED

Driving force 0.0000E+00

Moles 1.0000E+00, Mass 4.5321E+01, Volume fraction 0.0000E+00

Mass fractions:

B 9.31169E-01 A 6.88312E-02

LIQUID

Status FIXED

Driving force 0.0000E+00

Moles 1.0000E+00, Mass 3.8896E+01, Volume fraction 0.0000E+00

Mass fractions:

B 8.09680E-01 A 1.90320E-01

EXPERIMENT T=1203:DT \$1203.82:10 NO=1

EXPERIMENT W(LIQUID,A)=0.19:DX \$0.19032:2E-2 NO=2

EXPERIMENT W(BCC#1,A)=6.9E-2:DX \$6.88312E-2:2E-2 NO=3

EXPERIMENT W(FCC,A)=6E-2:DX \$5.97312E-2:2E-2 NO=4

ED_EXP: @@ Now equilibrium 4 is on the high B side

ED_EXP: save

ED_EXP: ba

PARROT: resc

PARROT: opt 0

Use 29 experiments, maximum is 2000

Use 740 real workspace, maximum is 50000

PARROT: l-r C SCREEN

=====

*** SUCCESSFUL OPTIMIZATION. ***
 NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
 MINIMUM SAVE ON FILE: Y
 ERROR FOR INEQUALITIES = 1.00000000E+00
 RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
 MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
 ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03222961E+04	2.03222961E+04	2.03222961E+04	0.00000000E+00
V2	-2.93449014E+01	-2.93449014E+01	-2.93449014E+01	0.00000000E+00
V11	-2.17824331E+04	-2.17824331E+04	-2.17824331E+04	0.00000000E+00
V12	1.53193306E+01	1.53193306E+01	1.53193306E+01	0.00000000E+00
V15	2.41287695E+04	2.41287695E+04	2.41287695E+04	0.00000000E+00
V16	-8.25177708E+00	-8.25177708E+00	-8.25177708E+00	0.00000000E+00
V17	3.08380219E+03	3.08380219E+03	3.08380219E+03	0.00000000E+00
V19	2.21586119E+04	2.21586119E+04	2.21586119E+04	0.00000000E+00
V20	-7.05926518E+00	-7.05926518E+00	-7.05926518E+00	0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.20075115E-02
 DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 6.00375577E-04

SYMBOL	STATUS	VALUE/FUNCTION	
FUNCTION R	298.15	8.314510000000000	; 6000 N REF0 !
2 RTLN P	20000000	+R*T*LN(1E-05*P)	
FUNCTION V1	298.15	20322.2960954001	; 6000 N REF0 !
FUNCTION V2	298.15	-29.3449013535391	; 6000 N REF0 !
FUNCTION V11	298.15	-21782.4331470453	; 6000 N REF0 !
FUNCTION V12	298.15	15.3193306162049	; 6000 N REF0 !
FUNCTION V15	298.15	24128.7695290274	; 6000 N REF0 !
FUNCTION V16	298.15	-8.25177707962393	; 6000 N REF0 !
FUNCTION V17	298.15	3083.80219468804	; 6000 N REF0 !
FUNCTION V19	298.15	22158.6118969593	; 6000 N REF0 !
FUNCTION V20	298.15	-7.05926517686829	; 6000 N REF0 !

LIQUID:L (A,B)1.0
 - This phase is a liquid

==== [A] ====
 G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
 G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
 L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
 L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
 DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
 HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1193.	10.	-0.3165	-3.1647E-02
1 W(LIQUID,B)=0.408	0.4077	2.00E-02	-2.5966E-04	-1.2983E-02
1 W(BCC#1,B)=0.13	0.1299	2.00E-02	-8.9156E-05	-4.4578E-03
2 T=1341	1341.	10.	1.6762E-02	1.6762E-03
2 HTR=3727	3719.	5.00E+02	-8.306	-1.6612E-02
3 T=1049	1049.	10.	0.1581	1.5808E-02
3 W(LIQUID,A)=0.27	0.2703	2.00E-02	3.0346E-04	1.5173E-02
3 W(BCC#1,A)=9.3E-2	9.3073E-02	2.00E-02	7.3356E-05	3.6678E-03
4 T=1203	1204.	10.	0.8177	8.1767E-02
4 W(LIQUID,A)=0.19	0.1903	2.00E-02	3.1961E-04	1.5981E-02
4 W(BCC#1,A)=6.9E-2	6.8831E-02	2.00E-02	-1.6881E-04	-8.4403E-03
4 W(FCC,A)=6E-2	5.9731E-02	2.00E-02	-2.6879E-04	-1.3439E-02
5 T=726	726.0	10.	-3.9296E-02	-3.9296E-03
5 X(BCC#1,B)=3.7E-2	3.7418E-02	2.00E-02	4.1774E-04	2.0887E-02
5 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.9542E-04	-9.7709E-03
6 X(BCC#1,B)=3.7E-2	3.7429E-02	2.00E-02	4.2879E-04	2.1440E-02
6 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.6846E-04	-8.4228E-03
10 W(LIQUID,A)=2E-2	1.9577E-02	2.00E-02	-4.2268E-04	-2.1134E-02
11 W(LIQUID,A)=4.2E-2	4.1871E-02	2.00E-02	-1.2909E-04	-6.4546E-03
12 W(LIQUID,A)=6.5E-2	6.4952E-02	2.00E-02	-4.8216E-05	-2.4108E-03
13 W(LIQUID,A)=9.3E-2	9.2753E-02	2.00E-02	-2.4714E-04	-1.2357E-02
20 W(LIQUID,A)=0.104	0.1039	2.00E-02	-1.4823E-04	-7.4116E-03
20 W(FCC,A)=3.8E-2	3.8206E-02	2.00E-02	2.0622E-04	1.0311E-02
21 W(LIQUID,A)=0.136	0.1366	2.00E-02	5.5883E-04	2.7942E-02
21 W(FCC,A)=4.7E-2	4.7091E-02	2.00E-02	9.1366E-05	4.5683E-03
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.5095E-04	-1.2547E-02
22 W(FCC,A)=5.9E-2	5.8955E-02	2.00E-02	-4.5463E-05	-2.2732E-03
23 W(LIQUID,A)=0.245	0.2450	2.00E-02	-2.8725E-05	-1.4362E-03
23 W(BCC#1,A)=8.5E-2	8.4998E-02	2.00E-02	-1.5924E-06	-7.9621E-05

PARROT:
 PARROT:Hit RETURN to continue
 PARROT: opt 30
 Use 29 experiments, maximum is 2000

Use 740 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

```

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.20075115E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.28462661E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.47298698E-02
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.22549263E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.26042028E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.02677648E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.09407110E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.04095798E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.16224820E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80123906E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0001E+00

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80665190E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 9.9998E-01 5 1.0003E+00
6 9.9991E-01 7 9.9998E-01 8 9.9983E-01 9 1.0002E+00

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 6.70490337E-03
1 1.0000E+00 2 1.0000E+00 3 9.9993E-01 4 9.9987E-01 5 1.0003E+00
6 1.0000E+00 7 9.9994E-01 8 9.9988E-01 9 1.0004E+00

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.58115292E-03
1 1.0001E+00 2 1.0001E+00 3 9.9977E-01 4 9.9963E-01 5 1.0003E+00
6 1.0002E+00 7 9.9986E-01 8 9.9999E-01 9 1.0009E+00

      AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 6.40884407E-03
1 1.0002E+00 2 1.0002E+00 3 9.9946E-01 4 9.9913E-01 5 1.0004E+00
6 1.0005E+00 7 9.9969E-01 8 1.0002E+00 9 1.0018E+00

      AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 6.18133787E-03
1 1.0005E+00 2 1.0005E+00 3 9.9885E-01 4 9.9815E-01 5 1.0004E+00
6 1.0012E+00 7 9.9936E-01 8 1.0007E+00 9 1.0036E+00

      AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 5.98610084E-03
1 1.0011E+00 2 1.0010E+00 3 9.9763E-01 4 9.9616E-01 5 1.0006E+00
6 1.0025E+00 7 9.9869E-01 8 1.0017E+00 9 1.0072E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 15 iterations
1 1.0011E+00 2 1.0010E+00 3 9.9763E-01 4 9.9616E-01 5 1.0006E+00
6 1.0025E+00 7 9.9869E-01 8 1.0017E+00 9 1.0072E+00

1 -3.4102E-02 2 -1.5978E-02 3 -5.3325E-03 4 2.9266E-03 5 -7.9591E-03
6 1.1423E-02 7 1.1769E-02 8 3.4022E-03 9 7.8408E-03 10 2.9223E-02
11 -5.9126E-03 12 -5.6076E-03 13 -3.2819E-03 14 2.3212E-02 15 -1.0523E-02
16 2.3674E-02 17 -9.3964E-03 18 -2.1057E-02 19 -6.4509E-03 20 -2.6190E-03
21 -1.2918E-02 22 -8.1194E-03 23 1.2186E-02 24 2.6873E-02 25 7.3889E-03
26 -1.3669E-02 27 2.3055E-03 28 -7.0926E-03 29 -1.8890E-03
```

THE SUM OF SQUARES IS 5.98610084E-03
PARROT: l-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:36:19

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 16

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03437437E+04	2.03222961E+04	2.03222961E+04	1.02353969E-01
V2	-2.93745531E+01	-2.93449014E+01	-2.93449014E+01	9.37147854E-02
V11	-2.17307923E+04	-2.17824331E+04	-2.17824331E+04	2.00613298E-01
V12	1.52604511E+01	1.53193306E+01	1.53193306E+01	3.28967060E-01
V15	2.41421943E+04	2.41287695E+04	2.41287695E+04	1.34897011E-01

V16 -8.27252866E+00 -8.25177708E+00 -8.25177708E+00 4.84759622E-01
V17 3.07975241E+03 3.08380219E+03 3.08380219E+03 2.31442375E-01
V19 2.21953870E+04 2.21586119E+04 2.21586119E+04 5.66892740E-01
V20 -7.11044476E+00 -7.05926518E+00 -7.05926518E+00 1.53808382E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.20075115E-02 TO 5.98610084E-03
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99305042E-04

SYMBOL	STATUS	VALUE/FUNCTION	
FUNCTION R	298.15	8.31451000000000	; 6000 N REFO !
2 RTINP	20000000	+R*T*LN(1E-05*P)	
FUNCTION V1	298.15	20343.7437470016	; 6000 N REFO !
FUNCTION V2	298.15	-29.3745530843477	; 6000 N REFO !
FUNCTION V11	298.15	-21730.7922542636	; 6000 N REFO !
FUNCTION V12	298.15	15.2604511121194	; 6000 N REFO !
FUNCTION V15	298.15	24142.1943065085	; 6000 N REFO !
FUNCTION V16	298.15	-8.27252865883767	; 6000 N REFO !
FUNCTION V17	298.15	3079.75241112698	; 6000 N REFO !
FUNCTION V19	298.15	22195.3870168468	; 6000 N REFO !
FUNCTION V20	298.15	-7.11044475557365	; 6000 N REFO !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====
G(LIQUID,A;0) 500 +14000-10*T; 2000 N

==== [B] ====
G(LIQUID,B;0) 500 +18000-12*T; 2000 N

==== [A, B] ====
L(LIQUID,A,B;0) 500 +V11+V12*T; 2000 N
L(LIQUID,A,B;1) 500 +V13+V14*T; 2000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1193.	10.	-0.3410	-3.4102E-02
1 W(LIQUID,B)=0.408	0.4077	2.00E-02	-3.1956E-04	-1.5978E-02
1 W(BCC#1,B)=0.13	0.1299	2.00E-02	-1.0665E-04	-5.3325E-03
2 T=1341	1341.	10.	2.9266E-02	2.9266E-03
2 HTR=3727	3723.	5.00E+02	-3.980	-7.9591E-03
3 T=1049	1049.	10.	0.1142	1.1423E-02
3 W(LIQUID,A)=0.27	0.2702	2.00E-02	2.3539E-04	1.1769E-02
3 W(BCC#1,A)=9.3E-2	9.3068E-02	2.00E-02	6.8043E-05	3.4022E-03
4 T=1203	1203.	10.	7.8408E-02	7.8408E-03
4 W(LIQUID,A)=0.19	0.1906	2.00E-02	5.8447E-04	2.9223E-02
4 W(BCC#1,A)=6.9E-2	6.8882E-02	2.00E-02	-1.1825E-04	-5.9126E-03
4 W(FCC,A)=6E-2	5.9888E-02	2.00E-02	-1.1215E-04	-5.6076E-03
5 T=726	726.0	10.	-3.2819E-02	-3.2819E-03
5 X(BCC#1,B)=3.7E-2	3.7464E-02	2.00E-02	4.6424E-04	2.3212E-02
5 X(BCC#2,A)=0.114	0.1138	2.00E-02	-2.1046E-04	-1.0523E-02
6 X(BCC#1,B)=3.7E-2	3.7473E-02	2.00E-02	4.7348E-04	2.3674E-02
6 X(BCC#2,A)=0.114	0.1138	2.00E-02	-1.8793E-04	-9.3964E-03
10 W(LIQUID,A)=2E-2	1.9579E-02	2.00E-02	-4.2114E-04	-2.1057E-02
11 W(LIQUID,A)=4.2E-2	4.1871E-02	2.00E-02	-1.2902E-04	-6.4509E-03
12 W(LIQUID,A)=6.5E-2	6.4948E-02	2.00E-02	-5.2380E-05	-2.6190E-03
13 W(LIQUID,A)=9.3E-2	9.2742E-02	2.00E-02	-2.5836E-04	-1.2918E-02
20 W(LIQUID,A)=0.104	0.1038	2.00E-02	-1.6239E-04	-8.1194E-03
20 W(FCC,A)=3.8E-2	3.8244E-02	2.00E-02	2.4372E-04	1.2186E-02
21 W(LIQUID,A)=0.136	0.1365	2.00E-02	5.3747E-04	2.6873E-02
21 W(FCC,A)=4.7E-2	4.7148E-02	2.00E-02	1.4778E-04	7.3889E-03
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.7337E-04	-1.3669E-02
22 W(FCC,A)=5.9E-2	5.9046E-02	2.00E-02	4.6110E-05	2.3055E-03
23 W(LIQUID,A)=0.245	0.2449	2.00E-02	-1.4185E-04	-7.0926E-03
23 W(BCC#1,A)=8.5E-2	8.4962E-02	2.00E-02	-3.7780E-05	-1.8890E-03

PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03437437E+04	2.03222961E+04	2.03222961E+04	1.02353969E-01
V2	-2.93745531E+01	-2.93449014E+01	-2.93449014E+01	9.37147854E-02
V11	-2.17307923E+04	-2.17824331E+04	-2.17824331E+04	2.00613298E-01
V12	1.52604511E+01	1.53193306E+01	1.53193306E+01	3.28967060E-01
V15	2.41421943E+04	2.41287695E+04	2.41287695E+04	1.34897011E-01
V16	-8.27252866E+00	-8.25177708E+00	-8.25177708E+00	4.84759622E-01
V17	3.07975241E+03	3.08380219E+03	3.08380219E+03	2.31442375E-01
V19	2.21953870E+04	2.21586119E+04	2.21586119E+04	5.66892740E-01
V20	-7.11044476E+00	-7.05926518E+00	-7.05926518E+00	1.53808382E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.20075115E-02 TO 5.98610084E-03
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99305042E-04

PARROT: s-o-v 11-12

PARROT: ed

ED_EXP: read 1

ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix	phases	or comments
1	AINV	2	1.	1192.7			LIQUID	A2B BCC
2	AINV	2	1.	1341.0			LIQUID	A2B
3	AINV	2	1.	1049.1			LIQUID	A2B BCC
4	AINV	2	1.	1203.1			LIQUID	BCC FCC

```

5 AINV 2 1. 726.0 A2B BCC BCC#2
6 AINV 2 1. 726.0 BCC BCC#2
10 ALF 2 1. 1594.0 LIQUID FCC
11 ALF 2 1. 1548.0 LIQUID FCC
12 ALF 2 1. 1499.0 LIQUID FCC
13 ALF 2 1. 1438.0 LIQUID FCC
20 ATIE 2 1. 1413.0 LIQUID FCC
21 ATIE 2 1. 1337.0 LIQUID FCC
22 ATIE 2 1. 1213.0 LIQUID FCC
23 ATIE 2 1. 1100.0 LIQUID BCC
100 AA < unused > 1573.0 LIQUID
101 AA < unused > 1573.0 LIQUID
102 AA < unused > 1573.0 LIQUID
103 AA < unused > 1573.0 LIQUID
104 AA < unused > 1573.0 LIQUID
105 AA < unused > 1573.0 LIQUID
106 AA < unused > 1573.0 LIQUID
107 AA < unused > 1573.0 LIQUID
108 AA < unused > 1573.0 LIQUID
110 AH < unused > 1773.0 LIQUID
111 AH < unused > 1773.0 LIQUID
112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID

```

ED_EXP: s-we 1 100-118

ED_EXP: s-e 1

Equilibrium number 1 , label AINV

ED_EXP: c-a

Eq	Lab	Iter	Weight	Temp	Exp	Fix	phases	or comments
1	AINV	2	1.	1192.7		LIQUID	A2B BCC	
2	AINV	2	1.	1341.0		LIQUID	A2B	
3	AINV	2	1.	1049.1		LIQUID	A2B BCC	
4	AINV	2	1.	1203.1		LIQUID	BCC FCC	
5	AINV	2	1.	726.0		A2B BCC	BCC#2	
6	AINV	2	1.	726.0		BCC	BCC#2	
10	ALF	2	1.	1594.0		LIQUID	FCC	
11	ALF	2	1.	1548.0		LIQUID	FCC	
12	ALF	2	1.	1499.0		LIQUID	FCC	
13	ALF	2	1.	1438.0		LIQUID	FCC	
20	ATIE	2	1.	1413.0		LIQUID	FCC	
21	ATIE	2	1.	1337.0		LIQUID	FCC	
22	ATIE	2	1.	1213.0		LIQUID	FCC	
23	ATIE	2	1.	1100.0		LIQUID	BCC	
100	AA	2	1.	1573.0		LIQUID		
101	AA	2	1.	1573.0		LIQUID		
102	AA	2	1.	1573.0		LIQUID		
103	AA	2	1.	1573.0		LIQUID		
104	AA	2	1.	1573.0		LIQUID		
105	AA	2	1.	1573.0		LIQUID		
106	AA	2	1.	1573.0		LIQUID		
107	AA	2	1.	1573.0		LIQUID		
108	AA	2	1.	1573.0		LIQUID		
110	AH	2	1.	1773.0		LIQUID		
111	AH	2	1.	1773.0		LIQUID		
112	AH	2	1.	1773.0		LIQUID		
113	AH	2	1.	1773.0		LIQUID		
114	AH	2	1.	1773.0		LIQUID		
115	AH	2	1.	1773.0		LIQUID		
116	AH	2	1.	1773.0		LIQUID		
117	AH	2	1.	1773.0		LIQUID		
118	AH	2	1.	1773.0		LIQUID		

ED_EXP: save

ED_EXP: ba

PARROT: opt 30

Use 47 experiments, maximum is 2000
 Use 1082 real workspace, maximum is 50000
 The following output is provided by subroutine VA05A

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      8.37679617E-02
1  1.0011E+00  2  1.0010E+00  3  1.0000E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      8.45969411E-02
1  1.0012E+00  2  1.0010E+00  3  1.0000E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      8.64911748E-02
1  1.0011E+00  2  1.0010E+00  3  1.0000E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      8.29336311E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      8.34054122E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0001E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      8.32698547E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0007E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      8.29176401E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      8.29247254E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9879E-01  8  1.0017E+00  9  1.0072E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      8.31153392E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9869E-01  8  1.0018E+00  9  1.0072E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      8.28951450E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9869E-01  8  1.0017E+00  9  1.0073E+00

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      8.22514632E-02
1  1.0010E+00  2  1.0011E+00  3  1.0001E+00  4  9.9998E-01  5  1.0006E+00
6  1.0027E+00  7  9.9870E-01  8  1.0016E+00  9  1.0073E+00

```

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 8.16971362E-02
1 1.0011E+00 2 1.0011E+00 3 1.0002E+00 4 9.9994E-01 5 1.0006E+00
6 1.0027E+00 7 9.9871E-01 8 1.0016E+00 9 1.0073E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 8.10070099E-02
1 1.0010E+00 2 1.0011E+00 3 1.0002E+00 4 9.9990E-01 5 1.0006E+00
6 1.0029E+00 7 9.9874E-01 8 1.0015E+00 9 1.0072E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 8.00973997E-02
1 1.0011E+00 2 1.0011E+00 3 1.0002E+00 4 9.9981E-01 5 1.0006E+00
6 1.0032E+00 7 9.9880E-01 8 1.0014E+00 9 1.0070E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 7.86823948E-02
1 1.0011E+00 2 1.0012E+00 3 1.0002E+00 4 9.9966E-01 5 1.0008E+00
6 1.0038E+00 7 9.9892E-01 8 1.0011E+00 9 1.0067E+00

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 7.64152026E-02
1 1.0012E+00 2 1.0014E+00 3 1.0002E+00 4 9.9936E-01 5 1.0010E+00
6 1.0050E+00 7 9.9916E-01 8 1.0004E+00 9 1.0060E+00

AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 7.28312654E-02
1 1.0015E+00 2 1.0017E+00 3 1.0002E+00 4 9.9879E-01 5 1.0014E+00
6 1.0074E+00 7 9.9965E-01 8 9.9923E-01 9 1.0046E+00

AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 6.84499747E-02
1 1.0019E+00 2 1.0024E+00 3 1.0002E+00 4 9.9764E-01 5 1.0023E+00
6 1.0124E+00 7 1.0006E+00 8 9.9680E-01 9 1.0019E+00

AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 6.73854820E-02
1 1.0023E+00 2 1.0029E+00 3 1.0001E+00 4 9.9672E-01 5 1.0031E+00
6 1.0163E+00 7 1.0014E+00 8 9.9501E-01 9 1.0002E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 18 iterations
1 1.0023E+00 2 1.0029E+00 3 1.0001E+00 4 9.9672E-01 5 1.0031E+00
6 1.0163E+00 7 1.0014E+00 8 9.9501E-01 9 1.0002E+00
1 -5.7838E-02 2 -9.3605E-03 3 1.4183E-02 4 2.0794E-02 5 -2.5747E-02
6 -5.2100E-02 7 1.9269E-02 8 2.6822E-02 9 1.3105E-02 10 2.7154E-02
11 8.7707E-03 12 1.3244E-02 13 -4.8660E-02 14 2.1790E-02 15 4.7290E-03
16 2.8670E-02 17 2.1551E-02 18 -2.2040E-02 19 -8.2402E-03 20 -4.9755E-03
21 -1.5646E-02 22 -1.0901E-02 23 1.5213E-02 24 2.4270E-02 25 1.4695E-02
26 -1.4885E-02 27 2.0283E-02 28 -1.2750E-02 29 1.5398E-02 30 -9.5909E-03
31 -1.6832E-02 32 2.7435E-02 33 8.7018E-02 34 1.2433E-01 35 1.0168E-01
36 -1.7320E-02 37 7.0577E-02 38 -1.9477E-02 39 1.6078E-02 40 4.5471E-02
41 4.8181E-02 42 4.6207E-02 43 4.1549E-02 44 3.4207E-02 45 2.2181E-02
46 7.4714E-03 47 -1.1922E-02

THE SUM OF SQUARES IS 6.73854820E-02
PARROT: 1-r C SCREEN

=====

OUTPUT FROM P A R R O T. DATE 2025. 5.12 9:36:19

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 19

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03690187E+04	2.03222961E+04	2.03222961E+04	2.99244829E-02
V2	-2.94289046E+01	-2.93449014E+01	-2.93449014E+01	2.27402510E-02
V11	-2.17329018E+04	-2.17307923E+04	-2.17307923E+04	3.48515483E-02
V12	1.52104284E+01	1.52604511E+01	1.52604511E+01	5.50818393E-02
V15	2.42024493E+04	2.41287695E+04	2.41287695E+04	8.32414822E-02
V16	-8.38635212E+00	-8.25177708E+00	-8.25177708E+00	2.56685209E-01
V17	3.08808170E+03	3.08380219E+03	3.08380219E+03	2.30230278E-01
V19	2.20479877E+04	2.21586119E+04	2.21586119E+04	4.86430870E-01
V20	-7.06074722E+00	-7.05926518E+00	-7.05926518E+00	1.22189124E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.37679617E-02 TO 6.73854820E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77330216E-03

SYMBOL	STATUS	VALUE/FUNCTION	
FUNCTION R	298.15	8.314510000000000	; 6000 N REF0 !
2 RTLN	20000000	+R*T*LN(1E-05*P)	
FUNCTION V1	298.15	20369.0186609360	; 6000 N REF0 !
FUNCTION V2	298.15	-29.4289045595743	; 6000 N REF0 !
FUNCTION V11	298.15	-21732.9018403046	; 6000 N REF0 !
FUNCTION V12	298.15	15.2104284441835	; 6000 N REF0 !
FUNCTION V15	298.15	24202.4492751557	; 6000 N REF0 !
FUNCTION V16	298.15	-8.38635211765797	; 6000 N REF0 !
FUNCTION V17	298.15	3088.08169510659	; 6000 N REF0 !
FUNCTION V19	298.15	22047.9876616182	; 6000 N REF0 !
FUNCTION V20	298.15	-7.06074721568414	; 6000 N REF0 !

LIQUID:L (A,B)1.0
- This phase is a liquid

==== [A] ====

G(LIQUID,A;0) 500 +14000-10*T; 2000 N


```
==== [B] ====
G(LIQUID,B;0)                500 +18000-12*T;                2000 N
```

```
==== [A, B] ====
L(LIQUID,A,B;0)              500 +V11+V12*T;                2000 N
L(LIQUID,A,B;1)              500 +V13+V14*T;                2000 N
```

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1192.	10.	-0.5784	-5.7838E-02
1 W(LIQUID,B)=0.408	0.4078	2.00E-02	-1.8721E-04	-9.3605E-03
1 W(BCC#1,B)=0.13	0.1303	2.00E-02	2.8366E-04	1.4183E-02
2 T=1341	1341.	10.	0.2079	2.0794E-02
2 HTR=3727	3714.	5.00E+02	-12.87	-2.5747E-02
3 T=1049	1048.	10.	-0.5210	-5.2100E-02
3 W(LIQUID,A)=0.27	0.2704	2.00E-02	3.8539E-04	1.9269E-02
3 W(BCC#1,A)=9.3E-2	9.3536E-02	2.00E-02	5.3645E-04	2.6822E-02
4 T=1203	1203.	10.	0.1311	1.3105E-02
4 W(LIQUID,A)=0.19	0.1905	2.00E-02	5.4309E-04	2.7154E-02
4 W(BCC#1,A)=6.9E-2	6.9175E-02	2.00E-02	1.7541E-04	8.7707E-03
4 W(FCC,A)=6E-2	6.0265E-02	2.00E-02	2.6487E-04	1.3244E-02
5 T=726	725.5	10.	-0.4866	-4.8660E-02
5 X(BCC#1,B)=3.7E-2	3.7436E-02	2.00E-02	4.3580E-04	2.1790E-02
5 X(BCC#2,A)=0.114	0.1141	2.00E-02	9.4580E-05	4.7290E-03
6 X(BCC#1,B)=3.7E-2	3.7573E-02	2.00E-02	5.7340E-04	2.8670E-02
6 X(BCC#2,A)=0.114	0.1144	2.00E-02	4.3102E-04	2.1551E-02
10 W(LIQUID,A)=2E-2	1.9559E-02	2.00E-02	-4.4080E-04	-2.2040E-02
11 W(LIQUID,A)=4.2E-2	4.1835E-02	2.00E-02	-1.6480E-04	-8.2402E-03
12 W(LIQUID,A)=6.5E-2	6.4900E-02	2.00E-02	-9.9511E-05	-4.9755E-03
13 W(LIQUID,A)=9.3E-2	9.2687E-02	2.00E-02	-3.1291E-04	-1.5646E-02
20 W(LIQUID,A)=0.104	0.1038	2.00E-02	-2.1801E-04	-1.0901E-02
20 W(FCC,A)=3.8E-2	3.8304E-02	2.00E-02	3.0425E-04	1.5213E-02
21 W(LIQUID,A)=0.136	0.1365	2.00E-02	4.8540E-04	2.4270E-02
21 W(FCC,A)=4.7E-2	4.7294E-02	2.00E-02	2.9390E-04	1.4695E-02
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.9770E-04	-1.4885E-02
22 W(FCC,A)=5.9E-2	5.9406E-02	2.00E-02	4.0566E-04	2.0283E-02
23 W(LIQUID,A)=0.245	0.2447	2.00E-02	-2.5500E-04	-1.2750E-02
23 W(BCC#1,A)=8.5E-2	8.5308E-02	2.00E-02	3.0796E-04	1.5398E-02
100 ACR(B)=0.94	0.9397	2.85E-02	-2.7299E-04	-9.5909E-03
101 ACR(B)=0.84	0.8395	2.82E-02	-4.7444E-04	-1.6832E-02
102 ACR(B)=0.74	0.7408	2.81E-02	7.6969E-04	2.7435E-02
103 ACR(B)=0.64	0.6424	2.81E-02	2.4423E-03	8.7018E-02
104 ACR(B)=0.54	0.5435	2.82E-02	3.5094E-03	0.1243
105 ACR(B)=0.44	0.4429	2.85E-02	2.9021E-03	0.1017
106 ACR(B)=0.34	0.3395	2.90E-02	-5.0277E-04	-1.7320E-02
107 ACR(B)=0.23	0.2321	2.97E-02	2.0965E-03	7.0577E-02
108 ACR(B)=0.12	0.1194	3.06E-02	-5.9601E-04	-1.9477E-02
110 HMR(LIQUID)=-1964	-1956.	5.00E+02	8.039	1.6078E-02
111 HMR(LIQUID)=-3500	-3477.	5.00E+02	22.74	4.5471E-02
112 HMR(LIQUID)=-4588	-4564.	5.00E+02	24.09	4.8181E-02
113 HMR(LIQUID)=-5239	-5216.	5.00E+02	23.10	4.6207E-02
114 HMR(LIQUID)=-5454	-5433.	5.00E+02	20.77	4.1549E-02
115 HMR(LIQUID)=-5233	-5216.	5.00E+02	17.10	3.4207E-02
116 HMR(LIQUID)=-4575	-4564.	5.00E+02	11.09	2.2181E-02
117 HMR(LIQUID)=-3481	-3477.	5.00E+02	3.736	7.4714E-03
118 HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.961	-1.1922E-02

PARROT:

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Calculate the phase diagram one last time.

PARROT: mac tcex36cpd

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

POLY:

POLY: @@ In PARROT, the global minimization is turned off automatically.

POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY: @@ message will be given.

POLY:

POLY: advanced-option global yes,,

Settings for global minimization:

*** WARNING *** Global equilibrium calculation may create new composition sets

and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY:

POLY: def-com,,,,

POLY: s-a-v 1 w(b) 0 1,,,,

The condition W(B)=.1234 created

POLY: s-a-v 2 t 300 1700,,,,

The condition T=942.2 created

POLY: s-c t=500

POLY: l-c

W(B)=0.1234, T=500

DEGREES OF FREEDOM 2

POLY: c-e

Creating condition P=1E5

Creating condition N=1

Using global minimization procedure

Calculated 628 grid points in 0.004 s

Found the set of lowest grid points in 0.000 s

Calculated POLY solution 0.004 s, total time 0.008 s

POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

POLY: map

Version 3 mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
BCC#1
** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.819E-01 7.255E+02
** A2B
BCC#1
** BCC#2

Phase region boundary 4 at: 3.626E-01 7.255E+02
** A2B
BCC#1
Calculated. 15 equilibria

Phase region boundary 5 at: 3.771E-01 1.192E+03
** LIQUID
** A2B
BCC#1

Phase region boundary 6 at: 2.828E-01 1.192E+03
** LIQUID
BCC#1
Calculated 27 equilibria

Phase region boundary 7 at: 4.863E-01 1.192E+03
** LIQUID
A2B
Calculated. 28 equilibria

Phase region boundary 8 at: 6.500E-01 1.048E+03
** LIQUID
A2B
** BCC#1

Phase region boundary 9 at: 7.639E-01 1.048E+03
A2B
** BCC#1
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.273E-01 1.048E+03
LIQUID
** BCC#1
Calculated. 8 equilibria

Phase region boundary 11 at: 8.748E-01 1.203E+03
LIQUID
** BCC#1
** FCC

Phase region boundary 12 at: 8.800E-01 1.203E+03
LIQUID
** FCC
Calculated 33 equilibria

Phase region boundary 13 at: 9.353E-01 1.203E+03
BCC#1
** FCC
Calculated 20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated. 13 equilibria

Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
BCC#1
** BCC#2
Calculated.. 13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated.. 13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated.. 13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated 10 equilibria

Phase region boundary 26 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.. 3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.. 14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated 10 equilibria

Phase region boundary 29 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.. 3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.. 9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated.. 4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated 26 equilibria

Phase region boundary 33 at: 8.858E-01 1.230E+03
** LIQUID
FCC
Calculated.. 2 equilibria

Terminating at known equilibrium

Phase region boundary 34 at: 8.858E-01 1.230E+03

** LIQUID
FCC

Calculated 29 equilibria

Phase region boundary 35 at: 6.415E-03 1.397E+03

LIQUID
** BCC#1

Calculated 13 equilibria

Phase region boundary 36 at: 6.415E-03 1.397E+03

LIQUID
** BCC#1

Calculated 13 equilibria

Terminating at known equilibrium

Phase region boundary 37 at: 2.299E-01 1.244E+03

LIQUID
** BCC#1

Calculated 20 equilibria

Phase region boundary 38 at: 2.299E-01 1.244E+03

LIQUID
** BCC#1

Calculated 4 equilibria

Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.240E+03

LIQUID
** A2B

Calculated 14 equilibria

Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03

LIQUID
** A2B

Calculated 8 equilibria

Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03

LIQUID
** FCC

Calculated 20 equilibria

Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03

LIQUID
** FCC

Calculated 8 equilibria

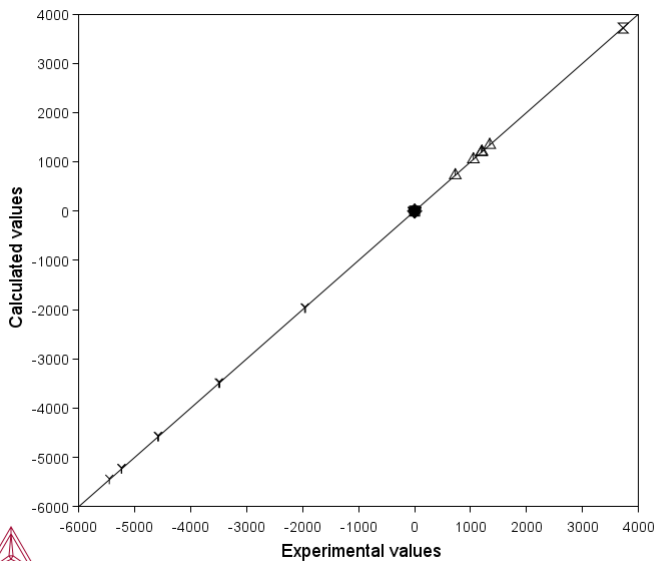
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3

CPU time for mapping 1 seconds

POLY: post

POST: s-l d

POST: plot



POST:

POST: set-inter

POST:Hit RETURN to continue

POST: @@ Add the experimental data

POST: a-e-d y exp36 0; 1

POST:

POST: SET EXP_FILE_FORMAT 5

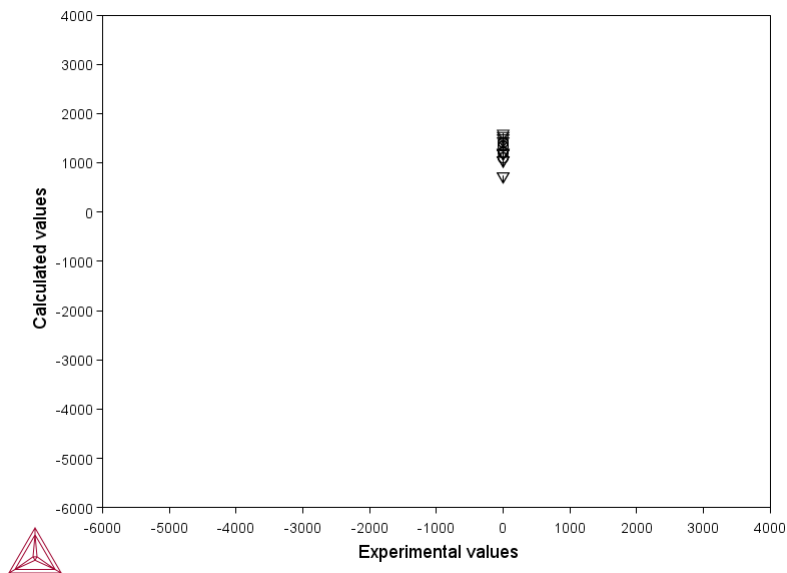
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED

POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
POLY: read,,,
POLY:
POLY:
POLY: s-a-v 2 none
POLY: s-c t=1773
POLY: c-e
Using global minimization procedure
Calculated      628 grid points in      0.006 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.004 s, total time      0.010 s
POLY: sh hmr
HMR=13116.472
POLY: l-st c
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)      P(Pa)
A      ENTERED      SER
B      ENTERED      SER
POLY: s-r-s a liq * 1e5
POLY: s-r-s b liq * 1e5
POLY: save tcex36h y

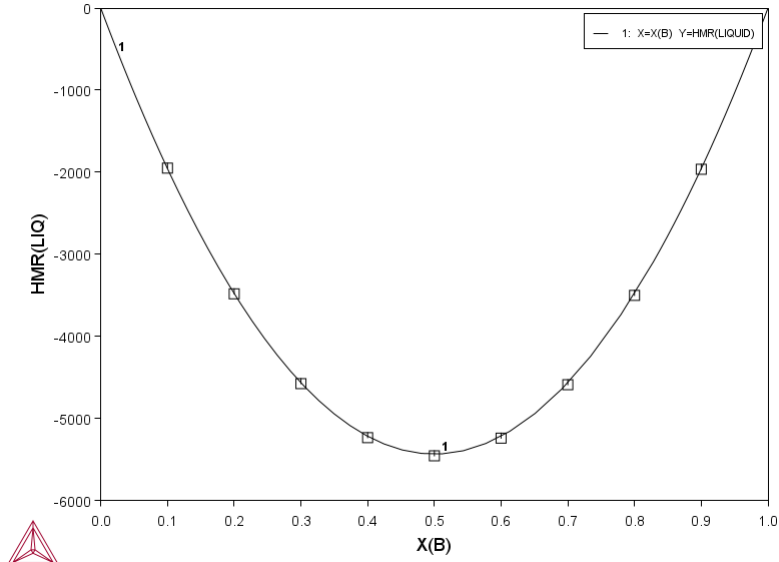
This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: step normal
No initial equilibrium, using default
Step will start from axis value      0.123400
...OK

Phase Region from      0.123400      for:
LIQUID
Global test at      3.23400E-01 .... OK
Global test at      5.73400E-01 .... OK
Global test at      8.23400E-01 .... OK
Global test at      9.53400E-01 .... OK
Global test at      1.00000E+00 .... OK
Terminating at      1.00000
Calculated      51 equilibria

Phase Region from      0.123400      for:
LIQUID
Global test at      8.34000E-02 .... OK
Global test at      3.34000E-02 .... OK
Terminating at      0.250000E-11
Calculated      28 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36h.POLY3
POLY: post
POST: s-d-a x x(b)
POST: s-d-a y hmr(liq)
POST: a-e-d y exp36 0; 2
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

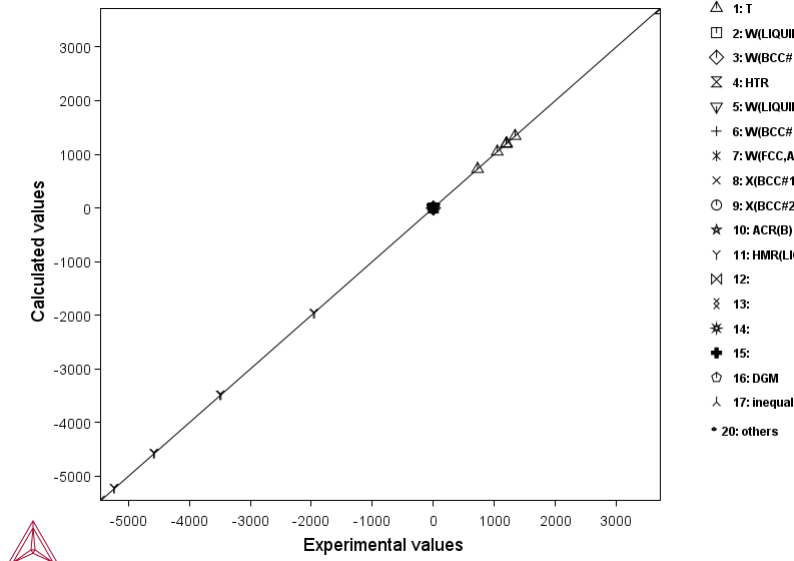
```



POST: Hit RETURN to continue
 POST: @@ We can see the fitting results by the following method
 POST: @@ Data points falling on the diagonal line indicates
 POST: @@ perfect fitting.
 POST: @@
 POST: ba
 POLY: ba

PARROT VERSION 5.3

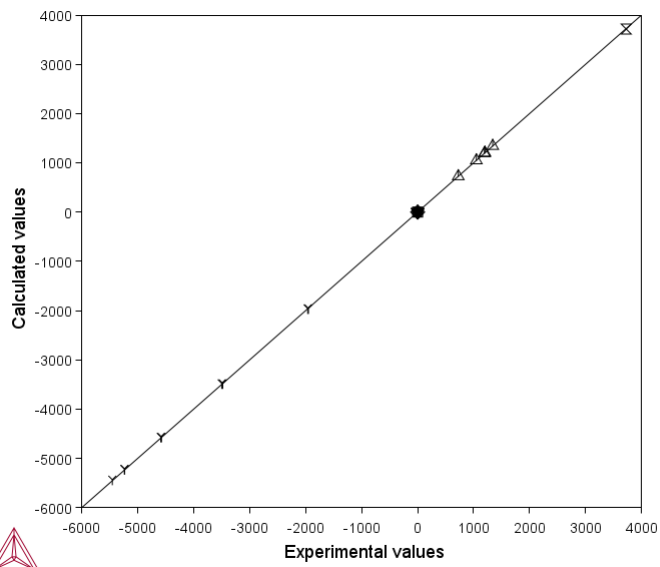
Global minimization used as test only
 PARROT: l-result gra pexp36 1,



POST: s-s-s y n -6000 4000
 POST: s-s-s x n -6000 4000
 POST: SET_EXP_FILE_FORMAT 5
 POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 *** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
 POST: SET_EXP_FILE_FORMAT 10
 POST: plot



POST: b
PARROT: set-inter
PARROT:



- 1: T
- 2: W(LIQU)
- 3: W(BCC#
- 4: HTR
- 5: W(LIQU)
- 6: W(BCC#
- 7: W(FCC,A
- 8: X(BCC#1
- 9: X(BCC#2
- 10: ACR(B)
- 11: HMR(LI
- 12:
- 13:
- 14:
- 15:
- 16: DGM
- 17: inequal
- 20: others

tcex36a-tcex36cpd

PARROT>About

NO SUCH COMMAND, USE HELP

PARROT:PARROT:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36cpd.TCM.test"

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

POLY:

POLY: @@ In PARROT, the global minimization is turned off automatically.

POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY: @@ message will be given.

POLY:

POLY: advanced-option global yes,,

Settings for global minimization:

*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY:

POLY: def-com,,,,

POLY: s-a-v 1 w(b) 0 1,,,,

The condition W(B)=.1234 created

POLY: s-a-v 2 t 300 1700,,,,

The condition T=942.2 created

POLY: s-c t=500

POLY: l-c

W(B)=0.1234, T=500

DEGREES OF FREEDOM 2

POLY: c-e

Creating condition P=1E5

Creating condition N=1

Using global minimization procedure

Calculated 628 grid points in 0.002 s

Found the set of lowest grid points in 0.001 s

Calculated POLY solution 0.006 s, total time 0.009 s

POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02

BCC#1

** BCC#2

Calculated.. 2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02

BCC#1

** BCC#2

Calculated. 14 equilibria

Phase region boundary 3 at: 6.819E-01 7.255E+02

** A2B

BCC#1

** BCC#2

Phase region boundary 4 at: 3.626E-01 7.255E+02

** A2B

BCC#1

Calculated. 15 equilibria

Phase region boundary 5 at: 3.771E-01 1.192E+03
 ** LIQUID
 ** A2B
 BCC#1

Phase region boundary 6 at: 2.828E-01 1.192E+03
 ** LIQUID
 BCC#1
 Calculated 27 equilibria

Phase region boundary 7 at: 4.863E-01 1.192E+03
 ** LIQUID
 A2B
 Calculated. 28 equilibria

Phase region boundary 8 at: 6.500E-01 1.048E+03
 ** LIQUID
 A2B
 ** BCC#1

Phase region boundary 9 at: 7.639E-01 1.048E+03
 A2B
 ** BCC#1
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 10 at: 8.273E-01 1.048E+03
 LIQUID
 ** BCC#1
 Calculated. 8 equilibria

Phase region boundary 11 at: 8.748E-01 1.203E+03
 LIQUID
 ** BCC#1
 ** FCC

Phase region boundary 12 at: 8.800E-01 1.203E+03
 LIQUID
 ** FCC
 Calculated 33 equilibria

Phase region boundary 13 at: 9.353E-01 1.203E+03
 BCC#1
 ** FCC
 Calculated 20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 ** BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

```

Phase region boundary 25 at: 3.647E-01 7.700E+02
** A2B
   BCC#1
Calculated 10 equilibria

Phase region boundary 26 at: 3.647E-01 7.700E+02
** A2B
   BCC#1
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.647E-01 7.700E+02
** A2B
   BCC#1
Calculated. 14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.910E-01 7.700E+02
** A2B
   BCC#1
Calculated 10 equilibria

Phase region boundary 29 at: 7.910E-01 7.700E+02
** A2B
   BCC#1
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.910E-01 7.700E+02
** A2B
   BCC#1
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
** LIQUID
   BCC#1
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
** LIQUID
   BCC#1
Calculated 26 equilibria

Phase region boundary 33 at: 8.858E-01 1.230E+03
** LIQUID
   FCC
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.858E-01 1.230E+03
** LIQUID
   FCC
Calculated 29 equilibria

Phase region boundary 35 at: 6.415E-03 1.397E+03
** LIQUID
   BCC#1
Calculated 13 equilibria

Phase region boundary 36 at: 6.415E-03 1.397E+03
** LIQUID
   BCC#1
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.299E-01 1.244E+03
** LIQUID
   BCC#1
Calculated 20 equilibria

Phase region boundary 38 at: 2.299E-01 1.244E+03
** LIQUID
   BCC#1
Calculated. 4 equilibria
Terminating at known equilibrium

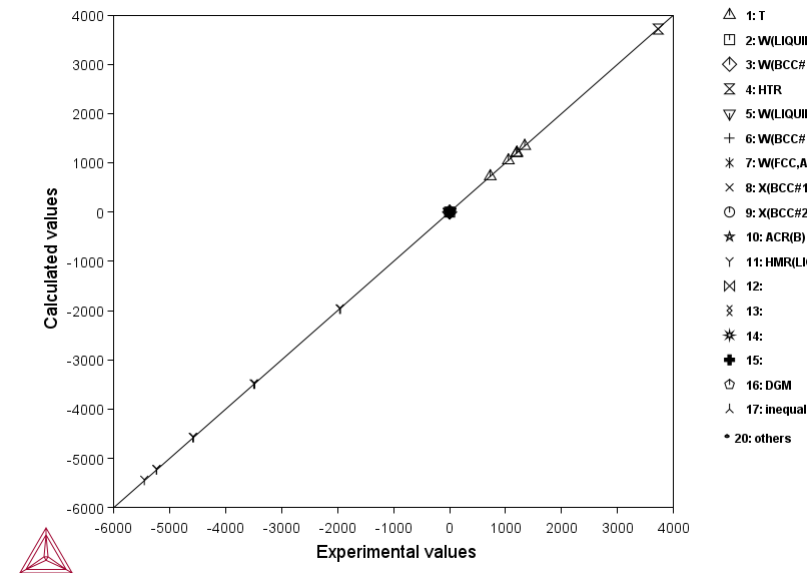
Phase region boundary 39 at: 6.122E-01 1.240E+03
** LIQUID
   A2B
Calculated. 14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03
** LIQUID
   A2B
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
** LIQUID
   FCC
Calculated. 20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
** LIQUID
   FCC
Calculated 8 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping 1 seconds
POLY: post
POST: s-l d
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



POST:
POST: set-inter
POST:

tcex37

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex37\tcex37.TCM.test"

SYS: @@ Calculating an Isothermal Section

SYS:

SYS: @@ This example shows how to use command

SYS: @@ lines to enter and calculate an isothermal

SYS: @@ section using the POLY3 module.

SYS:

SYS: go data

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11:_sw fedemo

Current database: Iron Demo Database v6.0

VA /- DEFINED

TDB_FEDEMO: def-sys

ELEMENTS: fe cr ni

CR

NI

DEFINED

TDB_FEDEMO: l-s c

GAS:G :CR CR2 FE FE2 NI NI2:

#Gas # # # #6038cfcf41046d48150aa2e6

LIQUID:L :CR FE NI:

#Liquid # # # #6038cfda41046d48150aa2e7

BCC_A2 :CR FE NI:VA:

#Body-Centered Cubic (W, A2, bcc) #cI2 #Im-3m # #602e7f15105f8553a825b4e4

C14_LAVES :CR FE NI:CR FE NI:

#MgZn2 Hexagonal Laves (C14) #hP12 #P6_3/mmc # #602e7f15105f8553a825b52b

CBCC_A12 :CR FE NI:VA:

#alpha-Mn (A12) #cI58 #I-43m # #602e7f15105f8553a825b4dc

CHI_A12 :CR FE NI:CR:CR FE NI:

#alpha-Mn (A12) #cI58 #I-43m # #602e7f15105f8553a825b4dc

CUB_A13 :CR FE NI:VA:

#beta-Mn (A13) #cP20 #P4_132 # #602e7f15105f8553a825b4dd

FCC_A1 :CR FE NI:VA:

#Face-Centered Cubic (Cu, Al, fcc) #cF4 #Fm-3m # #602e7f15105f8553a825b4d9

HCP_A3 :CR FE NI:VA:

#Hexagonal Close Packed (Mg, A3, hcp) #hP2 #P6_3/mmc #

#602e7f15105f8553a825b4e6

SIGMA_D8B :CR FE NI:CR:CR FE NI:

#sigma-CrFe (D8b) #tP30 #P4_2/mnm # #602e7f15105f8553a825b5b9

TDB_FEDEMO:Hit RETURN to continue

TDB_FEDEMO: get

09:40:12,838 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_FEDEMO: go p-3

POLY version 3.32

POLY: l-st

Option /CPS/: cps

*** STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
CR	ENTERED	SER		
FE	ENTERED	SER		
NI	ENTERED	SER		

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
SIGMA_D8B	ENTERED	0.000000E+00	0.000000E+00
HCP_A3	ENTERED	0.000000E+00	0.000000E+00
FCC_A1	ENTERED	0.000000E+00	0.000000E+00
CUB_A13	ENTERED	0.000000E+00	0.000000E+00
CHI_A12	ENTERED	0.000000E+00	0.000000E+00
CBCC_A12	ENTERED	0.000000E+00	0.000000E+00
C14_LAVES	ENTERED	0.000000E+00	0.000000E+00
BCC_A2	ENTERED	0.000000E+00	0.000000E+00
LIQUID	ENTERED	0.000000E+00	0.000000E+00
GAS	ENTERED	0.000000E+00	0.000000E+00

*** STATUS FOR ALL SPECIES

CR	ENTERED	FE	ENTERED	NI	ENTERED	VA	ENTERED
CR2	ENTERED	FE2	ENTERED	NI2	ENTERED		

POLY: @@ Set conditions for a point inside the diagram

POLY: s-c x(cr)=0.2 x(ni)=0.4

POLY: s-c t=1673 p=1e5 n=1

POLY: l-c

X(CR)=0.2, X(NI)=0.4, T=1673, P=100000, N=1

DEGREES OF FREEDOM 0

POLY: c-e

Using global minimization procedure

Calculated 17097 grid points in 0.347 s

Found the set of lowest grid points in 0.003 s

Calculated POLY solution 0.089 s, total time 0.439 s

POLY: l-e

OUTPUT TO SCREEN OR FILE /SCREEN/: SCREEN

```

Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0  , database: FEDEMO

Conditions:
X(CR)=0.2, X(NI)=0.4, T=1673, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1673.00 K ( 1399.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.62140E+01
Total Gibbs energy -1.08423E+05, Enthalpy 4.89973E+04, Volume 7.34210E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
CR              2.0000E-01  1.8499E-01 7.8623E-04 -9.9434E+04 SER
FE              4.0000E-01  3.9739E-01 4.0953E-04 -1.0851E+05 SER
NI              4.0000E-01  4.1762E-01 3.0004E-04 -1.1283E+05 SER

FCC_A1          Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.6214E+01, Volume fraction 1.0000E+00 Mass fractions:
NI 4.17618E-01 FE 3.97389E-01 CR 1.84993E-01
POLY: s-a-v
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: s-a-v 2
Condition /NONE/: x(cr)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: save tcex37 y
POLY:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16

Phase region boundary 1 at: 9.201E-03 4.019E-02
** BCC_A2
FCC_A1
Calculated 14 equilibria

Phase region boundary 2 at: 9.201E-03 4.019E-02
** BCC_A2
FCC_A1
Calculated. 31 equilibria

Phase region boundary 3 at: 1.950E-01 3.373E-01
** LIQUID
** BCC_A2
FCC_A1

Phase region boundary 4 at: 2.267E-01 3.103E-01
** LIQUID
FCC_A1
Calculated 53 equilibria

Phase region boundary 5 at: 1.883E-01 3.539E-01
** LIQUID
BCC_A2
Calculated 49 equilibria

Phase region boundary 6 at: 1.950E-01 3.373E-01
** BCC_A2
FCC_A1
Calculated 51 equilibria

Phase region boundary 7 at: 3.334E-01 3.082E-01
** LIQUID
FCC_A1
Calculated. 10 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 3.334E-01 3.082E-01
** LIQUID
FCC_A1
Calculated 39 equilibria

Phase region boundary 9 at: 6.543E-01 3.046E-01
** LIQUID
FCC_A1
Calculated. 35 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 6.543E-01 3.046E-01

```

```

** LIQUID
FCC_A1
Calculated                      23  equilibria

Phase region boundary 11 at:    1.678E-01  3.000E-01
BCC_A2
** FCC_A1
Calculated                      34  equilibria

Phase region boundary 12 at:    1.678E-01  3.000E-01
BCC_A2
** FCC_A1
Calculated.                     4  equilibria
Terminating at known equilibrium

Phase region boundary 13 at:    3.086E-01  5.984E-01
** LIQUID
BCC_A2
Calculated.                     21  equilibria
Terminating at known equilibrium

Phase region boundary 14 at:    3.086E-01  5.984E-01
** LIQUID
BCC_A2
Calculated                      25  equilibria

Phase region boundary 15 at:    1.097E-02  4.525E-02
BCC_A2
** FCC_A1
Calculated                      15  equilibria

Phase region boundary 16 at:    1.097E-02  4.525E-02
BCC_A2
** FCC_A1
Calculated.                     31  equilibria
Terminating at known equilibrium

Phase region boundary 17 at:    3.342E-01  6.558E-01
LIQUID
** BCC_A2
Calculated.                     26  equilibria
Terminating at known equilibrium

Phase region boundary 18 at:    3.342E-01  6.558E-01
LIQUID
** BCC_A2
Calculated                      13  equilibria

Phase region boundary 19 at:    6.736E-01  3.160E-01
LIQUID
** FCC_A1
Calculated.                     37  equilibria
Terminating at known equilibrium

Phase region boundary 20 at:    6.736E-01  3.160E-01
LIQUID
** FCC_A1
Calculated                      18  equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex37\tcex37.POLY3
CPU time for mapping              9  seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

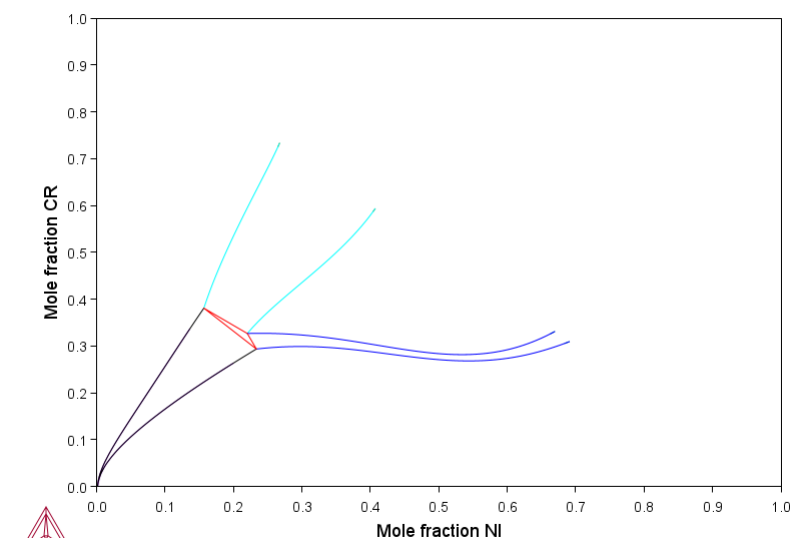
```

Setting automatic diagram axes

POST: @@ Use default axis on the diagram
POST:
POST: set-title example 37a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```

example 37a



```

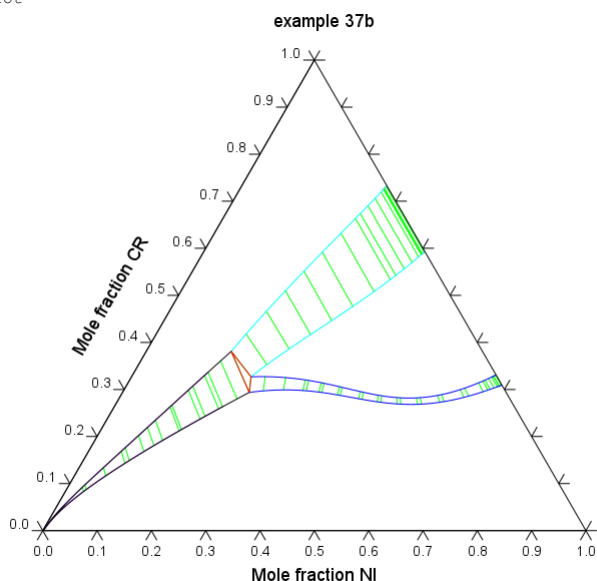
POST:
POST:
POST: Hit RETURN to continue
POST: @@ By default a diagram is always square. set it triangular,
POST: @@ add tie-lines and set scaling on the axis
POST: s-d-t
POST: TRIANGULAR DIAGRAM (Y OR N) /N/: y
POST: s-t-s

```

```

PLOTting EVERY TIE-LINE NO /0/: 3
POST: s-sc
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 1
POST: s-s y n 0 1
POST: set-title example 37b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

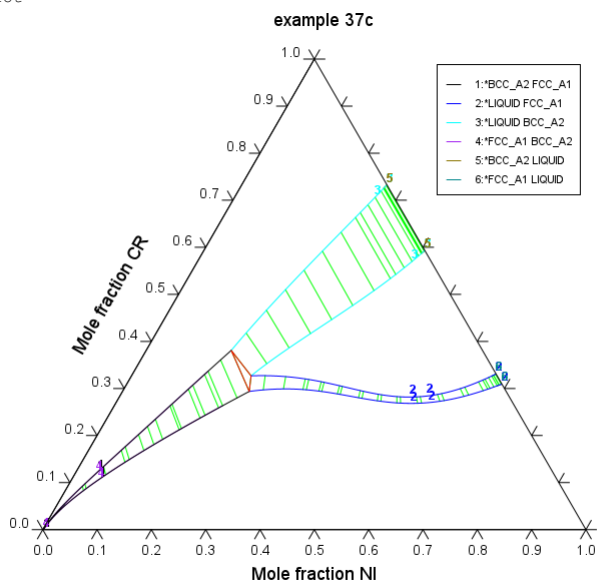
```



```

POST:
POST:
POST: Hit RETURN to continue
POST: @@ To identify the phases also set labels
POST: @@ To add text in phase regions use a dataplot file
POST: set-lab b
POST: set-title example 37c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



```

POST:
POST: set-inter
POST:

```

tcex38

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex38\tcex38.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating the Morral *rose*

SYS:

SYS: @@ This example uses the Gibbs energy system

SYS: @@ (GES) module to calculate the Morral rose,

SYS: @@ which are miscibility gaps.

SYS:

SYS: set-log ex38,,,

SYS: go g

... the command in full is GOTO_MODULE

GIBBS ENERGY SYSTEM

09:41:17,668 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

GES6: reinstantiate,,,

GES6:

GES6: @@ Enter a phase with just a ternary interaction parameter

GES6: e-e a b c

... the command in full is ENTER_ELEMENT

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

GES6: a-e-d a fcc_a1 10,,,

... the command in full is AMEND_ELEMENT_DATA

GES6: a-e-d b fcc_a1 10,,,

... the command in full is AMEND_ELEMENT_DATA

GES6: a-e-d c fcc_a1 10,,,

... the command in full is AMEND_ELEMENT_DATA

GES6:

GES6:

GES6: e-ph fcc_a1,,1 A B C,,,

... the command in full is ENTER_PHASE

GES6:

GES6:

GES6: e-par l(fcc_a1,a,b,c),,50000,,,

... the command in full is ENTER_PARAMETER

l(FCC_A1,A,B,C;0)

GES6: l-d

... the command in full is LIST_DATA

OUTPUT TO SCREEN OR FILE /SCREEN/: SCREEN

OPTIONS?:

Property type /ALL/: ALL

Element	Stable Element Reference	Mass	H298-H0	S298
VA	UNKNOWN	0.0000E+00	0.0000E+00	0.0000E+00
A	FCC_A1	1.0000E+01	0.0000E+00	0.0000E+00
B	FCC_A1	1.0000E+01	1.2220E+03	5.9000E+00
C	FCC_A1	1.0000E+01	1.0540E+03	5.7400E+00

FCC_A1 (A,B,C)1.0

==== [A, B, C] ====

l(FCC_A1,A,B,C;0) 298.15 +50000; 6000 N

GES6:

GES6:

GES6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: s-c t=600 p=1e5 n=1 x(b)=.3 x(c)=.1

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

09:41:20,309 [Thread-0] INFO Database: Preparing system for use: UNKNOWN_1747042877937

09:41:21,272 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1

Calculated 1965 grid points in 1.565 s

Found the set of lowest grid points in 0.001 s

Creating a new composition set FCC_A1#2

Calculated POLY solution 0.090 s, total time 1.656 s

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/:

Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:

T=600, P=100000, N=1, X(B)=0.3, X(C)=0.1

DEGREES OF FREEDOM 0

Temperature 600.00 K (326.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01

Total Gibbs energy -3.58989E+03, Enthalpy 6.74567E+02, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
A	6.0000E-01	6.0000E-01	5.7356E-01	-2.7732E+03	SER
B	3.0000E-01	3.0000E-01	3.8092E-01	-4.8149E+03	SER
C	1.0000E-01	1.0000E-01	3.8092E-01	-4.8149E+03	SER

FCC A1#1 Status ENTERED Driving force 0.0000E+00

Moles 8.7781E-01, Mass 8.7781E+00, Volume fraction 0.0000E+00 Mass fractions:


```

A 6.00000E-01 B 3.32342E-01 C 6.76579E-02

FCC_A1#2 Status ENTERED Driving force 0.0000E+00
Moles 1.2219E-01, Mass 1.2219E+00, Volume fraction 0.0000E+00 Mass fractions:
A 6.00000E-01 C 3.32342E-01 B 6.76579E-02
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 1 x(b) 0 1 0.01
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 x(c) 0 1 0.01
... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: save tcex38 y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Trying global minimization! 3
Generating start point 1
Generating start point 2
Trying global minimization! 3
Generating start point 3
Generating start point 4
Trying global minimization! 3
Generating start point 5
Generating start point 6
Trying global minimization! 3
Generating start point 7
Generating start point 8
Trying global minimization! 3
Generating start point 9
Generating start point 10
Working hard
Trying global minimization! 3
Generating start point 11
Generating start point 12

Phase region boundary 1 at: 2.333E-01 2.333E-01
FCC_A1#1
** FCC_A1#2
Calculated 31 equilibria

Phase region boundary 2 at: 2.333E-01 2.333E-01
FCC_A1#1
** FCC_A1#2
Creating a new composition set FCC_A1#3
Calculated 10 equilibria

Phase region boundary 3 at: 2.333E-01 2.333E-01
FCC_A1#1
** FCC_A1#2
Calculated. 5 equilibria

Phase region boundary 4 at: 2.699E-01 2.699E-01
FCC_A1#1
** FCC_A1#2
** FCC_A1#3

Phase region boundary 5 at: 4.603E-01 2.699E-01
FCC_A1#1
** FCC_A1#3
Calculated 47 equilibria

Phase region boundary 6 at: 2.699E-01 4.603E-01
FCC_A1#2
** FCC_A1#3
Calculated 45 equilibria

Phase region boundary 7 at: 2.699E-01 2.699E-01
FCC_A1#1
** FCC_A1#2
Calculated 36 equilibria

Phase region boundary 8 at: 6.633E-01 1.683E-01
FCC_A1#1
** FCC_A1#2
Calculated 26 equilibria

Phase region boundary 9 at: 6.633E-01 1.683E-01
FCC_A1#1
** FCC_A1#2
Calculated 33 equilibria

Phase region boundary 10 at: 6.633E-01 1.683E-01
FCC_A1#1
** FCC_A1#2
Calculated. 22 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 2.333E-01 2.333E-01
FCC_A1#1
** FCC_A1#2
Calculated 34 equilibria

Phase region boundary 12 at: 2.333E-01 2.333E-01
FCC_A1#1
** FCC_A1#2
Calculated 10 equilibria

Phase region boundary 13 at: 2.333E-01 2.333E-01
FCC_A1#1

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** FCC_A1#2
Calculated.                    5 equilibria
Terminating at known equilibrium

Phase region boundary 14 at:    1.683E-01  6.633E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    32 equilibria

Phase region boundary 15 at:    1.683E-01  6.633E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    22 equilibria
Terminating at known equilibrium

Phase region boundary 16 at:    1.683E-01  6.633E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    30 equilibria

Phase region boundary 17 at:    2.333E-01  5.333E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    19 equilibria

Phase region boundary 18 at:    2.333E-01  5.333E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    9 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:    2.333E-01  5.333E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    43 equilibria

Phase region boundary 20 at:    6.633E-01  1.683E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    26 equilibria

Phase region boundary 21 at:    6.633E-01  1.683E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    33 equilibria

Phase region boundary 22 at:    6.633E-01  1.683E-01
  FCC_A1#1
** FCC_A1#2
Calculated.                    22 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex38\tcex38.POLY3
CPU time for mapping          4 seconds

```

POLY:

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:

POST: s-d-a x m-f b
... the command in full is SET_DIAGRAM_AXIS

POST: s-d-a y m-f c
... the command in full is SET_DIAGRAM_AXIS

POST: s-d-ty y,,,,
... the command in full is SET_DIAGRAM_TYPE

POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS

POST: s-s y n 0 1
... the command in full is SET_SCALING_STATUS

POST: s-t-s 10
... the command in full is SET_TIELINE_STATUS

POST: set-title example 38a

POST:

POST: SET_EXP_FILE_FORMAT 5

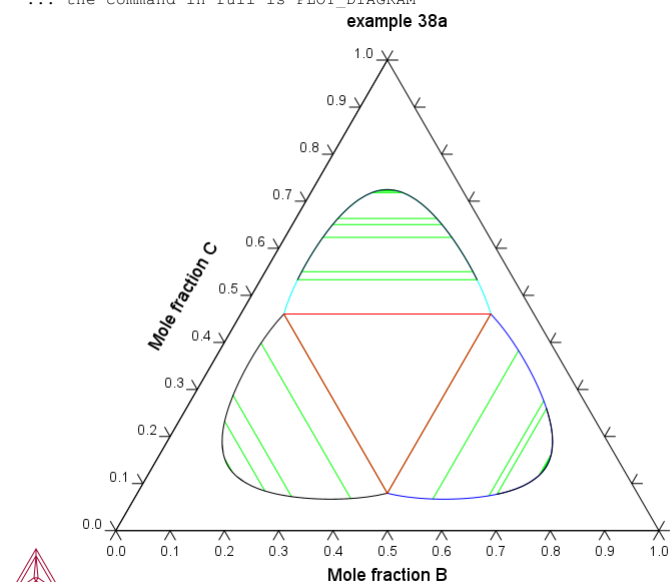
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI

The composition set FCC A1#3 created from the store file

POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot
... the command in full is PLOT_DIAGRAM



```

POST:
POST:Hit RETURN to continue
POST:
POST: back
POLY: read,,
... the command in full is READ_WORKSPACES
POLY:
POLY: @@ We will calculate at a higher temperature
POLY: @@ with a stable phase in the middle.
POLY: s-c t=696
... the command in full is SET_CONDITION
POLY: s-c x(b)=.44 x(c)=.28
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1965 grid points in      0.019 s
Found the set of lowest grid points in      0.001 s
Creating a new composition set FCC_A1#3
Calculated POLY solution      0.038 s, total time      0.058 s
POLY:
POLY: save tcex38b y
... the command in full is SAVE_WORKSPACES
POLY:
POLY:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Working hard
Trying global minimization! 3
Generating start point 1
Generating start point 2
Trying global minimization! 3
Generating start point 3
Generating start point 4
Trying global minimization! 3
Generating start point 5
Generating start point 6

Phase region boundary 1 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated      34 equilibria

Phase region boundary 2 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated      6 equilibria

Phase region boundary 3 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated      6 equilibria

Phase region boundary 4 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated      6 equilibria

Phase region boundary 5 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated      6 equilibria

Phase region boundary 6 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated      6 equilibria

Phase region boundary 7 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated.      6 equilibria

Phase region boundary 8 at: 2.998E-01 2.998E-01
FCC_A1#1
** FCC_A1#2
** FCC_A1#3

Phase region boundary 9 at: 3.618E-01 2.650E-01
FCC_A1#1
** FCC_A1#3
Calculated      7 equilibria

Phase region boundary 10 at: 3.618E-01 2.650E-01
FCC_A1#1
** FCC_A1#3
Calculated.      5 equilibria

Phase region boundary 11 at: 3.732E-01 2.650E-01
FCC_A1#1
** FCC_A1#2
** FCC_A1#3

Phase region boundary 12 at: 4.004E-01 2.998E-01
FCC_A1#1
** FCC_A1#2
Calculated      77 equilibria

Phase region boundary 13 at: 3.732E-01 3.618E-01
** FCC_A1#2
FCC_A1#3

```

```

Calculated                4 equilibria

Phase region boundary 14 at: 3.732E-01 3.618E-01
** FCC_A1#2
   FCC_A1#3
Calculated.                3 equilibria

Phase region boundary 15 at: 3.618E-01 3.732E-01
** FCC_A1#1
** FCC_A1#2
   FCC_A1#3

Phase region boundary 16 at: 2.650E-01 3.732E-01
** FCC_A1#1
   FCC_A1#3
Calculated                9 equilibria

Phase region boundary 17 at: 2.650E-01 3.732E-01
** FCC_A1#1
   FCC_A1#3
Calculated.                7 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 2.998E-01 4.004E-01
** FCC_A1#1
   FCC_A1#2
Calculated                58 equilibria

Phase region boundary 19 at: 2.998E-01 2.998E-01
   FCC_A1#1
** FCC_A1#2
Calculated                30 equilibria

Phase region boundary 20 at: 2.683E-01 2.683E-01
   FCC_A1#1
** FCC_A1#2
Calculated                35 equilibria

Phase region boundary 21 at: 2.683E-01 2.683E-01
   FCC_A1#1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 22 at: 2.683E-01 2.683E-01
   FCC_A1#1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 23 at: 2.683E-01 2.683E-01
   FCC_A1#1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 24 at: 2.683E-01 2.683E-01
   FCC_A1#1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 25 at: 2.683E-01 2.683E-01
   FCC_A1#1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 26 at: 2.683E-01 2.683E-01
   FCC_A1#1
** FCC_A1#2
Calculated.                6 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 2.683E-01 4.633E-01
   FCC_A1#1
** FCC_A1#2
Calculated                9 equilibria

Phase region boundary 28 at: 2.683E-01 4.633E-01
   FCC_A1#1
** FCC_A1#2
Calculated                9 equilibria

Phase region boundary 29 at: 2.683E-01 4.633E-01
   FCC_A1#1
** FCC_A1#2
Calculated                9 equilibria

Phase region boundary 30 at: 2.683E-01 4.633E-01
   FCC_A1#1
** FCC_A1#2
Calculated                9 equilibria

Phase region boundary 31 at: 2.683E-01 4.633E-01
   FCC_A1#1
** FCC_A1#2
Calculated                9 equilibria

Phase region boundary 32 at: 2.683E-01 4.633E-01
   FCC_A1#1
** FCC_A1#2
Calculated.                9 equilibria
Terminating at known equilibrium

Phase region boundary 33 at: 2.683E-01 4.633E-01
   FCC_A1#1
** FCC_A1#2
Calculated                44 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex38\tcex38b.POLY3
CPU time for mapping                2 seconds
POLY:
POLY:
POLY: post
      POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 38b

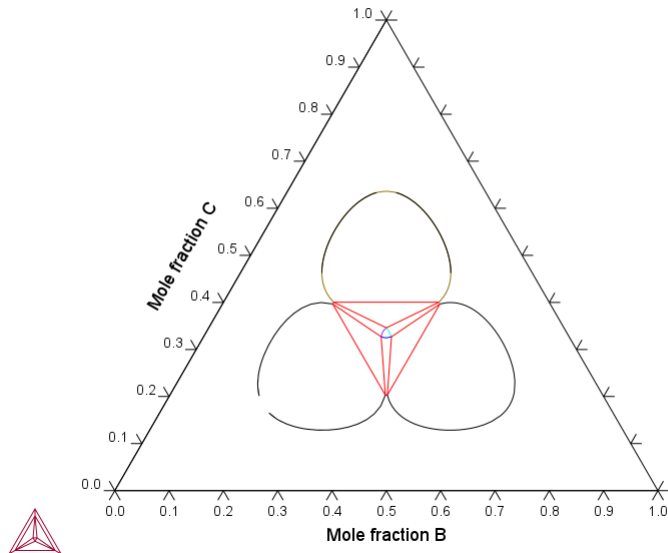
```

```

POST: s-d-ty y,,,,
... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 38b



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POST:
POST:Hit RETURN to continue
POST:
POST: back
POLY: @@ =====
POLY: @@ Now a quaternary.
POLY: @@
POLY: @@ Square rose by John Morral
POLY: @@
POLY: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES6: reinitiate,,,,
GES6: e-e a b c d
... the command in full is ENTER_ELEMENT
GES6: a-e-d a liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d b liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d c liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d d liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: e-ph liquid
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B C D
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES6: e-par g(liquid,a,b,c,d)
... the command in full is ENTER_PARAMETER
G(LIQUID,A,B,C,D;0)
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: 100000
&
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES6:
GES6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: reinitiate,,,,
... the command in full is REINITIATE_MODULE
POLY: s-c t=170 p=1e5 n=1 x(d)=.25 x(a)=.3 x(a)+x(c)=.5
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=170, P=100000, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
DEGREES OF FREEDOM 0
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
09:41:26,837 [Thread-0] INFO Database: Preparing system for use: UNKNOWN_1747042886673
09:41:27,400 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
Testing POLY result by global minimization procedure
Calculated 1787 grid points in 0.013 s
Creating a new composition set LIQUID#2
32 ITS, CPU TIME USED 3 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:

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Options /VWCS/: VXCS
Output from POLY-3, equilibrium =      1, label A0  , database: User dat

Conditions:
T=170, P=100000, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
DEGREES OF FREEDOM 0

Temperature 170.00 K ( -103.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -1.58399E+03, Enthalpy 2.18612E+02, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A                3.0000E-01  3.0000E-01 3.1587E-01 -1.6289E+03 SER
B                2.5000E-01  2.5000E-01 2.9182E-01 -1.7409E+03 SER
C                2.0000E-01  2.0000E-01 3.5423E-01 -1.4669E+03 SER
D                2.5000E-01  2.5000E-01 3.5423E-01 -1.4669E+03 SER

LIQUID#1                Status ENTERED      Driving force 0.0000E+00
Moles 5.8530E-01, Mass 5.8530E+00, Volume fraction 0.0000E+00 Mole fractions:
D 3.71549E-01 A 3.00000E-01 B 2.50000E-01 C 7.84507E-02

LIQUID#2                Status ENTERED      Driving force 0.0000E+00
Moles 4.1470E-01, Mass 4.1470E+00, Volume fraction 0.0000E+00 Mole fractions:
C 3.71549E-01 A 3.00000E-01 B 2.50000E-01 D 7.84507E-02
POLY: s-a-v 1 x(a)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY: s-a-v 2 x(d)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY:
POLY: add +1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY: save tcex38c y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Creating a new composition set LIQUID#3
Calculated 45 equilibria

Phase region boundary 2 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated. 41 equilibria

Phase region boundary 3 at: 2.500E-01 5.217E-02
LIQUID#1
** LIQUID#2
** LIQUID#3

Phase region boundary 4 at: 2.500E-01 5.217E-02
LIQUID#1
** LIQUID#2
LIQUID#3
Creating a new composition set LIQUID#4
Calculated 31 equilibria

Phase region boundary 5 at: 2.500E-01 5.217E-02
LIQUID#1
** LIQUID#2
LIQUID#3
Calculated. 15 equilibria

Phase region boundary 6 at: 1.816E-01 1.816E-01
LIQUID#1
** LIQUID#2
LIQUID#3
** LIQUID#4

Phase region boundary 7 at: 3.184E-01 1.816E-01
LIQUID#1
LIQUID#2
** LIQUID#3
Calculated. 15 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 3.184E-01 1.816E-01
LIQUID#1
LIQUID#2
** LIQUID#4
Calculated. 14 equilibria

Phase region boundary 9 at: 4.478E-01 2.500E-01
** LIQUID#1
LIQUID#2
** LIQUID#4

Phase region boundary 10 at: 4.478E-01 2.500E-01
LIQUID#2
** LIQUID#4
Calculated. 43 equilibria

Phase region boundary 11 at: 2.500E-01 4.478E-01
LIQUID#2
** LIQUID#3
** LIQUID#4

Phase region boundary 12 at: 2.500E-01 4.478E-01

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    LIQUID#2
    LIQUID#3
    ** LIQUID#4
Calculated                20 equilibria

Phase region boundary 13 at:  2.500E-01  4.478E-01
    LIQUID#2
    LIQUID#3
    ** LIQUID#4
Calculated.                15 equilibria
Terminating at known equilibrium

Phase region boundary 14 at:  2.500E-01  4.478E-01
    LIQUID#2
    ** LIQUID#3
Calculated.                41 equilibria

Phase region boundary 15 at:  5.217E-02  2.500E-01
    LIQUID#2
    ** LIQUID#3
    ** LIQUID#4

Phase region boundary 16 at:  5.217E-02  2.500E-01
    LIQUID#2
    ** LIQUID#3
    LIQUID#4
Calculated                20 equilibria

Phase region boundary 17 at:  5.217E-02  2.500E-01
    LIQUID#2
    ** LIQUID#3
    LIQUID#4
Calculated.                15 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  5.217E-02  2.500E-01
    LIQUID#2
    ** LIQUID#4
Calculated.                41 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  5.217E-02  2.500E-01
    LIQUID#2
    LIQUID#3
    ** LIQUID#4
Calculated.                15 equilibria
Terminating at known equilibrium

Phase region boundary 20 at:  2.500E-01  4.478E-01
    LIQUID#2
    ** LIQUID#3
    LIQUID#4
Calculated                20 equilibria

Phase region boundary 21 at:  2.500E-01  4.478E-01
    LIQUID#2
    ** LIQUID#3
    LIQUID#4
Calculated.                15 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  4.478E-01  2.500E-01
    ** LIQUID#1
    LIQUID#2
Calculated.                43 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  4.478E-01  2.500E-01
    ** LIQUID#1
    LIQUID#2
    LIQUID#4
Calculated.                15 equilibria
Terminating at known equilibrium

Phase region boundary 24 at:  4.478E-01  2.500E-01
    LIQUID#1
    ** LIQUID#2
Calculated                6 equilibria

Phase region boundary 25 at:  4.478E-01  2.500E-01
    LIQUID#1
    ** LIQUID#2
Calculated                2 equilibria

Phase region boundary 26 at:  4.478E-01  2.500E-01
    LIQUID#1
    ** LIQUID#2
Calculated                2 equilibria

Phase region boundary 27 at:  4.478E-01  2.500E-01
    LIQUID#1
    ** LIQUID#2
Calculated                2 equilibria

Phase region boundary 28 at:  4.478E-01  2.500E-01
    LIQUID#1
    ** LIQUID#2
Calculated                2 equilibria

Phase region boundary 29 at:  4.478E-01  2.500E-01
    LIQUID#1
    ** LIQUID#2
Calculated                2 equilibria
Calculated                2 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex38\tcex38c.POLY3
CPU time for mapping                2 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

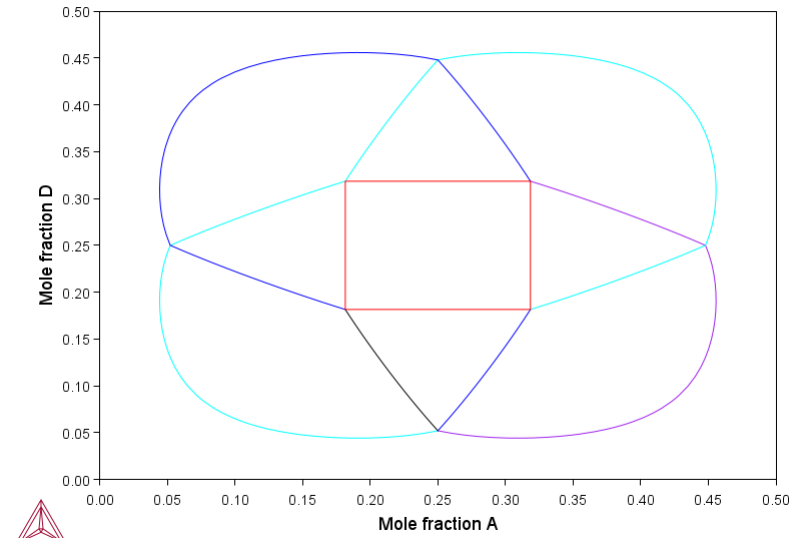
Setting automatic diagram axes

POST:
POST:
POST: set-title example 38c
POST:
POST:

```

```
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
The composition set LIQUID#3 created from the store file
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 38c



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```


SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating reversible Carnot cycles of a heat engine

SYS:

SYS: @@ This example shows how to calculate the reversible

SYS: @@ Carnot cycle of a heat engine using one mole of an ideal

SYS: @@ gas with two fictitious species A and A2. The GES, POLY3

SYS: @@ and POST modules are used.

SYS:

SYS: @@ One application of the Second Law is to the efficiencies

SYS: @@ of heat engines, pumps and refrigerators. Whenever there

SYS: @@ is a difference of temperature, work can be produced -

SYS: @@ the principle of heat engines. The Gibbs energy also

SYS: @@ enables the prediction of the maximum work that a process

SYS: @@ may achieve. The goal of this example is to help relate

SYS: @@ the results to different thermodynamic quantities.

SYS:

SYS: set-log ex39,,,

SYS:

SYS: go g

... the command in full is GOTO_MODULE

GIBBS ENERGY SYSTEM

09:42:27,055 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

GES6: rei,,,,

... the command in full is REINITIATE

GES6: e-e a

... the command in full is ENTER_ELEMENT

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

GES6: a-e-d a gas 10,,,,

... the command in full is AMEND_ELEMENT_DATA

GES6: e-sp A2 A2

... the command in full is ENTER_SPECIES

GES6: e-ph gas g 1 A A2; N N

... the command in full is ENTER_PHASE

GES6: @@ The Gibbs free energy for these species could be described

GES6: @@ by the general formula: $G_m = a + bT + cT \ln T + dT^2 + \dots + RT \ln(P)$

GES6:

GES6: @@ To calculate the Carnot cycle you have to give some numerical

GES6: @@ values to the a, b, c, etc. constants of the G_m expression.

GES6: @@ It is important to understand that the coefficients cannot

GES6: @@ be chosen arbitrarily, for example c should be negative as

GES6: @@ the heat capacity at constant pressure, $C_p = -T d^2G/dT^2$

GES6: @@ and thus $C_p = -c - 2dT$, must always be >0

GES6:

GES6: e-par g(gas,a) 298.15 6960-51*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,

... the command in full is ENTER_PARAMETER

G(GAS,A;0)-G(GAS,A;0)

GES6: e-par g(gas,a2) 298.15 130670-38*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,

... the command in full is ENTER_PARAMETER

G(GAS,A2;0)- 2 G(GAS,A;0)

GES6: l-d,,,,

... the command in full is LIST_DATA

Property type /ALL/:Hit RETURN to continue

Property type /ALL/:

Element	Stable Element Reference	Mass	H298-H0	S298
VA	UNKNOWN	0.0000E+00	0.0000E+00	0.0000E+00
A	GAS	1.0000E+01	0.0000E+00	0.0000E+00

Species	Stoichiometry
A2	A2

GAS:G (A,A2)1.0

- This phase is a gas

==== [A] =====

G(GAS,A2;0) 298.15 +130670-38*T-17*T*LN(T) 6000 N

+R*T*LN(1.0E-5*P);

G(GAS,A;0) 298.15 +6960-51*T-17*T*LN(T) 6000 N

+R*T*LN(1.0E-5*P);

GES6: @@ The Carnot cycle diagram gives the pressure and volume for

GES6: @@ the working media of a heat engine that operates between

GES6: @@ two temperatures T1 and T2, T1>T2.

GES6:

GES6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ The Carnot cycle is calculated for T1=500 K (the

POLY: @@ temperature of the hot reservoir) and T2=400 K

POLY: @@ (the temperature of the cold reservoir)

POLY: ent var t1=500;

... the command in full is ENTER_SYMBOL

POLY: ent var t2=400;

... the command in full is ENTER_SYMBOL

POLY:

POLY: @@ A Carnot cycle consists of four reversible stages:

POLY:

```

POLY: @@ Stage 1. Isothermal expansion at T1; the entropy change
POLY: @@ of the system is Q1/T1, where Q1 is the heat taken from
POLY: @@ the hot reservoir.
POLY:
POLY: s-c t=t1 p=1e7 n=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
09:42:29,858 [Thread=0] INFO Database: Preparing system for use: UNKNOWN_1747042947329
09:42:30,824 [Thread=0] INFO Phase: Preparing phase for use: GAS
Using global minimization procedure
Calculated 209 grid points in 0.023 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xn
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, P=10000000, N=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -5.22193E+04, Enthalpy 1.54600E+04, Volume 4.15726E-04

Component      Moles      M-Fraction Activity Potential Ref.stat
A               1.0000E+00  1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS              Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00 Mole fractions:
A 1.0000E+00
Constitution:
A 1.0000E+00 A2 8.75433E-20
POLY:Hit RETURN to continue
POLY:
POLY: @@ Set volume to 1 m3
POLY: s-c v
... the command in full is SET_CONDITION
Value /4.157255E-04/: 1
POLY: s-c n
... the command in full is SET_CONDITION
Value /1/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, P=10000000, V=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A               2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS              Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00 Mole fractions:
A 1.0000E+00
Constitution:
A 1.0000E+00 A2 8.75433E-20
POLY: s-c n
... the command in full is SET_CONDITION
Value /2405.433393/:
POLY: s-c p
... the command in full is SET_CONDITION
Value /10000000/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, N=2405.433393, V=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A               2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS              Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00 Mole fractions:
A 1.0000E+00
Constitution:
A 1.0000E+00 A2 8.75433E-20
POLY: enter var ha=h;
... the command in full is ENTER_SYMBOL
POLY: enter var sa=s;
... the command in full is ENTER_SYMBOL
POLY: s-c s
... the command in full is SET_CONDITION
Value /325596.1064/: sa
POLY: s-c v=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure

```

```

Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, N=2405.433393, S=SA
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
A              2.4054E+03  1.0000E+00  3.5061E-06 -5.2219E+04 SER

GAS              Status ENTERED   Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 8.75433E-20
POLY:Hit RETURN to continue
POLY:
POLY: show t,p,v,g,n,h,s
... the command in full is SHOW_VALUE
T=500
P=1E7
V=1.
G=-1.2561005E8
N=2405.4334
H=3.7188E7
S=325596.11
POLY:Hit RETURN to continue
POLY:
POLY: ent var ga=g;
... the command in full is ENTER_SYMBOL
POLY: ent var pa=p;
... the command in full is ENTER_SYMBOL
POLY: ent var va=v;
... the command in full is ENTER_SYMBOL
POLY: @@
POLY: @@
POLY: save tcex39a y
... the command in full is SAVE_WORKSPACES
POLY: s-c t=500
... the command in full is SET_CONDITION
POLY: s-c s=204200
... the command in full is SET_CONDITION
POLY: s-a-v l s 204000 205000,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 209 grid points in 0.007 s
17 ITS, CPU TIME USED 0 SECONDS
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 204200.
...OK

Phase Region from 204200. for:
GAS
Global test at 2.04400E+05 .... OK
Global test at 2.04650E+05 .... OK
Global test at 2.04900E+05 .... OK
Terminating at 205000.
Calculated 35 equilibria

Phase Region from 204200. for:
GAS
Global test at 2.04000E+05 .... OK
Terminating at 204000.
Calculated 11 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 2. Adiabatic expansion. No heat leaves the system,
POLY: @@ so the change in its entropy is zero. In the course of
POLY: @@ this expansion the temperature falls from T1 to T2, the
POLY: @@ temperature of cold reservoir.
POLY:
POLY: s-c s=205000
... the command in full is SET_CONDITION
POLY: s-c t=450
... the command in full is SET_CONDITION
POLY: s-a-v l t 400 500,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 209 grid points in 0.001 s
12 ITS, CPU TIME USED 0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

Phase Region from 450.000 for:
GAS
Global test at 4.70000E+02 .... OK
Global test at 4.95000E+02 .... OK
Terminating at 500.000
Calculated 23 equilibria

Phase Region from 450.000 for:
GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Terminating at 400.000
Calculated 23 equilibria

```

```

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 3. Isothermal compresion at T2. The heat Q2 is
POLY: @@ released to the cold reservoir, so the change in
POLY: @@ entropy of the system is -Q2/T2.
POLY:
POLY: s-c t=400
... the command in full is SET_CONDITION
POLY: s-c s=204200
... the command in full is SET_CONDITION
POLY: s-a-v l s 204000 205000,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          209 grid points in      0.003 s
      8 ITS, CPU TIME USED   0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value   204200.
...OK

Phase Region from   204200.      for:
GAS
Global test at 2.04400E+05 .... OK
Global test at 2.04650E+05 .... OK
Global test at 2.04900E+05 .... OK
Terminating at 205000.
Calculated 35 equilibria

Phase Region from   204200.      for:
GAS
Global test at 2.04000E+05 .... OK
Terminating at 204000.
Calculated 11 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 4. Adiabatic compression. No heat enters the system,
POLY: @@ so the change in entropy is zero. The temperature rises
POLY: @@ from T2 to T1.
POLY:
POLY: s-c s=204000
... the command in full is SET_CONDITION
POLY: s-c t=450
... the command in full is SET_CONDITION
POLY: s-a-v l t 400 500,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          209 grid points in      0.002 s
     10 ITS, CPU TIME USED   0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value   450.000
...OK

Phase Region from   450.000      for:
GAS
Global test at 4.70000E+02 .... OK
Global test at 4.95000E+02 .... OK
Terminating at 500.000
Calculated 23 equilibria

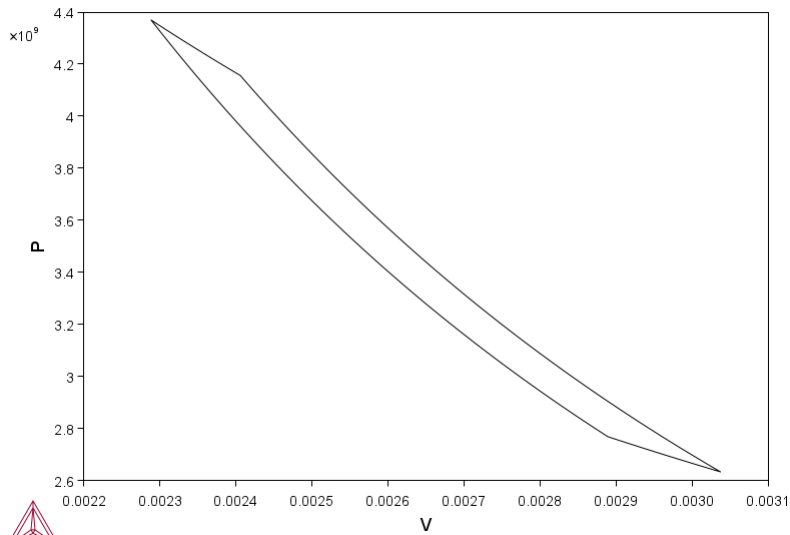
Phase Region from   450.000      for:
GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Terminating at 400.000
Calculated 23 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39a

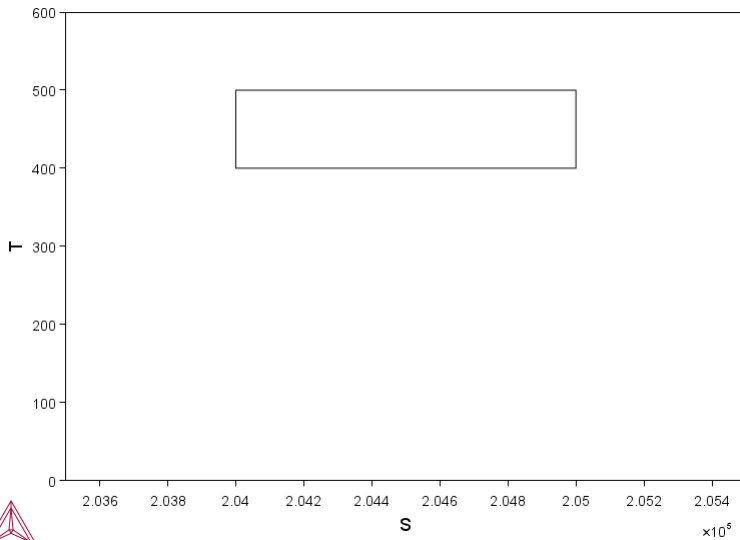


```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ The efficiency E of an engine which uses a Carnot
POST: @@ cycle is:
POST: @@ E=work performed/heat absorbed = W/Q1
POST: @@ If you plot the entropy versus temperature, you can
POST: @@ calculate the work performed just by calculating the
POST: @@ area of the surface depicted by the two squares and
POST: @@ by making the difference between them.
POST:
POST: s-d-a x s
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n 0 600
... the command in full is SET_SCALING_STATUS
POST: s-s x n 203500 205500
... the command in full is SET_SCALING_STATUS
POST: set-title example 39b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39b



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ The influence of the value of the temperature T1 (the
POST: @@ temperature of the hot reservoir) on the efficiency of the
POST: @@ Carnot cycle is important. Therefore we will make another
POST: @@ calculation for T1=800 K and compare with the one for
POST: @@ T1=500 K (example 39a and b). T2=400 K in both cases.
POST:
POST: ba
... the command in full is BACK
POLY: read,,,
... the command in full is READ_WORKSPACES
POLY: l-c
... the command in full is LIST_CONDITIONS
T=400, N=2405.433393, S=204000.
DEGREES OF FREEDOM 0
POLY: s-c s=None
... the command in full is SET_CONDITION

```

```

POLY: s-c t=800 p=1e7 n=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      209 grid points in      0.058 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
Output from POLY-3, equilibrium =      1, label A0 , database: User dat

Conditions:
T=800, P=10000000, N=1
DEGREES OF FREEDOM 0

Temperature      800.00 K (    526.85 C), Pressure  1.000000E+07
Number of moles of components  1.000000E+00, Mass in grams  1.000000E+01
Total Gibbs energy -9.41189E+04, Enthalpy  2.05600E+04, Volume  6.65161E-04

Component      Moles      M-Fraction Activity      Potential Ref.stat
A      1.0000E+00      1.0000E+00  7.1585E-07 -9.4119E+04 SER

GAS      Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 1.28633E-15
POLY: @@ Set volume to 1 m3
POLY: s-c v
... the command in full is SET_CONDITION
Value /6.651608E-04/: 1
POLY: s-c n
... the command in full is SET_CONDITION
Value /1/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
7 ITS, CPU TIME USED 0 SECONDS
POLY: s-c n
... the command in full is SET_CONDITION
Value /1503.395871/:
POLY: s-c p
... the command in full is SET_CONDITION
Value /10000000/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: enter var ha=h;
... the command in full is ENTER_SYMBOL
POLY: enter var sa=s;
... the command in full is ENTER_SYMBOL
POLY: s-c s
... the command in full is SET_CONDITION
Value /215509.7923/: sa
POLY: s-c v=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: show t,p,v,g,n,h,s
... the command in full is SHOW_VALUE
T=800
P=1E7
V=1.
G=-1.4149801E8
N=1503.3959
H=3.0909819E7
S=215509.79
POLY:Hit RETURN to continue
POLY:
POLY: save tcex39b y
... the command in full is SAVE_WORKSPACES
POLY: s-c s=272000
... the command in full is SET_CONDITION
POLY: s-a-v l s 270200 276200,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      209 grid points in      0.002 s
53 ITS, CPU TIME USED 0 SECONDS
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 272000.
...OK

Phase Region from 272000. for:
GAS
Global test at 2.73200E+05 .... OK
Global test at 2.74700E+05 .... OK
Global test at 2.76200E+05 .... OK
Terminating at 276200.
Calculated 31 equilibria

Phase Region from 272000. for:
GAS
Global test at 2.70800E+05 .... OK
Terminating at 270200.
Calculated 15 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c s=276200
... the command in full is SET_CONDITION
POLY: s-c t=750

```

```

... the command in full is SET_CONDITION
POLY: s-a-v l t 400 800,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      209 grid points in      0.002 s
      13 ITS, CPU TIME USED  0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value      750.000
...OK

Phase Region from      750.000      for:
      GAS
Terminating at      800.000
Calculated      8 equilibria

Phase Region from      750.000      for:
      GAS
Global test at      6.70000E+02 .... OK
Global test at      5.70000E+02 .... OK
Global test at      4.70000E+02 .... OK
Terminating at      400.000
Calculated      38 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c t=400
... the command in full is SET_CONDITION
POLY: s-c s=270250
... the command in full is SET_CONDITION
POLY: s-a-v l s 270200 276200,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      209 grid points in      0.002 s
      9 ITS, CPU TIME USED  0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value      270250.
...OK

Phase Region from      270250.      for:
      GAS
Global test at      2.71450E+05 .... OK
Global test at      2.72950E+05 .... OK
Global test at      2.74450E+05 .... OK
Global test at      2.75950E+05 .... OK
Terminating at      276200.
Calculated      43 equilibria

Phase Region from      270250.      for:
      GAS
Terminating at      270200.
Calculated      4 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c s=270200
... the command in full is SET_CONDITION
POLY: s-c t=750
... the command in full is SET_CONDITION
POLY: s-a-v l t 400 800,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      209 grid points in      0.002 s
      24 ITS, CPU TIME USED  0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value      750.000
...OK

Phase Region from      750.000      for:
      GAS
Terminating at      800.000
Calculated      8 equilibria

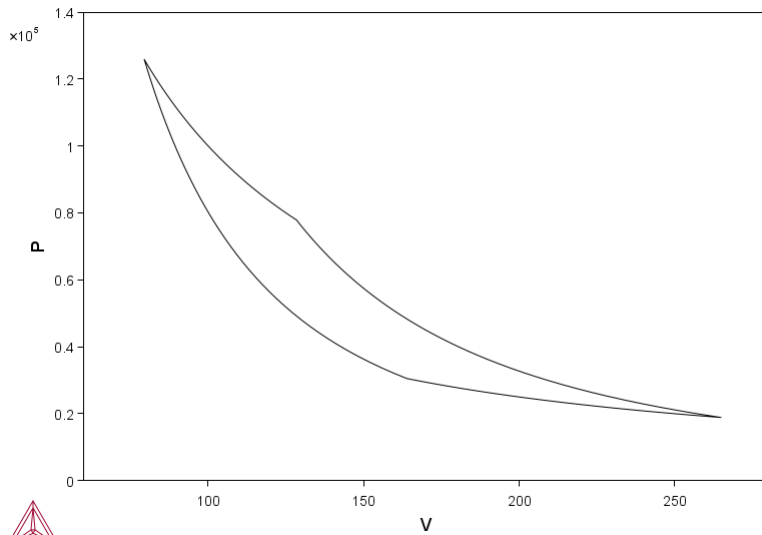
Phase Region from      750.000      for:
      GAS
Global test at      6.70000E+02 .... OK
Global test at      5.70000E+02 .... OK
Global test at      4.70000E+02 .... OK
Terminating at      400.000
Calculated      38 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY:
POLY: post
      POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39c

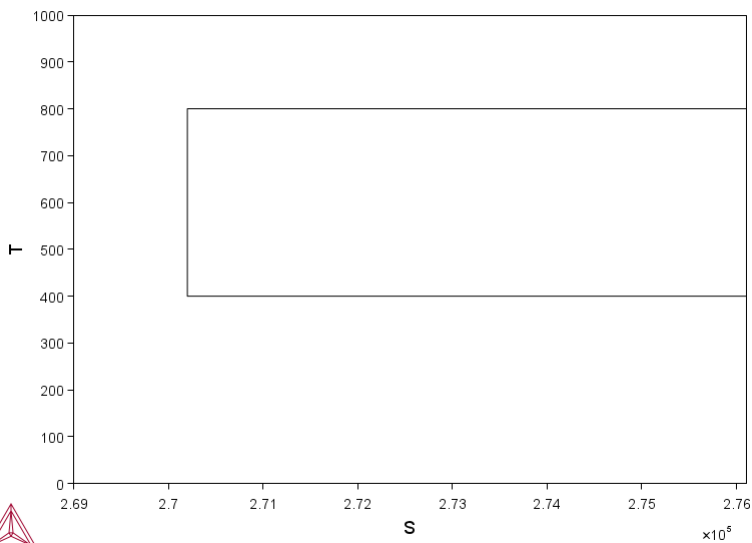


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x s
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 269000 276100
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1000
... the command in full is SET_SCALING_STATUS
POST: set-title example 39d
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39d



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ The efficiency for high value of T1 temperature is almost
POST: @@ double compared with that one for low value of T1
POST: @@ temperature (compare plot examples 39b with example 39d).
POST:
POST: @@ Now we will calculate the Carnot cycle for some real systems.
POST: @@ The most well known engine is the steam engine.
POST:
POST: @@ The Carnot cycle for steam engine
POST:
POST: ba
... the command in full is BACK
POLY: go da
... the command in full is GOTO_MODULE
TDB_TCFE11: rej sys
... the command in full is REJECT
VA /- DEFINED
DICTRA FCC_A1 REJECTED
REINITIATING GES .....
TDB_TCFE11: sw subdemo
... the command in full is SWITCH_DATABASE
Current database: Substance Demo Database v1.0
VA /- DEFINED
TDB_SUBDEMO: def-sp h2o1
... the command in full is DEFINE_SPECIES

```



```

H2O1 DEFINED
TDB_SUBDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
GAS:G      :H2O1:
H2O1_L     :H2O1:
TDB_SUBDEMO: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_SUBDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS    REF. STATE    T(K)          P(Pa)
VA              ENTERED    SER
H               ENTERED    SER
O               ENTERED    SER
*** STATUS FOR ALL PHASES
PHASE          STATUS    DRIVING FORCE    MOLES
H2O1_L         ENTERED    0.000000E+00    0.000000E+00
GAS            ENTERED    0.000000E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
H ENTERED      H2O1 ENTERED    O ENTERED      VA ENTERED
POLY: c-st p h2o_l=sus
... the command in full is CHANGE_STATUS
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS    REF. STATE    T(K)          P(Pa)
VA              ENTERED    SER
H               ENTERED    SER
O               ENTERED    SER
*** STATUS FOR ALL PHASES
PHASE          STATUS    DRIVING FORCE    MOLES
GAS            ENTERED    0.000000E+00    0.000000E+00
SUSPENDED PHASES:
H2O1_L
*** STATUS FOR ALL SPECIES
H ENTERED      H2O1 ENTERED    O ENTERED      VA ENTERED
POLY: @@ The Carnot cycle will be calculated for T1=350 K and T2=450 K
POLY:
POLY: s-c t=380 p=1e5 n=100 ac(o)=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      1 grid points in      0.001 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:
T=380, P=100000, N=100, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 380.00 K ( 106.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.04643E+07, Enthalpy -7.96861E+06, Volume 1.05317E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
H               6.6667E+01 6.6667E-01 2.6556E-22 -1.5697E+05 SER
O               3.3333E+01 3.3333E-01 1.0000E+00 0.0000E+00 SER

GAS              Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY: s-c p=None
... the command in full is SET_CONDITION
POLY: s-c s
... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY: s-c t=350
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      1 grid points in      0.000 s
11 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:
T=350, N=100, AC(O)=1, S=6100
DEGREES OF FREEDOM 0

Temperature 350.00 K ( 76.85 C), Pressure 3.863619E+05
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.01376E+07, Enthalpy -8.00259E+06, Volume 2.51067E-01

Component      Moles      M-Fraction Activity Potential Ref.stat
H               6.6667E+01 6.6667E-01 2.0244E-23 -1.5206E+05 SER
O               3.3333E+01 3.3333E-01 1.0000E+00 0.0000E+00 SER

```

```

GAS                      Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY: @@ step in S with t=350
POLY: s-a-v l s 6000 7000,,,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex39c y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

Phase Region from 6100.00 for:
GAS
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global test at 6.80000E+03 .... OK
Terminating at 7000.00
Calculated 39 equilibria

Phase Region from 6100.00 for:
GAS
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY:
POLY: read,,,,
... the command in full is READ_WORKSPACES
POLY: s-c s=6000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0.000 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: @@ step in T with S=6000
POLY: s-a-v l t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 350.000
...OK

Phase Region from 350.000 for:
GAS
Global test at 3.70000E+02 .... OK
Global test at 3.95000E+02 .... OK
Global test at 4.20000E+02 .... OK
Global test at 4.45000E+02 .... OK
Terminating at 450.000
Calculated 43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: read,,,,
... the command in full is READ_WORKSPACES
POLY: s-c t=450
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0.000 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Step in S with t=450
POLY: s-a-v l s 6000 7000,,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6000.00
...OK

Phase Region from 6000.00 for:
GAS
Global test at 6.20000E+03 .... OK
Global test at 6.45000E+03 .... OK
Global test at 6.70000E+03 .... OK
Global test at 6.95000E+03 .... OK
Terminating at 7000.00
Calculated 43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: s-c s=7000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0.000 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Step in T with S=7000
POLY: s-a-v l t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

Phase Region from 450.000 for:
GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Global test at 3.80000E+02 .... OK
Global test at 3.55000E+02 .... OK
Terminating at 350.000
Calculated 43 equilibria

```

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39c.POLY3

POLY:

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-p-f ##1,,,,,,,,

... the command in full is SET_PLOT_FORMAT
CURRENT DEVICE: TC-UNITE Driver

POST:

POST: s-d-a x v

... the command in full is SET_DIAGRAM_AXIS

POST: s-d-a y p

... the command in full is SET_DIAGRAM_AXIS

POST: set-title example 39e

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

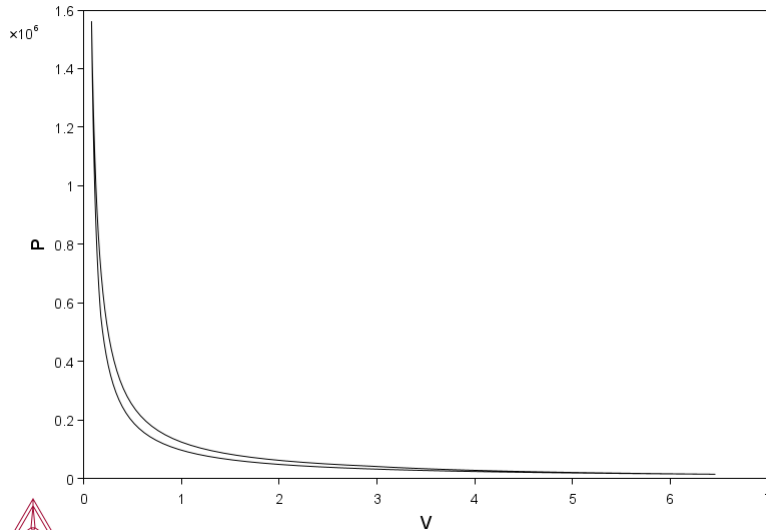
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 39e



POST:

POST:Hit RETURN to continue

POST:

POST: s-a-ty y log

... the command in full is SET_AXIS_TYPE

POST: s-lab b

... the command in full is SET_LABEL_CURVE_OPTION

POST: set-title example 39f

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

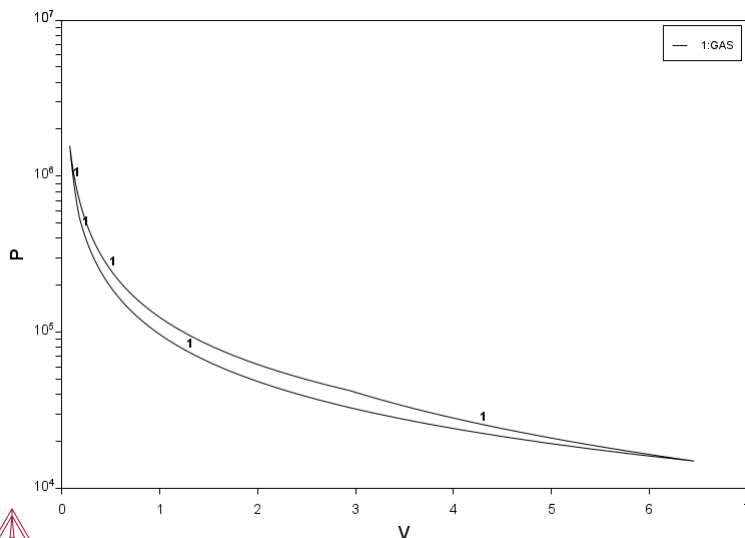
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 39f



POST:

POST:Hit RETURN to continue

POST:

POST: @@ It is a bit difficult to distinguish from the calculated

POST: @@ diagram, example 39e, where the adiabatic expansion and

POST: @@ compresion start. Therefore it is good to plot temperature

POST: @@ on the same diagram.

example 39g



Use the command `LIST_REFERENCES` to see the list of references for assessed data

```

SPECIES                                STOICHIOMETRY
  1 H                                80800000 H
  2 H2O1                             00000000 H2O1
  3 O                                 80800000 O
  4 VA                               81800000 VA

GES6: @@ patch
GES6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)            P(Pa)
VA              ENTERED    SER
H              ENTERED    SER
O              ENTERED    SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
H2O1_L         ENTERED    0.000000E+00    0.000000E+00
GAS            ENTERED    0.000000E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
H  ENTERED    H2O1 ENTERED    O  ENTERED    VA  ENTERED
POLY: c-st p h2o_l=e 0
... the command in full is CHANGE_STATUS
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)            P(Pa)
VA              ENTERED    SER
H              ENTERED    SER
O              ENTERED    SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
H2O1_L         ENTERED    0.000000E+00    0.000000E+00
GAS            ENTERED    0.000000E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
H  ENTERED    H2O1 ENTERED    O  ENTERED    VA  ENTERED
POLY: s-c t=380 p=1e5 n=100 ac(o)=1
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=380, P=100000, N=100, AC(O)=1
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      2 grid points in      0.000 s
      6 ITS, CPU TIME USED  0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VNNS/: xn
Output from POLY-3, equilibrium =      1, label A0 , database: SUBDEMO

Conditions:
T=380, P=100000, N=100, AC(O)=1
DEGREES OF FREEDOM 0

Temperature      380.00 K ( 106.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.04643E+07, Enthalpy -7.96861E+06, Volume 1.05317E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
H              6.6667E+01  6.6667E-01 2.6556E-22 -1.5697E+05 SER
O              3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

GAS            Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY: s-c p=none
... the command in full is SET_CONDITION
POLY: s-c s
... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY: s-c t=350
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      2 grid points in      0.000 s
      36 ITS, CPU TIME USED  0 SECONDS
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: SUBDEMO

Conditions:
T=350, N=100, AC(O)=1, S=6100
DEGREES OF FREEDOM 0

Temperature      350.00 K ( 76.85 C), Pressure 4.130269E+04
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.03545E+07, Enthalpy -8.21947E+06, Volume 1.98337E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
H              6.6667E+01  6.6667E-01 6.6188E-24 -1.5532E+05 SER
O              3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

GAS            Status ENTERED      Driving force 0.0000E+00
Moles 8.4450E+01, Mass 5.0711E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00

H2O1_L         Status ENTERED      Driving force 0.0000E+00
Moles 1.5550E+01, Mass 9.3379E+01, Volume fraction 0.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:

```

```

H2O1 1.00000E+00
POLY: @@ step in S with t=350
POLY: s-a-v l s 6000 7000,,,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex39d y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

Phase Region from 6100.00 for:
GAS
H2O1_L
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global check of removing phase at 6.71967E+03
Calculated 27 equilibria

Phase Region from 6719.67 for:
GAS
Global test at 6.90000E+03 .... OK
Terminating at 7000.00
Calculated 15 equilibria

Phase Region from 6100.00 for:
GAS
H2O1_L
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: read,,,,
... the command in full is READ_WORKSPACES
POLY: s-c s=6000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 2 grid points in 0.000 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: @@ step in T with S=6000
POLY: s-a-v l t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 350.000
...OK

Phase Region from 350.000 for:
GAS
H2O1_L
Global test at 3.70000E+02 .... OK
Global test at 3.95000E+02 .... OK
Global test at 4.20000E+02 .... OK
Global test at 4.45000E+02 .... OK
Terminating at 450.000
Calculated 43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: read,,,,
... the command in full is READ_WORKSPACES
POLY: s-c t=450
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 2 grid points in 0.000 s
6 ITS, CPU TIME USED 1 SECONDS
POLY: @@ Step in S with t=450
POLY: @@
POLY: s-a-v l s 6000 7000,,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6000.00
...OK

Phase Region from 6000.00 for:
GAS
H2O1_L
Global check of removing phase at 6.16203E+03
Calculated 9 equilibria

Phase Region from 6162.03 for:
GAS
Global test at 6.35000E+03 .... OK
Global test at 6.60000E+03 .... OK
Global test at 6.85000E+03 .... OK
Terminating at 7000.00
Calculated 37 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: s-c s=7000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 2 grid points in 0.000 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Step in T with S=7000
POLY: s-a-v l t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

```

```

Phase Region from    450.000    for:
  GAS
Global test at    4.30000E+02 .... OK
Global test at    4.05000E+02 .... OK
Global test at    3.80000E+02 .... OK
Global test at    3.55000E+02 .... OK
Terminating at      350.000
Calculated      43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex39\tcex39d.POLY3

```

POLY:

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: @@ The cycle shows the constant pressure at phase transformation.

POST: s-p-f ##1,,,,,,,,

... the command in full is SET_PLOT_FORMAT

CURRENT DEVICE: TC-UNITE Driver

POST:

POST: @@ To get a better understanding of this process it is possible

POST: @@ to plot the cycle using any set of thermodynamic state

POST: @@ variables. From the pressure-volume-temperature diagram,

POST: @@ example 39g, you can see the temperature variation on the

POST: @@ two adiabatical stages of the Carnot cycle.

POST: @@ The cycle shows the constant pressure at phase

POST: @@ transformation.

POST:

POST: s-d-a x v

... the command in full is SET_DIAGRAM_AXIS

POST: s-d-a y p

... the command in full is SET_DIAGRAM_AXIS

POST: set-title example 39h

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

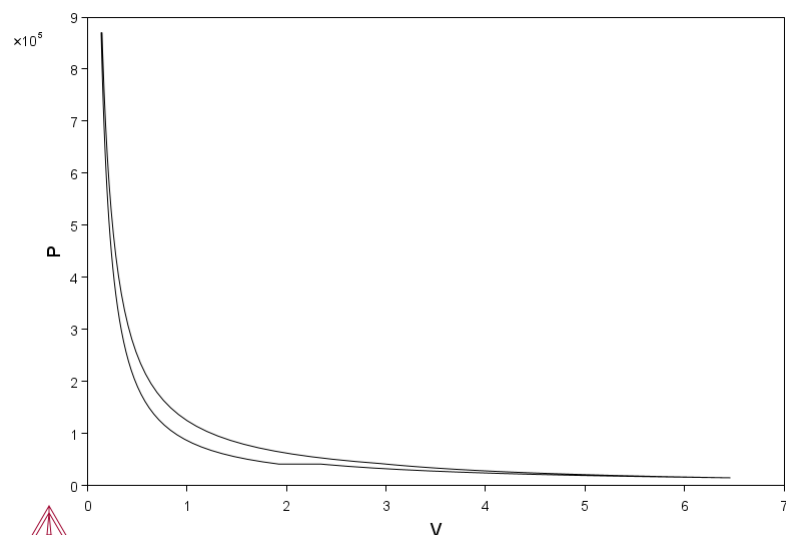
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 39h



POST:

POST: Hit RETURN to continue

POST:

POST: s-a-ty y log

... the command in full is SET_AXIS_TYPE

POST: s-lab b

... the command in full is SET_LABEL_CURVE_OPTION

POST: s-tit example 39i

... the command in full is SET_TITLE

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

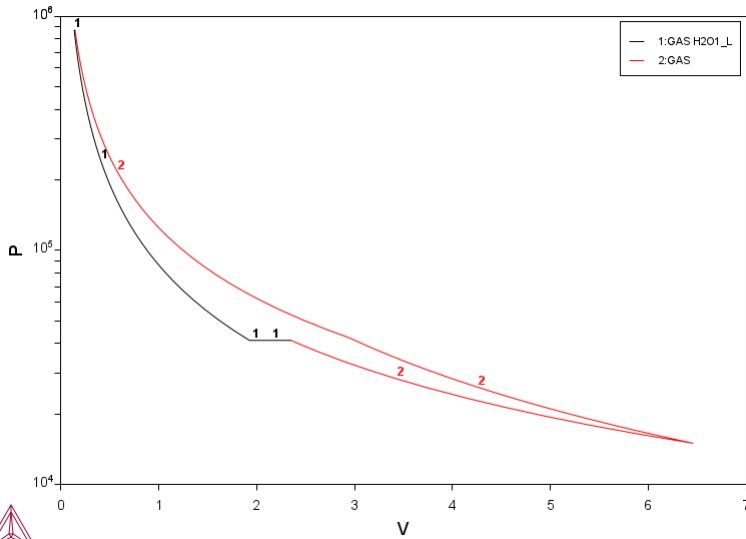
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 39i

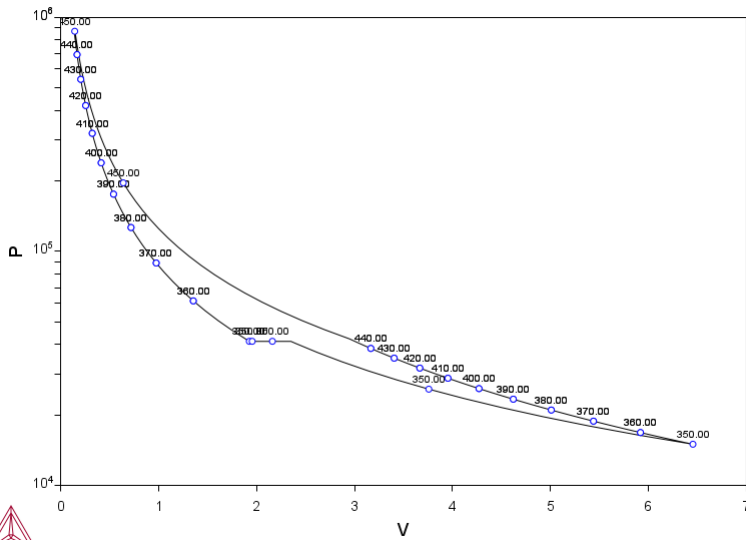


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39j
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39j

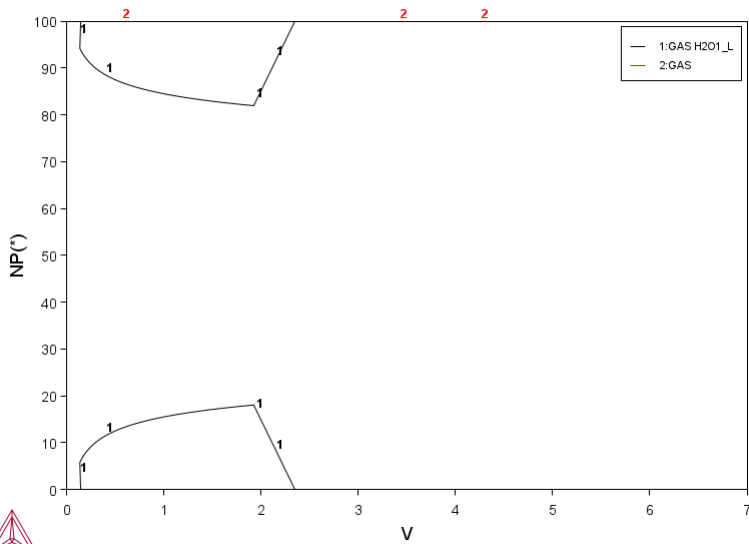


```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ Another interesting aspect is it plots the amount of phases
POST: @@ versus volume. You can get information about both the kind
POST: @@ and amount of phases that fill up a certain volume.
POST:
POST: s-d-a z none
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*),,,
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty Y,,,
... the command in full is SET_AXIS_TYPE
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39k
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

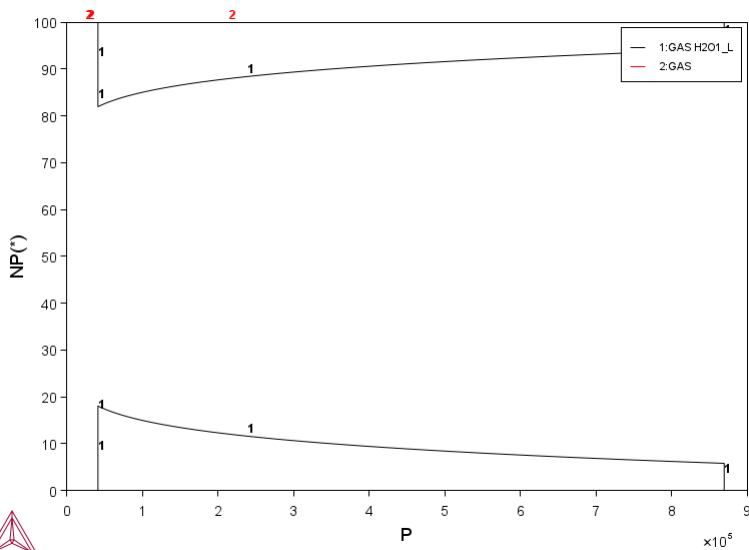
```


example 39k



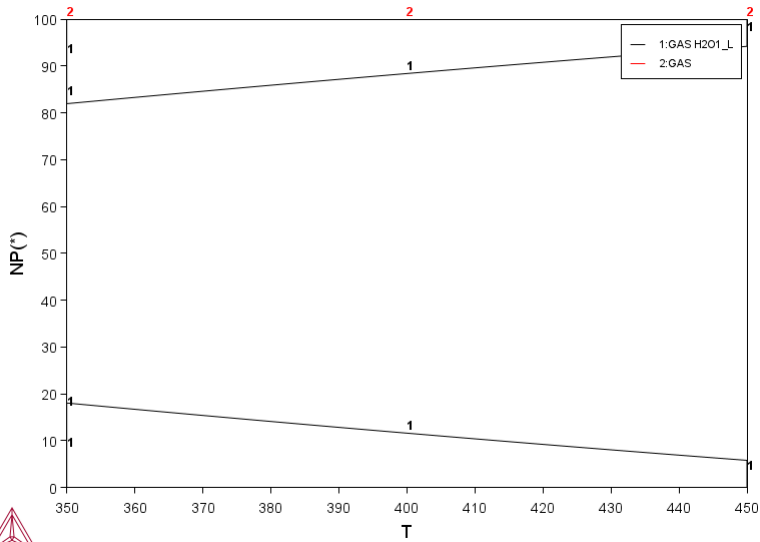
```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ The next plot shows the amount of phases versus pressure. It
POST: @@ gives important information on the phase transformation
POST: @@ pressure and on the ratio between the two phases in
POST: @@ equilibrium at a certain pressure.
POST:
POST: s-d-a x p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39l
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 39l



```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ By plotting the amount of phases versus temperature,
POST: @@ example 39k, it is possible to know the phase transformation
POST: @@ temperature and the ratio between the two phases in
POST: @@ equilibrium at a certain temperature.
POST:
POST: s-d-a x t
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39m
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 39m

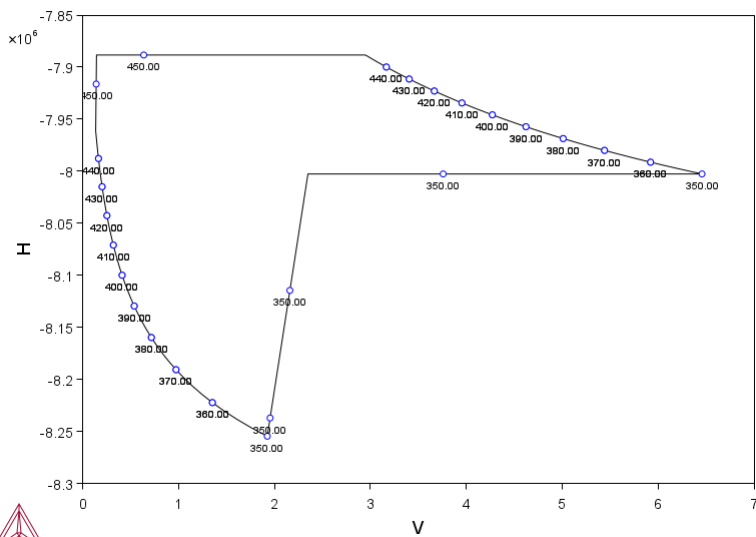


```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ The enthalpy and Gibbs energy for the Carnot cycle could
POST: @@ also be plotted using the same calculation but a different
POST: @@ set for diagram axis. Note the important drop of the
POST: @@ enthalpy at the phase transformation point, example 39L.
POST:
POST: s-lab none
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y h
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39n
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39n

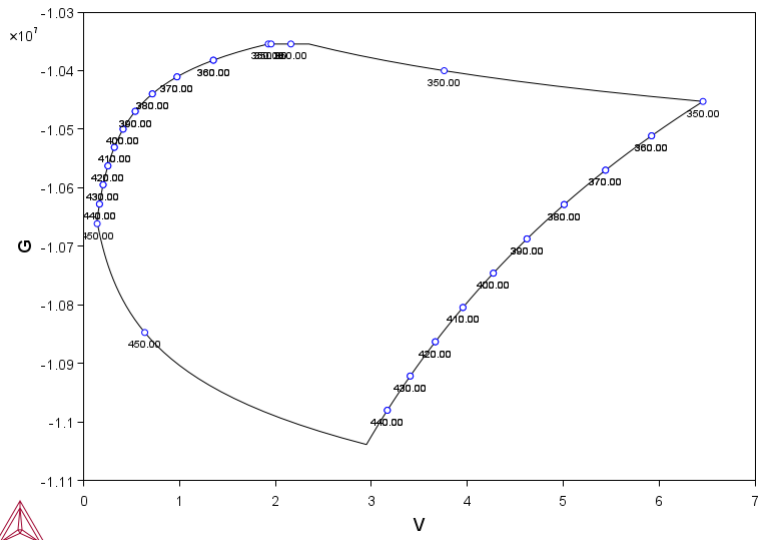


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y g
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39o
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39o



POST:
 POST:Hit RETURN to continue
 POST:
 POST: set-inter
 ... the command in full is SET_INTERACTIVE_MODE
 POST:

tcex40-TCEX40

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex40\TCEX40.TCM.test"
```

```
SYS: @@ Working with the POURBAIX module.
```

```
SYS: go sys
```

```
SYS: set-echo
```

```
SYS:
```

```
SYS: set-log TCEX40.LOG
```

```
Heading: Part 1 - Pourbaix Diagram Calculations with the advanced POURBAIX module
```

```
SYS: set-ges 5
```

```
... the command in full is SET_GES_VERSION
```

```
SYS:
```

```
SYS: @@ Part 1 - Pourbaix Diagram Calculations with the advanced POURBAIX module
```

```
SYS:
```

```
SYS:
```

```
SYS: @@ Delete both for Windows and Linux to be able to run macro twice without stumbling on existing EXP file
```

```
SYS:
```

```
SYS: @@ TCEX40: Thermo-Calc (Console Mode) Standard Example No 40
```

```
SYS: @@ =====
```

```
SYS: @@ Copyright: Thermo-Calc Software AB, Stockholm, Sweden
```

```
SYS: @@ Developer: Dr. Pingfang Shi, Thermo-Calc Software AB
```

```
SYS: @@ Date: 2014-05-18 (revision)
```

```
SYS: @@ Text updated July 2021 (AJW)
```

```
SYS:
```

```
SYS: @@ =====
```

```
SYS: @@ Example description:
```

```
SYS: @@ =====
```

```
SYS: @@ TCEX40 is the first in a series of examples to demonstrate
```

```
SYS: @@ the POURBAIX module calculations and plotting.
```

```
SYS: @@ - Uses Option 1: Start a new Pourbaix diagram calculation
```

```
SYS: @@ - Part 1 of a 5 part example.
```

```
SYS: @@ - Note that example 40D is deprecated as of version 2022a.
```

```
SYS: @@ - Uses the TCS Public Aqueous Solution Database (PAQ2);
```

```
SYS: @@ - For the Fe-H2O-NaCl heterogeneous interaction system
```

```
SYS:
```

```
SYS: @@ The example automatically calculates and plots a Pourbaix
```

```
SYS: @@ diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at
```

```
SYS: @@ 25 C and 1 bar. Other diagrams, along various phase
```

```
SYS: @@ boundaries for the same interactions resulting from the
```

```
SYS: @@ same Pourbaix module calculation, are also plotted.
```

```
SYS:
```

```
SYS: @@ =====
```

```
SYS: @@ Notes about the examples and the PAQ2 database:
```

```
SYS: @@ =====
```

```
SYS: @@ The so-called Pourbaix diagram is actually a phase diagram
```

```
SYS: @@ with independently-varied electropotential (Eh) and
```

```
SYS: @@ acidity (pH), for a heterogeneous interaction system at a
```

```
SYS: @@ certain bulk composition (that is by default always set as
```

```
SYS: @@ 1 kg of water solving a specified amount of metals and
```

```
SYS: @@ other solutes), under defined temperature and pressure
```

```
SYS: @@ conditions.
```

```
SYS:
```

```
SYS: @@ This example uses Option 1 followed by a choice of a
```

```
SYS: @@ single database, i.e., retrieving data from the PAQ2
```

```
SYS: @@ database. For this and other Thermo-Calc simulations,
```

```
SYS: @@ it can also be done with the TDB-GES-POLY-POST routine,
```

```
SYS: @@ which is used in example TCEX53.
```

```
SYS:
```

```
SYS: @@ The PAQ2 database is specially designed for Pourbaix
```

```
SYS: @@ diagram calculations (i.e., Eh-pH plots). It contains an
```

```
SYS: @@ AQUEOUS solution phase and REF_ELECTRODE phase (as a
```

```
SYS: @@ reference for electron in aqueous electrolyte systems),
```

```
SYS: @@ as well as some data for various solid phases (solution
```

```
SYS: @@ or stoichiometric) and a gaseous mixture phase.
```

```
SYS:
```

```
SYS: @@ A POLY3 file (POURBAIX.POLY3) is automatically saved at the
```

```
SYS: @@ end of the calculation. The POURBAIX.POLY3 file can be used
```

```
SYS: @@ with the other options and examples:
```

```
SYS: @@ Option 2: to plot other property diagrams of the calculated
```

```
SYS: @@ interaction system. See TCEX40B.
```

```
SYS: @@ Option 3: to make another Pourbaix calculation of the same
```

```
SYS: @@ chemical system but under different P-T-X
```

```
SYS: @@ conditions. See TCEX40C.
```

```
SYS:
```

```
SYS: @@ ** If you use the POLY3 file with the other examples it is
```

```
SYS: @@ important to make copies and rename these (for example
```

```
SYS: @@ TCEX40A.POLY3, TCEX40B.POLY3, etc.). This must be done
```

```
SYS: @@ outside of the Thermo-Calc software and after the TCEX40
```

```
SYS: @@ calculation and plotting is complete. This is so that the
```

```
SYS: @@ required POLY3 file structure is not lost.
```

```
SYS:
```

```
SYS: @@ ** A more advanced version of 40 and 40A can be found in
```

```
SYS: @@ TCEX40E, which also uses Option 1 but with multiple
```

```
SYS: @@ databases. However, licenses are required for three
```

```
SYS: @@ commercial Thermo-Calc databases. See the online help
```

```
SYS: @@ and the 40E macro text.
```

```
SYS: @@ -----
```

```
SYS:
```

```
SYS: @@... Now, let's start using the advanced POURBAIX module:
```

```
SYS: @@
```

```
SYS: go pour
```

```
... the command in full is GOTO_MODULE
```

```
WELCOME TO THE POURBAIX MODULE
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
for Quick Calculations of Pourbaix Diagrams
```

=====

Pingfang Shi and Bo Sundman
Thermo-Calc Software AB
Norra Stationsgatan 93
SE-113 47 Stockholm, Sweden

(Version 7.0, Mar. 2014)

Need any instruction on the POURBAIX module? /N/: ?

IMPORTANT NOTES for Calculating a POURBAIX Diagram:

- 1) The so-called Pourbaix diagram is actually a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (Eh, as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modelled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).
 - 2) One must have at least a database containing an AQUEOUS solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc database spectrum, or be chosen from an appropriate USER-specified database (it must be in the Thermo-Calc TDB format).
 - 3) Due to the restrictions of aqueous solution model used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ) or AQS (PAQS) for AQUEOUS solution phase. Among others, one should keep in mind the following regulations:
 - * The ELECTRON is defined as a special element (ZE) and as the only constituent in its reference phase REFERENCE ELECTRODE (for determining the electropotential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;
 - * The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;
 - * The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.
 - 4) Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H₂O, O₂ and H₂; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!
 - 5) All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a Gaseous mixture phase, a REF ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above). Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the TCAQ or AQS as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAl, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for Gaseous mixture phase and for various solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.
 - 6) The current advanced POURBAIX-Module has been designed and developed in an efficient and effective way that it only requires the user to just answer some simple and necessary questions, rather than to go through basic modules (i.e., TDB, GES5, POLY3 and POST) and type the ordinary command-lines. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.
 - 7) The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-PLOY3-POST calculation.
-

Enforce a PAUSE after plotting when running a MACRO? /N/: ?

Whenever running a Thermo-Calc MACRO (TCM) file, you may prefer to have a PAUSE after a specific diagram has been

plotted on SCREEN, for the multiple purposes of efficiently and easily manipulating the plotted diagram directly on the traditional TC-Graph window or Java-based TC-UNITE window, such as:

- * Printing it (of EMF/PS format) on connected printer(s);
- * Converting it (of EMF format) to (PDF) graphical files;
- * Saving it as an EMF graphical file;
- * Dumping it as a PNG or BMP graphical file;
- * Setting background colour for the current diagram and for all the sequential plots;
- * Setting default font/size for all the sequential plots;
- * Changing plotting Layers for all the sequential plots.

If no PAUSE is enforced, the POURBAIX Module will be going through all the sequential command-lines (answers) in the same POURBAIX session or till the SET_INTERACTIVE_MODE line in the MACRO file has been reached.

** By Y(y), a PAUSE is always enforced after each diagram;
** By N(n), no PAUSE will be enforced at any point at all.

Please then press <RETURN> at the PAUSE for continuation!

Enforce a PAUSE after plotting when running a MACRO? /N/: y

|
| 1. Start a completely new POURBAIX diagram calculation |
| 2. Open an old file & plot other property diagrams |
| 3. Open an old file & make another POURBAIX calculation |
| 4. Open an old file & make another STEPPING calculation |
|
|-----|

Select option /1/: ?

One of the four options (1/2/3/4) should be entered here:

- 1 -- Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram.
i.e., define a new chemical system;
specify the T-P-X conditions;
calculate the initial equilibria;
perform the pH-Eh mapping calculation;
plot pH-Eh & various property diagrams.
- 2 -- Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and just selectively plot other property diagrams.
i.e., open the old GES and POLY3 workspaces;
plot pH-Eh or various property diagrams.
- 3 -- Open an existing POLY3 file created by POURBAIX Module and make another POURBAIX diagram calculation.
i.e., open the old GES and POLY3 workspaces;
adopt the defined chemical system;
modify the T-P-X conditions;
calculate the initial equilibria;
perform the pH-Eh mapping calculation;
plot pH-Eh & various property diagrams.
- 4 -- Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation.
i.e., open the old GES and POLY3 workspaces;
adopt the defined chemical system;
specify one of the T-P-X conditions as the stepping variable;
calculate the initial equilibria;
perform the stepping calculation;
plot various property diagrams.

Select option /1/: 1

- 1 -- Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram.
i.e., define a new chemical system;
specify the T-P-X conditions;
calculate the initial equilibria;
perform the pH-Eh mapping calculation;
plot pH-Eh & various property diagrams.

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: ?

You may optionally choose to ignore the GAS mixture phase on a calculated/plotted Pourbaix diagram. However, such a plot is actually not a complete Pourbaix diagram, due to that the thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will not be calculated at all.

** By Y(y), GAS mixture phase shall be always considered;
** By N(n), GAS mixture phase will be completely ignored.

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: Y

Use single database? /Y/: Y

Combined Database: /PAQ2/: PAQ2

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data
Current database: Public Aqueous Solution (SIT) v2.5

H	O	ZE
VA DEFINED		
LIQUID:L REJECTED		
GRAPHITE	DIAMOND_A4	FC_ORTHORHOMBIC
MONOCLINIC REJECTED		
CBCC_A12	CUB_A13	CHI_A12
FE4N	FECN_CHI REJECTED	

CEMENTITE	M23C6	M7C3
M5C2	M3C2	KSI_CARBIIDE
PI REJECTED		
FE3C	NI3C	CR3C2
CR7C3	CR23C6 REJECTED	
COCO3	FECO3	NAHCO3
NA2CO3_S1	NA2CO3_S2	NICO3
CRC6O6 REJECTED		
CO3N	CRN	CR2N
FE2N	NI3N REJECTED	
NANO2_S1	NANO2_S2	NANO3
REJECTED		
COCL2	CRCL2	CRCL3
FECL2	FECL3	NICL2
REJECTED		
FECLO	NACLO4_S1	NACLO4_S2
REJECTED		

DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:

=====

Normally a POURBAIX diagram and related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

CHEMICAL SYSTEM (ELEMENTS):

Default defined elements (solvent H2O): H & O
and specially assigned ZE(electron) & VA(vacancy).
Prompt specified elements (solutes ELEM):
Fe Ni Co Cr C N S Na Cl

INITIAL BULK COMPOSITION:

Default defined composition (solvent): 1.0 kg of H2O
Prompt specified composition (solutes): x mole of ELEM

Notes: For accepting a default value, just RETURN at prompt;
For changing to a specific value, enter it at prompt.

=====

IMPORTANT NOTE for Entering Solutes in Chemical Formulas:
First element letter in UPPER case, and second lower case!
such as NaCl CO2 CoCl3 Fe0.93S NaSO4-1 H2SO4

Mass of Water (weight) = 1 kg

First solute: Fe
Molality of Fe [mol/kg] /.001/: .001
Second solute: NaCl .1
Next solute:

Defined chemical system and initial bulk composition:

Note: Solutes have been split up into chemical elements and their mole numbers. If confirmed, the POURBAIX Module will, in further steps, count the initial bulk composition in terms of chemical elements.

H2O	1.00000000	kg
ZE	(specially assigned)	
FE	0.1000000000E-02	mole
CL	0.1000000000E+00	mole
NA	0.1000000000E+00	mole

Confirm defined system and initial bulk composition? /Y/: Y

RETRIEVE THERMODYNAMIC DATA FROM THE DATABASE: PAQ2

H	O	ZE
VA DEFINED		
LIQUID:L REJECTED		
GRAPHITE	DIAMOND_A4	FC_ORTHORHOMBIC
MONOCLINIC REJECTED		
CBCC_A12	CUB_A13	CHI_A12
FE4N	FECN_CHI REJECTED	
CEMENTITE	M23C6	M7C3
M5C2	M3C2	KSI_CARBIIDE
PI REJECTED		
FE3C	NI3C	CR3C2
CR7C3	CR23C6 REJECTED	
COCO3	FECO3	NAHCO3
NA2CO3_S1	NA2CO3_S2	NICO3
CRC6O6 REJECTED		
CO3N	CRN	CR2N
FE2N	NI3N REJECTED	
NANO2_S1	NANO2_S2	NANO3
REJECTED		
COCL2	CRCL2	CRCL3
FECL2	FECL3	NICL2
REJECTED		
FECLO	NACLO4_S1	NACLO4_S2
REJECTED		
REINITIATING GES		
FE DEFINED		
CL DEFINED		
NA DEFINED		
/- DEFINED		

This database has following phases for the defined system

AQUEOUS:A	REF ELECTRODE	GAS:G
FCC_A1	BCC_A2	HCP_A3
HALITE	WUSTITE	MAGNETITE
HEMATITE	FE2O3_GAMMA	FE02H2
FE03H3	FE0OH	FE2O2O2H2
NAO2	NA2O_S1	NA2O_S2
NA2O_S3	NA2O2_S1	NA2O2_S2
NAOH_S1	NAOH_S2	NA2FE02
Reject phase(s) /NONE/: HCP_A3		
HCP A3 REJECTED		
Reject phase(s) /NONE/: NONE		

Restore phase(s) : /NONE/: NONE

.....

The following phases are retained in this system:

AQUEOUS:A	REF_ELECTRODE	GAS:G
FCC_A1	BCC_A2	HALITE
WUSTITE	MAGNETITE	HEMATITE
FE2O3_GAMMA	FE02H2	FE03H3
FE0OH-	FE2O2O2H2	NAO2
NA2O_S1	NA2O_S2	NA2O_S3
NA2O2_S1	NA2O2_S2	NAOH_S1
NAOH_S2	NA2FE02	

.....

OK? /Y/: Y

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

..... Reinitializing POLY3 workspaces

Enforce Global Minimization Technique in calculations? /N/: N

Save all functions, variables and tables in POLY3 file? /Y/: Y

Set numerical limits? /N/: N

SET CALCULATING PARAMETERS:

List of Default and Pre-defined Calculation Conditions:

Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole

T=298.15, P=100000, B(H2O)=1000, N(H+1)=0, N(ZE)=0, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

DEGREES OF FREEDOM 0

Confirm defined conditions? /Y/: Y

Calculating start points; please be patient!

LIST THE FIRST DEFAULT STARTING EQUILIBRIUM POINT:

Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:

T=298.15, P=100000, B(H2O)=1000, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1, LNACR(H+1)=-16.11809565, MUR(ZE)=100

DEGREES OF FREEDOM 0

Temperature 298.15 K (25.00 C), Pressure 1.000000E+05

Number of moles of components 5.57094E+01, Mass in grams 1.00590E+03

Total Gibbs energy -1.70696E+07, Enthalpy -1.59069E+07, Volume 0.00000E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
CL	1.0000E-01	1.7950E-03	1.4499E-30	-1.7032E+05	SER
FE	1.0000E-03	1.7950E-05	4.6321E-26	-1.4461E+05	SER
H+1	-3.0000E-03	-5.3851E-05	1.0000E-07	-3.9956E+04	SER
NA	1.0000E-01	1.7950E-03	1.7205E-50	-2.8406E+05	SER
H2O	5.5508E+01	9.9639E-01	9.9593E-01	-1.0110E+01	AQUEOUS
ZE	3.0000E-03	5.3851E-05	1.0412E+00	1.0000E+02	REF_ELEC

AQUEOUS Status ENTERED Driving force 0.0000E+00

Moles 5.5707E+01, Mass 1.0058E+03, Volume fraction 0.0000E+00 Mole fractions:

H2O 9.96410E-01 NA 1.79511E-03 FE 1.08146E-11

CL 1.79511E-03 ZE 2.03382E-11 H+1 -1.36468E-11

Constitution:	SiteFraction	Molality	Activity	log10Act
H2O	9.96410E-01	5.55084E+01	9.96012E-01	-0.0017
CL-1	1.79511E-03	1.00003E-01	7.76756E-02	-1.1097
NA+1	1.79511E-03	1.00003E-01	7.76756E-02	-1.1097
OH-1	2.31689E-09	1.29070E-07	1.00218E-07	-6.9991
H+1	2.30788E-09	1.28568E-07	1.00000E-07	-7.0000
FE+2	6.21477E-12	3.46215E-10	1.26203E-10	-9.8989
FE0H+1	4.59380E-12	2.55913E-10	1.99003E-10	-9.7011
O3	1.00000E-15	0.00000E+00	2.6033E-113	-112.5845
H2O2	1.00000E-15	0.00000E+00	3.63324E-46	-45.4397
HClO	1.00000E-15	0.00000E+00	3.55905E-45	-44.4487
H2	1.00000E-15	0.00000E+00	5.46000E-18	-17.2628
HClO2	1.00000E-15	0.00000E+00	1.38939E-87	-86.8572
FE0H+2	1.00000E-15	0.00000E+00	9.27035E-19	-18.0329
HO2-1	1.00000E-15	0.00000E+00	7.68880E-51	-50.1141
FE03H3-1	1.00000E-15	0.00000E+00	1.69673E-51	-50.7704
FECL+2	1.00000E-15	0.00000E+00	3.39801E-23	-22.4688
FE2O2H2+4	1.00000E-15	0.00000E+00	3.71405E-35	-34.4302
FE+3	1.00000E-15	0.00000E+00	1.53892E-23	-22.8128
O2	1.00000E-15	0.00000E+00	2.54948E-58	-57.5935
CLO4-1	1.00000E-15	0.00000E+00	8.8489E-133	-132.0531
CLO3-1	1.00000E-15	0.00000E+00	1.5694E-105	-104.8043
CLO2-1	1.00000E-15	0.00000E+00	1.45414E-82	-81.8374
CLO2	1.00000E-15	0.00000E+00	1.6417E-100	-99.7847
CLO-1	1.00000E-15	0.00000E+00	7.71560E-46	-45.1126
CL2	1.00000E-15	0.00000E+00	5.82418E-50	-49.2348

Solution Properties:

pH = 7.0000	Eh = 0.0010 V	I = 0.1000
pe = 0.0175	Ah = 0.1000 kJ	m* = 0.2000
Aw = 0.9960	Os = 1.1089	pKw = 13.9973
At1= 1.0000E-15	At2= 1.2907E-07	(equiv_mol/kg_H2O)


```

Y(AQUEOUS,FECL+2), Y(AQUEOUS,FE03H3-1), Y(AQUEOUS,FE0H+1),
Y(AQUEOUS,FE0H+2), Y(AQUEOUS,H+1), Y(AQUEOUS,H2), Y(AQUEOUS,H2O),
Y(AQUEOUS,H2O2), Y(AQUEOUS,HClO), Y(AQUEOUS,HClO2), Y(AQUEOUS,H02-1),
Y(AQUEOUS,NA+1), Y(AQUEOUS,O2), Y(AQUEOUS,O3), Y(AQUEOUS,OH-1), PH, EH
AYT=AC(CL-1,AQUEOUS), AC(CL2,AQUEOUS), AC(CLO-1,AQUEOUS),
AC(CLO2,AQUEOUS), AC(CLO2-1,AQUEOUS), AC(CLO3-1,AQUEOUS),
AC(CLO4-1,AQUEOUS), AC(FE+2,AQUEOUS), AC(FE+3,AQUEOUS),
AC(FE2O2H2+4,AQUEOUS), AC(FECL+2,AQUEOUS), AC(FE03H3-1,AQUEOUS),
AC(FE0H+1,AQUEOUS), AC(FE0H+2,AQUEOUS), AC(H+1,AQUEOUS),
AC(H2,AQUEOUS), AC(H2O,AQUEOUS), AC(H2O2,AQUEOUS), AC(HClO,AQUEOUS),
AC(HClO2,AQUEOUS), AC(H02-1,AQUEOUS), AC(NA+1,AQUEOUS), AC(O2,AQUEOUS),
AC(O3,AQUEOUS), AC(OH-1,AQUEOUS), PH, EH
ART=ACR(CL-1,AQUEOUS), ACR(CL2,AQUEOUS), ACR(CLO-1,AQUEOUS),
ACR(CLO2,AQUEOUS), ACR(CLO2-1,AQUEOUS), ACR(CLO3-1,AQUEOUS),
ACR(CLO4-1,AQUEOUS), ACR(FE+2,AQUEOUS), ACR(FE+3,AQUEOUS),
ACR(FE2O2H2+4,AQUEOUS), ACR(FECL+2,AQUEOUS), ACR(FE03H3-1,AQUEOUS),
ACR(FE0H+1,AQUEOUS), ACR(FE0H+2,AQUEOUS), ACR(H+1,AQUEOUS),
ACR(H2,AQUEOUS), ACR(H2O,AQUEOUS), ACR(H2O2,AQUEOUS),
ACR(HClO,AQUEOUS), ACR(HClO2,AQUEOUS), ACR(H02-1,AQUEOUS),
ACR(NA+1,AQUEOUS), ACR(O2,AQUEOUS), ACR(O3,AQUEOUS), ACR(OH-1,AQUEOUS),
PH, EH
AIT=AI1, AI2, AI3, AI4, AI5, AI6, AI7, AI8, AI9, AI10, AI11, AI12, AI13,
AI14, AI15, AI16, AI17, AI18, AI19, AI20, AI21, AI22, AI23, AI24, AI25,
PH, EH
RCT=RC1, RC2, RC3, RC4, RC5, RC6, RC7, RC8, RC9, RC10, RC11, RC12, RC13,
RC14, RC15, RC16, RC17, RC18, RC19, RC20, RC21, RC22, RC23, RC24, RC25,
PH, EH
MLT=ML1, ML2, ML3, ML4, ML5, ML6, ML7, ML8, ML9, ML10, ML11, ML12, ML13,
ML14, ML15, ML16, ML18, ML19, ML20, ML21, ML22, ML23, ML24, ML25, ISTR,
PH, EH

```

IMPORTANT FACTS:

The default definitions of the Eh and pH quantities in the advanced POURBAIX-Module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

Eh = MUR(ZE)/RNF

pH = -log10[AI(H+1,AQUEOUS)]

= -log10[ACR(H+1,AQUEOUS)*AH2O]

where RNF is the Faraday constant (96485.309 C/mol), and AH2O is the molecular weight of H2O (55.508435 g). MUR(ZE) is the electrochemical potential (ECP; in the unit of J/mol; w.r.t. the standard hydrogen electrode). ACR(H+1,AQUEOUS) is the site-fraction-based activity of the H+1 aqueous species in AQUEOUS solution phase, but AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is the molality-based activity of the H+1 aqueous species that should be used for defining the pH quantity.

Within an aqueous-bearing heterogeneous interaction system, the fundamental system-components must be H2O, H+1 and ZE, which are corresponding to the basic elements O & H and the hypothetical electron (ZE) in the aqueous solution phase. For the additional chemical elements in the system, their corresponding system-components shall be defined as in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S) or (for some) in their molecular forms (e.g., NaCl, H2S). The reference state for the H2O component must always be defined as the solvent species H2O in the AQUEOUS solution phase under the current temperature (*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

ML = Y(AQUEOUS,I)*AH2O/YH2O

RC = ACR(I,AQUEOUS)*YH2O/Y(AQUEOUS,I)

AI = RC*ML

= ACR(I,AQUEOUS)*AH2O

where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are the site-fractions of solvent H2O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

```

Axis No 1: LNACR(H+1)           Min: -34.532608Max: 2.3025851 Inc: 0.8
Axis No 2: MUR(ZE)             Min: -150000   Max: 200000   Inc: 7718.85

```

NOTE: The default settings (listed above) for two mapping variables [in terms of lnACR(H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

pH: 0.00 -> 14.00, at a step of 0.35

Eh: -1.55 -> 2.07, at a step of 0.08 [V]

The maximum pH limit has been calculated precisely and determined automatically by the POURBAIX-Module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

Accept the default settings for two mapping variables? /Y/: Y

LIST ALL THE INITIAL EQUILIBRIA FOR MAPPING:

```

No 1  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 2  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 3  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 4  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 5  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 6  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 7  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 8  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 9  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 10 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 11 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000

```

No 12 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 13 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 14 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 15 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 16 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 17 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 18 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 19 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 20 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.

MAP THE POURBAIX DIAGRAM:
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32
Generating start point 33
Generating start point 34
Generating start point 35
Generating start point 36
Generating start point 37
Generating start point 38
Generating start point 39
Generating start point 40
Working hard
Generating start point 41
Generating start point 42
Generating start point 43
Generating start point 44

Phase region boundary 1 at: -1.612E+01 7.817E+04
** GAS
AQUEOUS
HEMATITE
Calculated.. 26 equilibria
Terminating at axis limit.

Phase region boundary 2 at: -3.453E+01 3.296E+04
** GAS
AQUEOUS
HEMATITE
Calculated. 43 equilibria

Phase region boundary 3 at: -1.975E+00 1.132E+05
** GAS
AQUEOUS
** HEMATITE

Phase region boundary 4 at: -1.975E+00 1.132E+05
** GAS
AQUEOUS
Calculated.. 9 equilibria
Terminating at axis limit.

Phase region boundary 5 at: -1.975E+00 1.132E+05
AQUEOUS
** HEMATITE
Calculated. 30 equilibria

Phase region boundary 6 at: -1.420E+01 -2.225E+04
AQUEOUS
** HEMATITE
** MAGNETITE

Phase region boundary 7 at: -1.420E+01 -2.225E+04
AQUEOUS
** HEMATITE
MAGNETITE
Calculated.. 30 equilibria

Terminating at axis limit.

Phase region boundary 8 at: -1.420E+01 -2.225E+04
AQUEOUS
** MAGNETITE
Calculated. 4 equilibria

Phase region boundary 9 at: -1.625E+01 -4.067E+04
** GAS
AQUEOUS
** MAGNETITE

Phase region boundary 10 at: -1.625E+01 -4.067E+04
GAS
AQUEOUS
** MAGNETITE
Calculated 34 equilibria

Phase region boundary 11 at: -1.625E+01 -4.067E+04
** GAS
AQUEOUS
Calculated.. 28 equilibria
Terminating at axis limit.

Phase region boundary 12 at: -1.625E+01 -4.067E+04
** GAS
AQUEOUS
MAGNETITE
Calculated.. 27 equilibria
Terminating at axis limit.

Phase region boundary 13 at: -1.420E+01 -2.225E+04
AQUEOUS
HEMATITE
** MAGNETITE
Calculated.. 30 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 14 at: -1.975E+00 1.132E+05
GAS
AQUEOUS
** HEMATITE
Calculated 11 equilibria

Phase region boundary 15 at: -1.612E+01 7.817E+04
** GAS
AQUEOUS
HEMATITE
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: -1.612E+01 -2.701E+04
AQUEOUS
HEMATITE
** MAGNETITE
Calculated.. 26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 17 at: -1.612E+01 -2.701E+04
AQUEOUS
HEMATITE
** MAGNETITE
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: -1.116E+01 1.000E+02
AQUEOUS
** HEMATITE
Calculated. 7 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: -1.116E+01 1.000E+02
AQUEOUS
** HEMATITE
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: -1.612E+01 -2.701E+04
AQUEOUS
** HEMATITE
MAGNETITE
Calculated.. 26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at: -1.612E+01 -2.701E+04
AQUEOUS
** HEMATITE
MAGNETITE
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: -1.612E+01 -3.959E+04
AQUEOUS
** MAGNETITE
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: -1.612E+01 -3.959E+04
AQUEOUS
** MAGNETITE
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 24 at: -1.485E+01 -2.840E+04
AQUEOUS
** MAGNETITE
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: -1.485E+01 -2.840E+04
AQUEOUS
** MAGNETITE
Calculated. 2 equilibria

Terminating at known equilibrium

Phase region boundary 26 at: -1.668E+01 -2.840E+04
 AQUEOUS
 ** HEMATITE
 MAGNETITE
 Calculated.. 26 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 27 at: -1.668E+01 -2.840E+04
 AQUEOUS
 ** HEMATITE
 MAGNETITE
 Calculated. 5 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: -9.172E+00 9.539E+04
 ** GAS
 AQUEOUS
 HEMATITE
 Calculated.. 35 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 29 at: -9.172E+00 9.539E+04
 ** GAS
 AQUEOUS
 HEMATITE
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: -9.210E+00 9.529E+04
 ** GAS
 AQUEOUS
 HEMATITE
 Calculated.. 35 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 31 at: -9.210E+00 9.529E+04
 ** GAS
 AQUEOUS
 HEMATITE
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 32 at: -9.210E+00 1.461E+04
 AQUEOUS
 ** HEMATITE
 Calculated. 8 equilibria
 Terminating at known equilibrium

Phase region boundary 33 at: -9.210E+00 1.461E+04
 AQUEOUS
 ** HEMATITE
 Calculated. 25 equilibria
 Terminating at known equilibrium

Phase region boundary 34 at: -9.210E+00 -2.323E+04
 ** GAS
 AQUEOUS
 Calculated. 10 equilibria
 Terminating at known equilibrium

Phase region boundary 35 at: -9.210E+00 -2.323E+04
 ** GAS
 AQUEOUS
 Calculated.. 18 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 36 at: -5.086E+00 -1.300E+04
 ** GAS
 AQUEOUS
 Calculated. 16 equilibria
 Terminating at known equilibrium

Phase region boundary 37 at: -5.086E+00 -1.300E+04
 ** GAS
 AQUEOUS
 Calculated.. 13 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 38 at: -1.293E+01 -1.300E+04
 AQUEOUS
 ** HEMATITE
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 39 at: -1.293E+01 -1.300E+04
 AQUEOUS
 ** HEMATITE
 Calculated. 27 equilibria
 Terminating at known equilibrium

Phase region boundary 40 at: -9.210E+00 9.529E+04
 ** GAS
 AQUEOUS
 HEMATITE
 Calculated.. 35 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 41 at: -9.210E+00 9.529E+04
 ** GAS
 AQUEOUS
 HEMATITE
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 42 at: -9.210E+00 -2.323E+04
 ** GAS
 AQUEOUS
 Calculated. 10 equilibria

Terminating at known equilibrium

Phase region boundary 43 at: -9.210E+00 -2.323E+04

** GAS

AQUEOUS

Calculated.. 18 equilibria

Terminating at known equilibrium

Terminating at axis limit.

Phase region boundary 44 at: -9.210E+00 1.461E+04

AQUEOUS

** HEMATITE

Calculated. 8 equilibria

Terminating at known equilibrium

Phase region boundary 45 at: -9.210E+00 1.461E+04

AQUEOUS

** HEMATITE

Calculated. 23 equilibria

Terminating at known equilibrium

Phase region boundary 46 at: -1.975E+00 8.684E+04

AQUEOUS

** HEMATITE

Calculated. 26 equilibria

Terminating at known equilibrium

Phase region boundary 47 at: -1.975E+00 8.684E+04

AQUEOUS

** HEMATITE

Calculated. 5 equilibria

Terminating at known equilibrium

Phase region boundary 48 at: -1.262E+01 8.684E+04

** GAS

AQUEOUS

HEMATITE

Calculated.. 31 equilibria

Terminating at known equilibrium

Terminating at axis limit.

Phase region boundary 49 at: -1.262E+01 8.684E+04

** GAS

AQUEOUS

HEMATITE

Calculated. 15 equilibria

Terminating at known equilibrium

Phase region boundary 50 at: -1.612E+01 7.817E+04

** GAS

AQUEOUS

HEMATITE

Calculated.. 26 equilibria

Terminating at known equilibrium

Terminating at axis limit.

Phase region boundary 51 at: -1.612E+01 7.817E+04

** GAS

AQUEOUS

HEMATITE

Calculated. 19 equilibria

Terminating at known equilibrium

Phase region boundary 52 at: -1.612E+01 -2.701E+04

AQUEOUS

HEMATITE

** MAGNETITE

Calculated.. 26 equilibria

Terminating at known equilibrium

Terminating at axis limit.

Phase region boundary 53 at: -1.612E+01 -2.701E+04

AQUEOUS

HEMATITE

** MAGNETITE

Calculated. 4 equilibria

Terminating at known equilibrium

Phase region boundary 54 at: -2.438E+00 6.600E+04

AQUEOUS

** HEMATITE

Calculated. 24 equilibria

Terminating at known equilibrium

Phase region boundary 55 at: -2.438E+00 6.600E+04

AQUEOUS

** HEMATITE

Calculated. 9 equilibria

Terminating at known equilibrium

Phase region boundary 56 at: -2.103E+01 6.600E+04

** GAS

AQUEOUS

HEMATITE

Calculated.. 20 equilibria

Terminating at known equilibrium

Terminating at axis limit.

Phase region boundary 57 at: -2.103E+01 6.600E+04

** GAS

AQUEOUS

HEMATITE

Calculated. 26 equilibria

Terminating at known equilibrium

*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex40\POURBAIX.POLY3

CPU time for mapping 119 seconds

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

CURRENT DEVICE: TC-UNITE Driver

Plotting the diagram; please be patient!

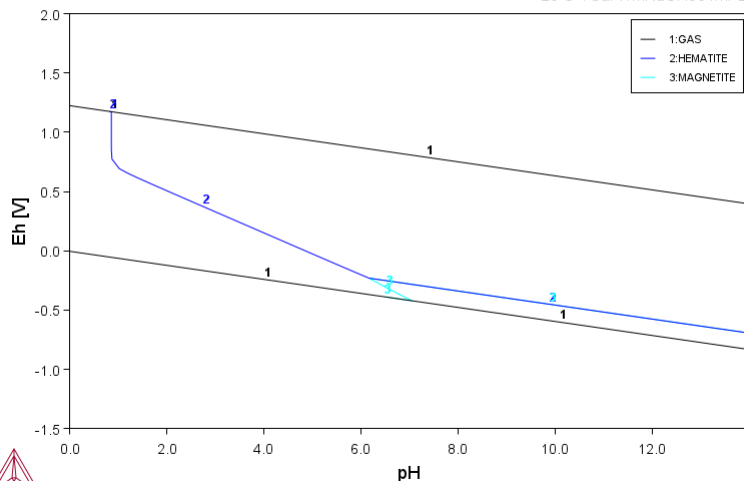
Pourbaix Diagram

2025.05.12.09.45.38

CL, FE, H+1, NA, H2O, ZE

T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



Hit RETURN to continue

Any missing phase boundary you could possibly think of? /N/: N

Change the pH/Eh steps for smoother curves? /N/: N

Zoom in? /N/: y

Change scaling of X-axis? /N/: N

Change scaling of Y-axis? /N/: y

Minimum /-1.2/: -1.0

Maximum /1.5/: 1.5

COMMAND NOT SUPPORTED IN THIS PLOT DRIVER

COMMAND NOT SUPPORTED IN THIS PLOT DRIVER

CURRENT DEVICE: TC-UNITE Driver

Plotting the diagram; please be patient!

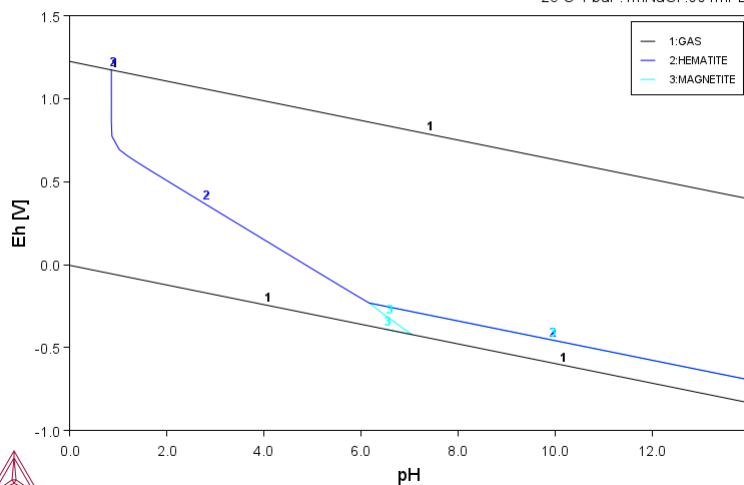
Pourbaix Diagram

2025.05.12.09.46.01

CL, FE, H+1, NA, H2O, ZE

T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: n

Hard copy of the diagram? /N/: n

Save X-Y coordinates of curve on text file? /N/: y

File name /POURBAIX/: TCEX40-1.EXP

FILE EXISTS, OVERWRITE (Y OR N) /N/: y

Modify the diagram? /N/: y

Zoom in? /N/: n

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: y

At what pH-Eh point add the label text?

X-pH /1.2/: 1.2

Y-Eh /.25/: 0.25

Automatic phase labels? /N/: N

Text? /Aqs/: Aqs

Text size: /.36/: 0.5

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /2.599732093/: 8

Y-Eh /.5/: 0.25

Automatic phase labels? /N/: N

Text? /Aqs/: Aqs+Hm

Text size: /.36/: 0.5

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /9.399732093/: 8

Y-Eh /.5/: -0.3

Automatic phase labels? /N/: N

Text? /Aqs/: Aqs+Mt

Text size: /.36/: 0.5

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /9.399732093/: 6

Y-Eh /-.05/: 1.1

Automatic phase labels? /N/: N

Text? /Aqs/: Gas (O2-dominant)

Text size: /.36/: 0.5

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /7.399732093/: 6

Y-Eh /1.35/: -0.8

Automatic phase labels? /N/: N

Text? /Aqs/: Gas (H2-dominant)

Text size: /.36/: 0.5

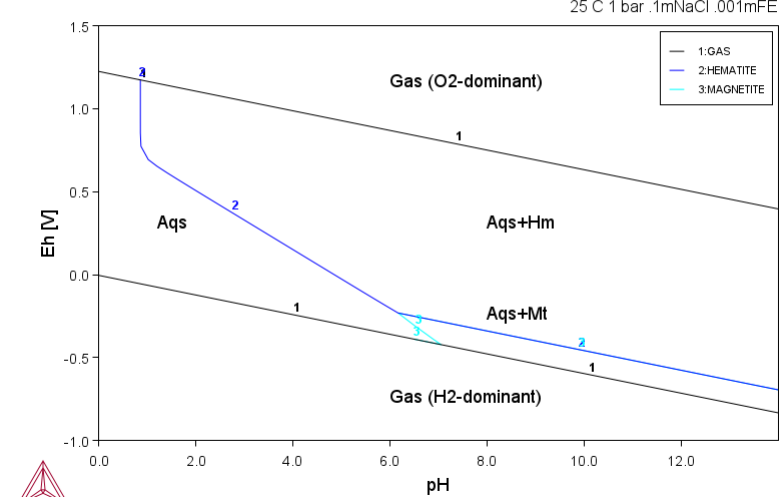
Another Label Text to be added? /N/: N

Pourbaix Diagram

2025.05.12.09.46.25

CL, FE, H+1, NA, H2O, ZE

T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1



Hit RETURN to continue

Modify Label-Texts on the Pourbaix diagram? /N/: y

These labels are defined

No 1 at 1.20000E+00 2.50000E-01 : Aqs

No 2 at 8.00000E+00 2.50000E-01 : Aqs+Hm

No 3 at 8.00000E+00-3.00000E-01 : Aqs+Mt

No 4 at 6.00000E+00 1.10000E+00 : Gas (O2-dominant)

No 5 at 6.00000E+00-8.00000E-01 : Gas (H2-dominant)

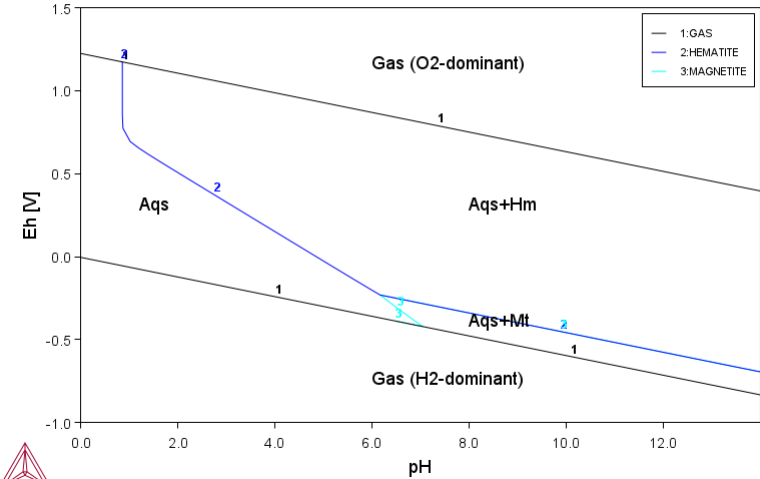
Which label to modify? /5/: 3

New X coordinate /8/: 8

New Y coordinate /-.3/: -0.45

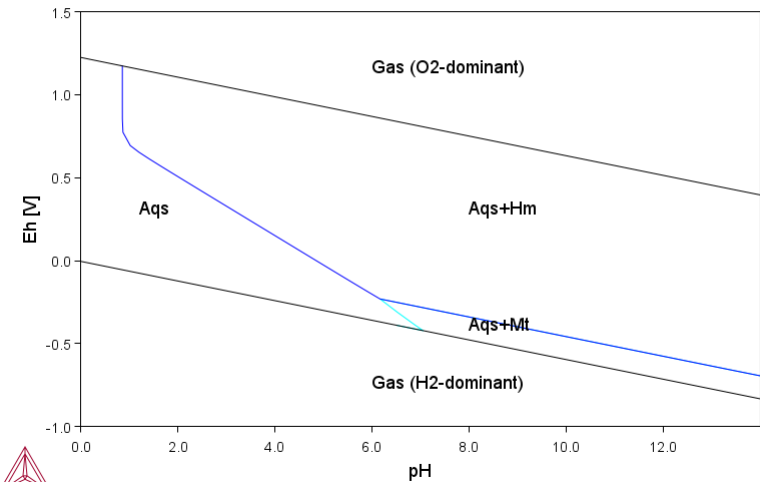
New text /Aqs+Mt/: Aqs+Mt

Another Label Text to be modified? /N/: N



Hit RETURN to continue

Modify Label-Curve-Option on the Pourbaix diagram? /N/: y
Curve-Label Option? /E/: ?
THE OPTIONS MEANS:
A LIST STABLE PHASES ALONG LINE
B AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
C LIST AXIS QUANTITIES
D AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
E AS B WITH CHANGING COLORS
F AS D WITH CHANGING COLORS
N NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /E/: n



Hit RETURN to continue

Another Curve-Label Option? /N/: N
Add Label-Texts onto the Pourbaix diagram? /N/: N
Modify Label-Texts on the Pourbaix diagram? /N/: N
Modify Label-Curve-Option on the Pourbaix diagram? /N/: N
Change the Subtitle of the diagram? /N/: N
Change Axis-Texts? /N/: N
Further Refine the diagram in POST Module? /N/: N
Hard copy of the diagram? /N/: N
Save X-Y coordinates of curve on text file? /N/: N
Modify the diagram? /N/: N
Any more diagram? /N/: y

Loading workspaces from the POLY3 file: POURBAIX
The loaded POLY3 file is of POURBAIX-MAPPING Calculation.
The current system consists of 6 elements:
CL FE H NA O ZE
List of Default and Pre-defined Calculation Conditions:

Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole

T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1,
LNACR(H+1)=-16.11809565, MUR(ZE)=66000.
FIXED PHASES
GAS=0
DEGREES OF FREEDOM -1

SET PLOTTING PARAMETERS:

```
-----
I
I The following properties are available to be selected I
I as axis variables for making other diagrams from the I
I same calculation: I
I I
I pH --- Acidity I
I Eh --- Electronic Potential [V] I
I Ah --- Electronic Affinity [kJ] I
I pe --- Electronic Activity [log10ACRe] I
I IS --- Ionic Strength I
I TM --- Total Concentration I
I Aw --- Activity of Water I
I Oc --- Osmotic Coefficient I
I MF(AQsp) --- Mole Fractions of aqueous species I
I ML(AQsp) --- Molalities of aqueous species I
I AI(AQsp) --- Activities of aqueous species I
I RC(AQsp) --- Activity Coefficients of Aq Species I
I
I where "AQsp" is the name of a specific aqueous species, I
I and "*" can be used as a wild sign for all "AQsp"; I
I It is unnecessary to give a complete aqueous species I
I names; however, the entered AQsp name must be unique. I
I If neither "AQsp" nor "*" is given here, all species I
I will be searched. I
I
I-----
```

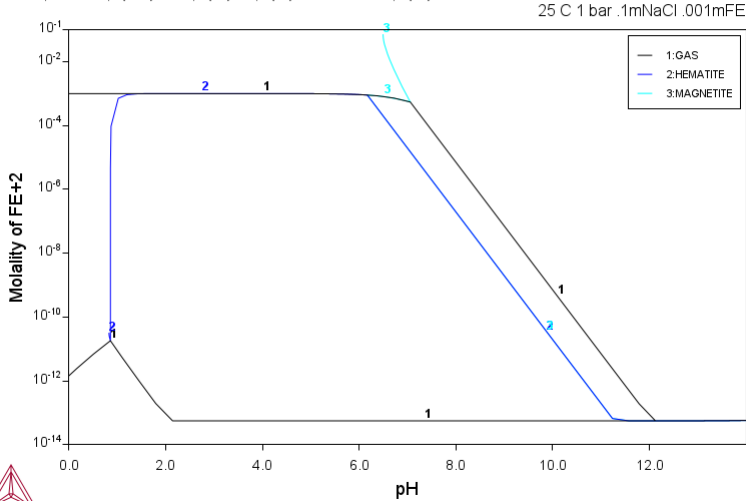
List of all the AQsp (aqueous species) in the defined system:

CL-1	CL2	CLO-1	CLO2	CLO2-1
CLO3-1	CLO4-1	FE+2	FE+3	FE2O2H2+4
FECL+2	FE03H3-1	FE0H+1	FE0H+2	H+1
H2	H2O	H2O2	HCLO	HCLO2
HO2-1	NA+1	O2	O3	OH-1

X-axis Variable: /PH/: ph
Y-axis Variable: /EH/: ml(fe+2)
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!

Property Diagram

2025.05.12.09.47.35
CL, FE, H+1, NA, H2O, ZE
T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1



Hit RETURN to continue

Change axis type? /N/: N

Zoom in? /N/: y
Change scaling of X-axis? /N/: y
Minimum /0/: 0
Maximum /13.99557858/: 14
Change scaling of Y-axis? /N/: y
Minimum /1E-40/: 1e-12
Maximum /1/: 1e-2

COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!

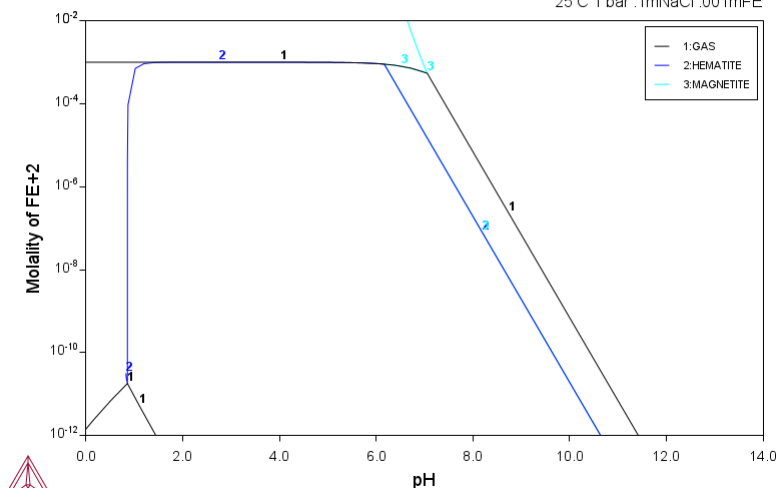
Property Diagram

2025.05.12 09:47:59

CL, FE, H+1, NA, H2O, ZE

T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: n

Add label texts onto the specified diagram? /N/: n

Change the subtitle of the diagram? /N/: n

Change axis text? /N/: n

Further refine the diagram in POST module? /N/: n

Hard copy of the diagram? /N/: n

Save X-Y coordinates of curve on text file? /N/: n

Modify the diagram? /N/: n

Any more diagram? /N/: y

Loading workspaces from the POLY3 file: POURBAIX

The loaded POLY3 file is of POURBAIX-MAPPING Calculation.

The current system consists of 6 elements:

CL FE H NA O ZE

List of Default and Pre-defined Calculation Conditions:

Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole

T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1,
LNACR(H+1)=-16.11809565, MUR(ZE)=66000.

FIXED PHASES

GAS=0

DEGREES OF FREEDOM -1

SET PLOTTING PARAMETERS:

```

-----
I
I The following properties are available to be selected I
I as axis variables for making other diagrams from the I
I same calculation: I
I I I I I
I pH --- Acidity I
I Eh --- Electronic Potential [V] I
I Ah --- Electronic Affinity [kJ] I
I pe --- Electronic Activity [log10ACRe] I
I IS --- Ionic Strength I
I TM --- Total Concentration I
I Aw --- Activity of Water I
I Oc --- Osmotic Coefficient I
I MF(AQsp) --- Mole Fractions of aqueous species I
I ML(AQsp) --- Molalities of aqueous species I
I AI(AQsp) --- Activities of aqueous species I
I RC(AQsp) --- Activity Coefficients of Aq Species I
I I I
I where "AQsp" is the name of a specific aqueous species, I
I and "*" can be used as a wild sign for all "AQsp"; I
I It is unnecessary to give a complete aqueous species I
I names; however, the entered AQsp name must be unique. I
I If neither "AQsp" nor "*" is given here, all species I
I will be searched. I
I I
I
-----

```

List of all the AQsp (aqueous species) in the defined system:

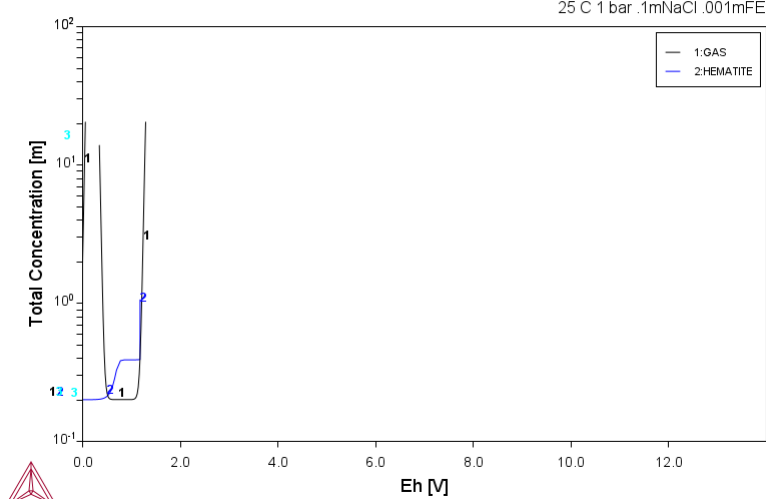
```

-----
CL-1      CL2      CLO-1      CLO2      CLO2-1
CLO3-1    CLO4-1    FE+2      FE+3      FE2O2H2+4
FECL+2    FEO3H3-1    FEOH+1    FEOH+2    H+1
H2         H2O         H2O2      HCLO      HCLO2
HO2-1     NA+1        O2         O3         OH-1
-----

```

X-axis Variable: /PH/: eh

Y-axis Variable: /ML/: tm
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!
Property Diagram
2025.05.12.09.48.22
CL, FE, H+1, NA, H2O, ZE
T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1

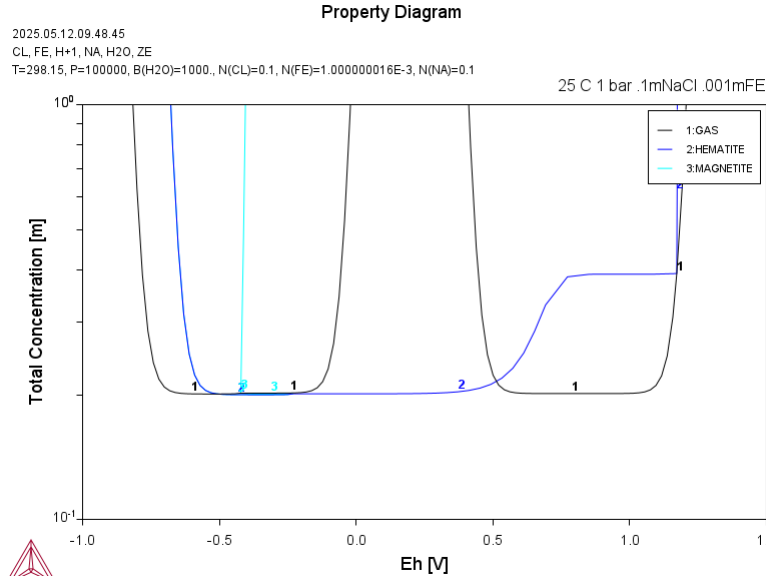


Hit RETURN to continue

Change axis type? /N/: N

Zoom in? /N/: y
Change scaling of X-axis? /N/: y
Minimum /-1.2/: -1.0
Maximum /1.5/: 1.5
Change scaling of Y-axis? /N/: y
Minimum /1E-08/: 0.1
Maximum /100/: 1

COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!



Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add label texts onto the specified diagram? /N/: N

Change the subtitle of the diagram? /N/: N

Change axis text? /N/: N

Further refine the diagram in POST module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: N

SYS:
SYS: @@... Up to this point, the POURBAIX module run is complete.
SYS:
SYS: SET_INTERACTIVE
... the command in full is SET_INTERACTIVE_MODE
SYS:

tcex41

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex41\tcex41.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculation of a solubility product

SYS:

SYS: @@ Note that a TCFE database license is required

SYS: @@ to run the example.

SYS:

SYS: set-log ex41,,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tofell

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/:

1st alloying element: c .19

2nd alloying element: mn 1.16

Next alloying element: si .2

Next alloying element: cr .72

Next alloying element: ni .2

Next alloying element: mo .08

Next alloying element: cu .26

Next alloying element: al .027

Next alloying element: n .0089

Next alloying element:

Temperature (C) /1000/: 1056

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

... the command in full is DEFINE_ELEMENTS

NI DEFINED

... the command in full is DEFINE_ELEMENTS

MO DEFINED

... the command in full is DEFINE_ELEMENTS

CU DEFINED

... the command in full is DEFINE_ELEMENTS

AL DEFINED

... the command in full is DEFINE_ELEMENTS

N DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	MC_ETA	MC_SHP
KSI_CARBIDE	Z_PHASE	FE4N_LP1
PI_A13	SIGMA_D8B	HIGH_SIGMA
MU_D85	P_PHASE	R_PHASE
CHI_A12	C14_LAVES	C15_LAVES
M3SI	MN9SI2	MN11SI19
MN6SI	G_PHASE	ETA_M5SIN
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	CU6Y	MOSI2_C11B
MO5SI3_D8M	AL8MN5_D810	NB5SI3_D8L
MSI2_C40	M11SI8	M6SI5
KAPPA_E21	AL4C3_D71	FE8SI2C
SIC_B3	MN5SIC	CRZN17
FEZN13	CUZN_EPSILON	NIZN_B2
NIZN_L10	NI2ZN11_D82	AL2FE
AL5FE4	AL5FE2	AL13FE4
AL7CR	AL2CR3	ALN_B4
SI3N4	MN3N2	MN6N5
MNP_B31	M2P_C22	M4SI1_G3
NI3ISI12	CO2SI_C37	M2SI_TETA
NISI_B31	NI3SI2	CR5SI3_D8M

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M6C_E93	M5C2
M3C2_D510	MC_ETA	MC_SHP
KSI_CARBIDE	Z_PHASE	FE4N_LP1
PI_A13	SIGMA_D8B	HIGH_SIGMA
MU_D85	P_PHASE	R_PHASE
CHI_A12	CI4_LAVES	CI5_LAVES
M3SI	MN9SI2	MN11SI19
MN6SI	G_PHASE	ETA_M5SIN
CR3SI_A15	FESI2_H	FESI2_L
MSI_B20	M5SI3_D88	NBNI3_D0A
NI3TI_D024	CU6Y	MOSI2_C11B
MO5SI3_D8M	AL8MN5_D810	NB5SI3_D8L
MSI2_C40	M11SI8	M6SI5
KAPPA_E21	AL4C3_D71	FE8SI2C
SIC_B3	MN5SIC	CRZN17
FEZN13	CUZN_EPSILON	NIZN_B2
NIZN_L10	NI2ZN11_D82	AL2FE
AL5FE4	AL5FE2	AL13FE4
AL7CR	AL2CR3	ALN_B4
SI3N4	MN3N2	MN6N5
MNP_B31	M2P_C22	M4SI1_G3
NI3SI12	CO2SI_C37	M2SI_TETA
NISI_B31	NI3SI2	CR5SI3_D8M

.....

OK? /Y/: Y

09:50:07,817 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set FCC_A1#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set HCP_A3#2

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 60421 grid points in 1.235 s

Found the set of lowest grid points in 0.045 s

Calculated POLY solution 1.451 s, total time 2.731 s

POLY:

POLY: l-e,,,

... the command in full is LIST_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=1329.15, W(C)=1.9E-3, W(MN)=1.16E-2, W(SI)=2E-3, W(CR)=7.2E-3, W(NI)=2E-3,
 W(MO)=8E-4, W(CU)=2.6E-3, W(AL)=2.7E-4, W(N)=8.9E-5, P=100000, N=1

DEGREES OF FREEDOM 0

Temperature 1329.15 K (1056.00 C), Pressure 1.000000E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.53245E+01
 Total Gibbs energy -6.89246E+04, Enthalpy 3.91344E+04, Volume 7.33623E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
AL	5.5361E-04	2.7000E-04	1.6366E-09	-2.2357E+05	SER
C	8.7517E-03	1.9000E-03	8.6866E-03	-5.2449E+04	SER
CR	7.6609E-03	7.2000E-03	7.7406E-05	-1.0462E+05	SER
CU	2.2636E-03	2.6000E-03	1.0186E-04	-1.0158E+05	SER
FE	9.6245E-01	9.7154E-01	2.2977E-03	-6.7145E+04	SER
MN	1.1682E-02	1.1600E-02	1.1151E-05	-1.2603E+05	SER
MO	4.6133E-04	8.0000E-04	1.0256E-05	-1.2695E+05	SER
N	3.5153E-04	8.9000E-05	5.1866E-07	-1.5993E+05	SER
NI	1.8853E-03	2.0000E-03	2.6599E-06	-1.4187E+05	SER
SI	3.9398E-03	2.0000E-03	5.0540E-09	-2.1111E+05	SER

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
 Moles 9.9975E-01, Mass 5.5319E+01, Volume fraction 9.9978E-01 Mass fractions:
 FE 9.71631E-01 CR 7.20067E-03 NI 2.00019E-03 C 1.90018E-03 AL 2.09122E-04
 MN 1.16011E-02 CU 2.60024E-03 SI 2.00019E-03 MO 8.00074E-04 N 5.73920E-05

ALN_B4 Status ENTERED Driving force 0.0000E+00
 Moles 2.4973E-04, Mass 5.1181E-03, Volume fraction 2.1734E-04 Mass fractions:
 AL 6.58274E-01 SI 0.00000E+00 MO 0.00000E+00 FE 0.00000E+00 CR 0.00000E+00
 N 3.41726E-01 NI 0.00000E+00 MN 0.00000E+00 CU 0.00000E+00 C 0.00000E+00

POLY:Hit RETURN to continue

POLY:

POLY: def-dia

... the command in full is DEFINE_DIAGRAM

Same elements as before? /Y/: Y

For binary or ternary diagrams you may prefer the special modules

You must specify a value for all compositions and the temperature even
 if you want to use it as axis.

Mass (weight) percent of AL /.027/: .027

Mass (weight) percent of C /.19/: .19

Mass (weight) percent of CR /.72/: .72

Mass (weight) percent of CU /.26/: .26

Mass (weight) percent of MN /1.16/: 1.16

Mass (weight) percent of MO /.08/: .08

Mass (weight) percent of N /.0089/: .0089

Mass (weight) percent of NI /.2/: .2

```

Mass (weight) percent of SI /.2/: .2
Temperature (C) /1056/: 1056
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0.042 s
Calculated POLY solution      0.593 s, total time      0.635 s
You must now set an independent axis for your diagram
as one of the following conditions:
Condition 1 is temperature (Celsius)
Condition 2 is mass percent of C
Condition 3 is mass percent of MN
Condition 4 is mass percent of SI
Condition 5 is mass percent of CR
Condition 6 is mass percent of NI
Condition 7 is mass percent of MO
Condition 8 is mass percent of CU
Condition 9 is mass percent of AL
Condition 10 is mass percent of N
Give the number of the condition to vary /1/: 1
Minimum value (C) /800/: 650
Maximum value (C) /1800/: 1200

The second axis can be another of the conditions above and you will then
calculate a phase diagram.
Or you may want to plot how some other quantities depend on the selected
condition and you will then calculate a "property" diagram.

In addition to the conditions above you may use these selected
dependent quantities on the vertical axis:
Dependent 11 is mass fraction of all phases
Dependent 12 is composition of a phase
Dependent 13 is the fraction of a component in all phases
(In the post processor you may select many other quantities)
Give the number of the quantity on second axis /11/: 11 tcex41
No initial equilibrium, using default
Step will start from axis value      1329.15
...OK

Phase Region from      1329.15      for:
    ALN_B4
    FCC_A1#1
Global Check of removing phase at      1.38213E+03
Calculated      8 equilibria

Phase Region from      1382.13      for:
    FCC_A1#1
Global test at      1.45915E+03 .... OK
Terminating at      1473.15
Calculated      13 equilibria

Phase Region from      1329.15      for:
    ALN_B4
    FCC_A1#1
Global test at      1.24915E+03 .... OK
Global test at      1.14915E+03 .... OK
Global check of adding phase at      1.07187E+03
Calculated      28 equilibria

Phase Region from      1071.87      for:
    ALN_B4
    BCC_A2
    FCC_A1#1
Global test at      9.99150E+02 .... OK
Global check of adding phase at      9.95086E+02
Calculated      11 equilibria

Phase Region from      995.086      for:
    ALN_B4
    BCC_A2
    CEMENTITE_D011
    FCC_A1#1
Global Check of removing phase at      9.68450E+02
Calculated      6 equilibria

Phase Region from      968.450      for:
    ALN_B4
    BCC_A2
    CEMENTITE_D011
Terminating at      923.150
Calculated      8 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex41\tcex41.POLY3
    POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is REINITIATE_PLOT_SETTINGS
    POSTPROCESSOR VERSION 3.2

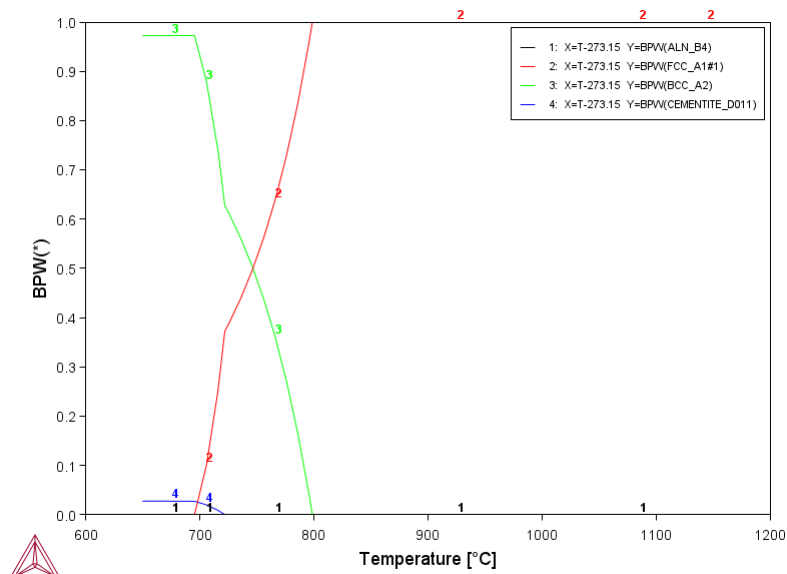
Setting automatic diagram axes

... the command in full is SET_AUTOMATIC_DIAGRAM_A

Setting automatic diagram axes

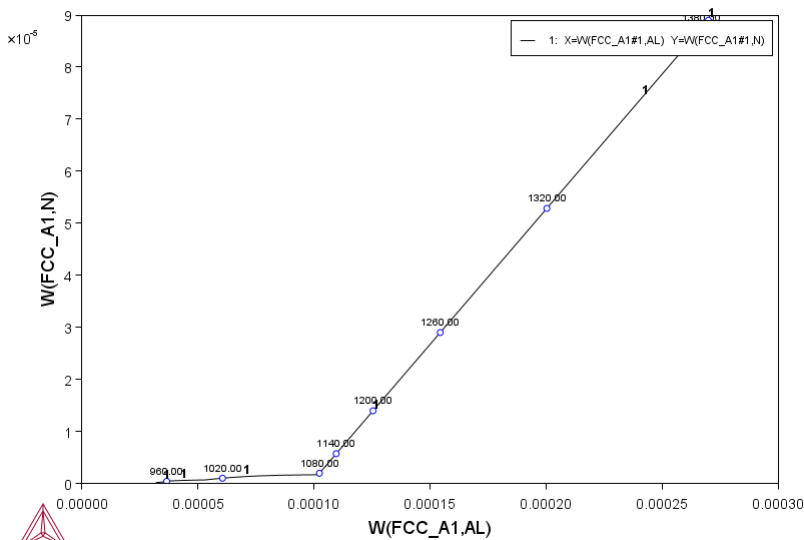
... the command in full is PLOT_DIAGRAM

```



```
POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x w(fcc_a1,a1)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(fcc_a1,n)
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: set-title example 41a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

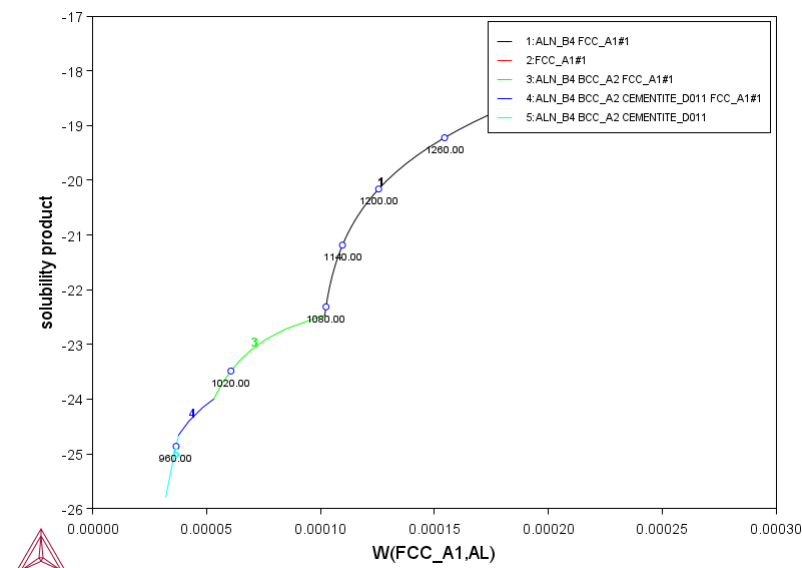
example 41a



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Now let's go back to POLY3 and enter a function
POST: @@ corresponding to the solubility product
POST:
POST: back
POLY: enter fun
... the command in full is ENTER_SYMBOL
Name: sp
Function: log(w(fcc_a1,a1)*w(fcc_a1,n));
POLY:
POLY: @@ Now go back to POST and plot the entered function
POLY: post
POST:
POST: s-d-a y sp
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-t-s y n solubility product
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: set-title example 41b
POST:
POST: sel-plot new
... the command in full is SELECT_PLOT
```



```
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex42

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex42\tcex42.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isopleth

SYS:

SYS: @@ This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to

SYS: @@ show a paraequilibrium calculation where there is formation of

SYS: @@ para-pearlite. It is an isopleth calculation and shows the

SYS: @@ Step_with_Options command using the Paraequilibrium option.

SYS: @@ Note that a TCFE database license is required to run

SYS: @@ the example.

SYS:

SYS: set-log ex42,,,

SYS: go da

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw tcfell

... the command in full is SWITCH_DATABASE

TDB_TCFE11: d-sys fe c mn

... the command in full is DEFINE_SYSTEM

FE C MN

DEFINED

TDB_TCFE11: rej ph gra m5c2 diamond_fcc_a4

... the command in full is REJECT

*** ERROR DIAMOND_FCC_A4 INPUT IGNORED

GRAPHITE_A9 M5C2 REJECTED

TDB_TCFE11: get

... the command in full is GET_DATA

09:51:48,994 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_TCFE11: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: @@ To work with u-fractions, just set the status of component C to SPECIAL

POLY:

POLY: c-s com c

... the command in full is CHANGE_STATUS

Status: /ENTERED/: special

POLY: l-st

... the command in full is LIST_STATUS

Option /CPS/:

*** STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T (K)	P (Pa)

VA	ENTERED	SER		

C	SPECIAL	SER		

FE	ENTERED	SER		

MN	ENTERED	SER		

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES

NBNI3_D0A	ENTERED	0.000000E+00	0.000000E+00

M7C3_D101	ENTERED	0.000000E+00	0.000000E+00

M23C6_D84	ENTERED	0.000000E+00	0.000000E+00

KSI_CARBIDE	ENTERED	0.000000E+00	0.000000E+00

HCP_A3	ENTERED	0.000000E+00	0.000000E+00

G PHASE	ENTERED	0.000000E+00	0.000000E+00

FE4N_LP1	ENTERED	0.000000E+00	0.000000E+00

FCC_L12	ENTERED	0.000000E+00	0.000000E+00

FCC_A1	ENTERED	0.000000E+00	0.000000E+00

DIAMOND_A4	ENTERED	0.000000E+00	0.000000E+00

CUZN_EPSILON	ENTERED	0.000000E+00	0.000000E+00

CUB_A13	ENTERED	0.000000E+00	0.000000E+00

CEMENTITE_D011	ENTERED	0.000000E+00	0.000000E+00

CBCC_A12	ENTERED	0.000000E+00	0.000000E+00

C15_LAVES	ENTERED	0.000000E+00	0.000000E+00

C14_LAVES	ENTERED	0.000000E+00	0.000000E+00

BCC_B2	ENTERED	0.000000E+00	0.000000E+00

BCC_A2	ENTERED	0.000000E+00	0.000000E+00

```

AL5FE4          ENTERED      0.000000E+00   0.000000E+00
LIQUID          ENTERED      0.000000E+00   0.000000E+00
GAS             ENTERED      0.000000E+00   0.000000E+00
*** STATUS FOR ALL SPECIES
C      ENTERED   C4      ENTERED   FE      ENTERED   FE+4      ENTERED   MN+3      ENTERED
C2     ENTERED   C5     ENTERED   FE+2     ENTERED   MN      ENTERED   MN+4     ENTERED
C3     ENTERED   C60    ENTERED   FE+3     ENTERED   MN+2     ENTERED   VA      ENTERED
POLY:
POLY:Hit RETURN to continue
POLY: s-c t=900 p=1e5 n=1 w(c)=0.002 w(mn)=0.025
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      23045 grid points in      0.563 s
Found the set of lowest grid points in      0.005 s
Calculated POLY solution      0.217 s, total time      0.785 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE11

Conditions:
T=900, P=100000, N=1, W(C)=2E-3, W(MN)=2.5E-2
DEGREES OF FREEDOM 0

Temperature      900.00 K ( 626.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.54204E+01
Total Gibbs energy -3.64344E+04, Enthalpy 2.02443E+04, Volume 7.24781E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C      9.2099E-03  2.0000E-03 1.6686E-01 -1.3399E+04 SER
FE     9.6562E-01  9.7500E-01 8.1714E-03 -3.5972E+04 SER
MN     2.5169E-02  2.5000E-02 2.3252E-04 -6.2607E+04 SER

BCC_A2          Status ENTERED      Driving force 0.0000E+00
Moles 3.6326E-02, Mass 5.3797E+01, Volume fraction 9.6992E-01 Mass fractions:
FE 9.81934E-01 MN 1.80378E-02 C 2.86448E-05

CEMENTITE_D011      Status ENTERED      Driving force 0.0000E+00
Moles 3.6326E-02, Mass 1.6238E+00, Volume fraction 3.0085E-02 Mass fractions:
FE 6.78866E-01 MN 2.53958E-01 C 6.71754E-02
POLY: s-a-v l w(c) 0 0.02
... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 2.5E-04
POLY: s-a-v 2 t 800 1200 10
... the command in full is SET_AXIS_VARIABLE
POLY: sa tcex42a y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32

Phase region boundary 1 at: 1.965E-02 8.100E+02
      BCC_A2
      CEMENTITE_D011
** DIAMOND_A4
Calculated..      15 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 1.632E-02 8.000E+02
      BCC_A2

```

CEMENTITE_D011
 ** DIAMOND_A4
 Calculated.. 17 equilibria
 Terminating at axis limit.

Phase region boundary 3 at: 1.965E-02 8.100E+02
 BCC_A2
 CEMENTITE_D011
 ** DIAMOND_A4
 Calculated.. 3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 4 at: 2.500E-04 8.899E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 3 equilibria

Phase region boundary 5 at: 1.687E-05 8.830E+02
 BCC_A2
 ** CEMENTITE_D011
 ** FCC_A1

Phase region boundary 6 at: 1.687E-05 8.830E+02
 BCC_A2
 ** FCC_A1
 Calculated 29 equilibria

Phase region boundary 7 at: 1.687E-05 8.830E+02
 BCC_A2
 ** CEMENTITE_D011
 Calculated.. 10 equilibria
 Terminating at axis limit.

Phase region boundary 8 at: 1.687E-05 8.830E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 33 equilibria

Phase region boundary 9 at: 6.844E-03 9.776E+02
 ** BCC_A2
 ** CEMENTITE_D011
 FCC_A1

Phase region boundary 10 at: 6.844E-03 9.776E+02
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 38 equilibria
 Terminating at axis limit.

Phase region boundary 11 at: 6.844E-03 9.776E+02
 ** BCC_A2
 FCC_A1
 Calculated 45 equilibria

Phase region boundary 12 at: 6.844E-03 9.776E+02
 ** BCC_A2
 CEMENTITE_D011
 FCC_A1
 Calculated.. 54 equilibria
 Terminating at axis limit.

Phase region boundary 13 at: 1.687E-05 8.830E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 85 equilibria
 Terminating at axis limit.

Phase region boundary 14 at: 2.500E-04 8.899E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 81 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 15 at: 6.750E-03 9.542E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 28 equilibria
 Terminating at known equilibrium

Phase region boundary 16 at: 6.750E-03 9.542E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 55 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 17 at: 1.325E-02 9.705E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 54 equilibria
 Terminating at known equilibrium

Phase region boundary 18 at: 1.325E-02 9.705E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 29 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 19 at: 1.965E-02 8.100E+02
 BCC_A2
 CEMENTITE_D011
 ** DIAMOND_A4
 Calculated.. 15 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 1.965E-02 8.100E+02
 BCC_A2
 CEMENTITE_D011
 ** DIAMOND_A4
 Calculated.. 3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 21 at: 1.975E-02 8.103E+02
 BCC_A2
 CEMENTITE_D011
 ** DIAMOND_A4
 Calculated.. 15 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 1.975E-02 8.103E+02
 BCC_A2
 CEMENTITE_D011
 ** DIAMOND_A4
 Calculated.. 3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 23 at: 1.009E-03 9.367E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 8 equilibria
 Terminating at known equilibrium

Phase region boundary 24 at: 1.009E-03 9.367E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 28 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.542E-03 9.367E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 16 equilibria
 Terminating at known equilibrium

Phase region boundary 26 at: 3.542E-03 9.367E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated.. 68 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 27 at: 1.020E-03 1.063E+03
 ** BCC_A2
 FCC_A1
 Calculated.. 32 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 1.020E-03 1.063E+03
 ** BCC_A2
 FCC_A1
 Calculated 22 equilibria

Phase region boundary 29 at: 9.115E-03 1.063E+03
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 9.115E-03 1.063E+03
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 29 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 31 at: 1.287E-02 1.190E+03
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 36 equilibria
 Terminating at known equilibrium

Phase region boundary 32 at: 1.287E-02 1.190E+03
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 4 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 33 at: 2.500E-04 1.081E+03
 ** BCC_A2
 FCC_A1
 Calculated 4 equilibria

Phase region boundary 34 at: 2.500E-04 1.081E+03
 ** BCC_A2
 FCC_A1
 Calculated.. 28 equilibria
 Terminating at known equilibrium

Phase region boundary 35 at: 6.750E-03 9.786E+02
 ** BCC_A2
 FCC_A1
 Calculated 48 equilibria

Phase region boundary 36 at: 6.750E-03 9.786E+02
 ** BCC_A2
 FCC_A1
 Calculated.. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 37 at: 1.325E-02 9.814E+02
 ** BCC_A2
 CEMENTITE_D011

```

FCC_A1
Calculated. 27 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 1.325E-02 9.814E+02
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.. 29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 39 at: 1.287E-02 1.190E+03
** CEMENTITE_D011
FCC_A1
Calculated. 36 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 1.287E-02 1.190E+03
** CEMENTITE_D011
FCC_A1
Calculated.. 4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 41 at: 1.975E-02 9.841E+02
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated. 53 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 1.975E-02 9.841E+02
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex42\tcex42a.POLY3
CPU time for mapping 21 seconds

```

```

POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

```

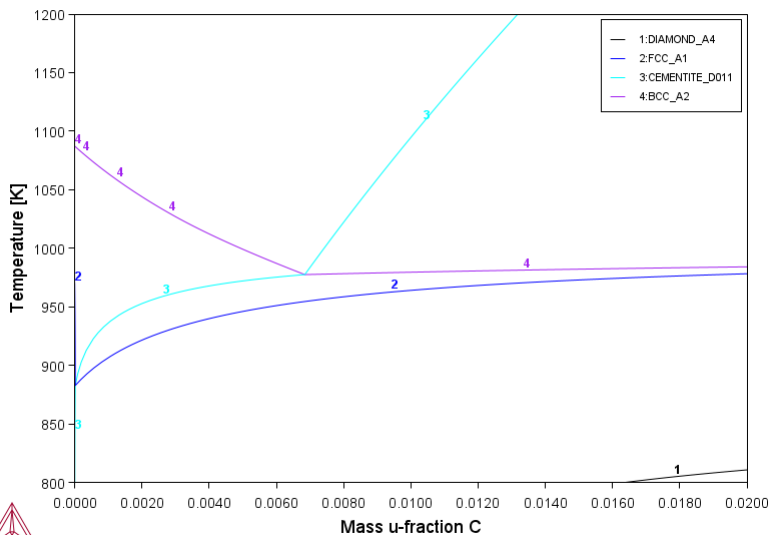
Setting automatic diagram axes

```

POST: s-lab e
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-text x n Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: set-title example 42a
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 42a



```

POST:
POST: Hit RETURN to continue
POST:
POST: make tcex42 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: back
POLY: read tcex42a
... the command in full is READ_WORKSPACES
POLY: s-a-v 1 t 800 1200 10
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY: sa tcex42b y
... the command in full is SAVE_WORKSPACES
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

```

This command calculates a paraequilibrium between two phases.

You must calculate an equilibrium with the overall composition first.

Name of first phase: fcc_a1

Name of second phase: bcc_a2

Fast diffusing component: /C/: C

Fast diffusing component: /NONE/:

Output during stepping is:

axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

```
Phase Region from      900.000      for:
  BCC_A2
  FCC_A1
  9.000000E+02    0.176    0.824    4.978820E-02    6.632554E-04    -2.411191E-01
  8.900000E+02    0.161    0.839    5.422637E-02    6.913419E-04    -2.814989E-02
  8.800000E+02    0.148    0.852    5.873850E-02    7.164862E-04    1.826378E-01
  8.700000E+02    0.137    0.863    6.331514E-02    7.386191E-04    3.918139E-01
  8.600000E+02    0.127    0.873    6.794785E-02    7.576965E-04    5.998836E-01
  8.500000E+02    0.119    0.881    7.262910E-02    7.736968E-04    8.072994E-01
  8.400000E+02    0.111    0.889    7.735219E-02    7.866192E-04    1.014471E+00
  8.300000E+02    0.105    0.895    8.211115E-02    7.964818E-04    1.221773E+00
  8.200000E+02    0.099    0.901    8.690064E-02    8.033198E-04    1.429553E+00
  8.100000E+02    0.093    0.907    9.171593E-02    8.071848E-04    1.638132E+00
  8.000000E+02    0.089    0.911    9.655277E-02    8.081431E-04    1.847816E+00
```

```
Phase Region from      900.000      for:
  BCC_A2
  FCC_A1
  9.000000E+02    0.176    0.824    4.978820E-02    6.632554E-04    -2.411191E-01
  9.100000E+02    0.193    0.807    4.543455E-02    6.323238E-04    -4.569199E-01
  9.200000E+02    0.214    0.786    4.117723E-02    5.986755E-04    -6.763019E-01
  9.300000E+02    0.239    0.761    3.702936E-02    5.624744E-04    -9.001396E-01
  9.400000E+02    0.270    0.730    3.300554E-02    5.239251E-04    -1.129464E+00
  9.500000E+02    0.308    0.692    2.912186E-02    4.832788E-04    -1.365508E+00
  9.600000E+02    0.355    0.645    2.539605E-02    4.408411E-04    -1.609759E+00
  9.700000E+02    0.415    0.585    2.184745E-02    3.969810E-04    -1.864037E+00
  9.800000E+02    0.493    0.507    1.849705E-02    3.521428E-04    -2.130596E+00
  9.900000E+02    0.597    0.403    1.536739E-02    3.068594E-04    -2.412255E+00
  1.000000E+03    0.739    0.261    1.248241E-02    2.617708E-04    -2.712568E+00
  1.010000E+03    0.942    0.058    9.854299E-03    2.173378E-04    -3.037453E+00
  1.020000E+03    1.258    -0.258    7.421605E-03    1.722830E-04    -3.406198E+00
  1.030000E+03    1.821    -0.821    5.162033E-03    1.261960E-04    -3.851549E+00
  1.040000E+03    3.087    -2.087    3.064308E-03    7.892826E-05    -4.452579E+00
  1.050000E+03    8.516    -7.516    1.118312E-03    3.035919E-05    -5.537500E+00
```

*** Buffer savend on file c:\jenkins\WORKSP~1\DEV_PI~1\GENERA~1\examples\tcex42\TCEX42~2.POL

*** ERROR 3 IN NS01AD: Numerical error

POLY:

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x w(*,c)

... the command in full is SET_DIAGRAM_AXIS

COLUMN NUMBER /*/: *

POST: s-d-a y t-k

... the command in full is SET_DIAGRAM_AXIS

POST: s-a-text x n Mass u-fraction C

... the command in full is SET_AXIS_TEXT_STATUS

POST: set-tie 5

... the command in full is SET_TIELINE_STATUS

POST: set-title example 42b

POST: sel-plot new

... the command in full is SELECT_PLOT

POST:

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

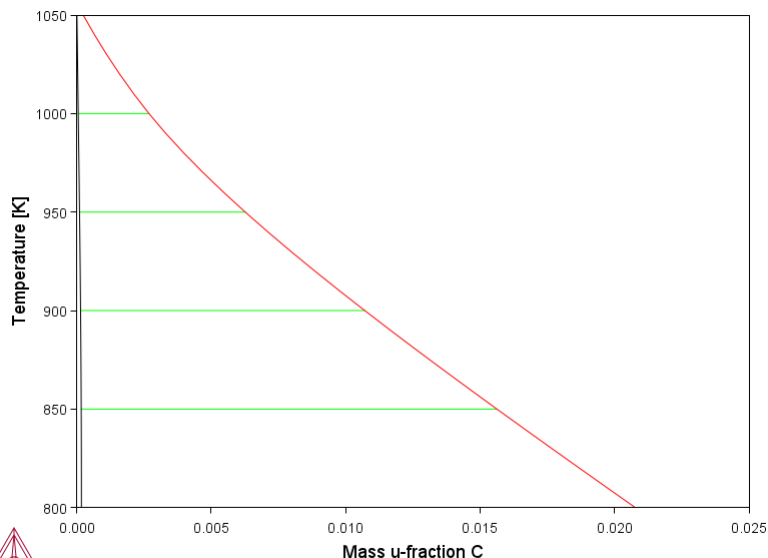
... the command in full is MAKE_EXPERIMENTAL_DATAFI

POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM



POST:

POST:Hit RETURN to continue

POST:

POST: ap-e y tcex42

... the command in full is APPEND_EXPERIMENTAL_DATA

PROLOGUE NUMBER: /0/: 0

DATASET NUMBER(s): /-1/: 1

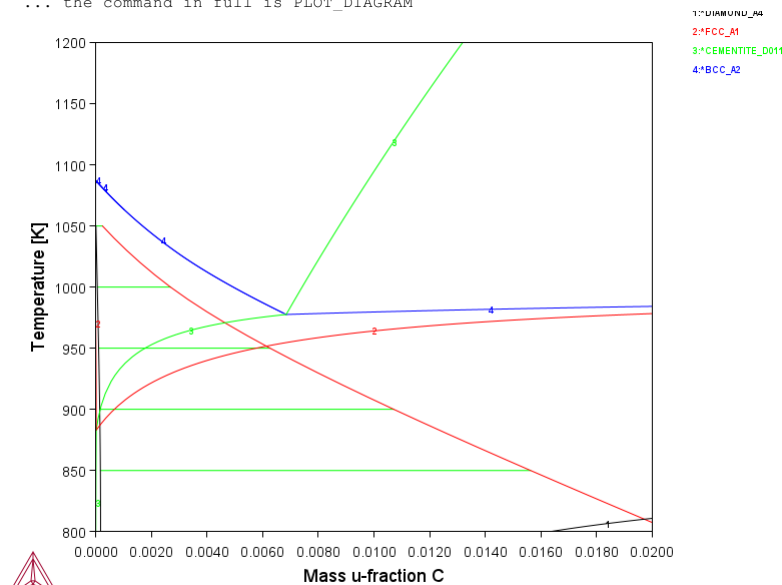
POST: s-s x n 0 0.02

... the command in full is SET_SCALING_STATUS

```

POST: s-s y n 800 1200
... the command in full is SET_SCALING_STATUS
POST: set-title example 42c
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



```

POST:Hit RETURN to continue
POST:
POST: back
POLY: read tcex42b
... the command in full is READ_WORKSPACES
POLY: s-c w(c)=0.01
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 23045 grid points in 0.148 s
Found the set of lowest grid points in 0.003 s
Calculated POLY solution 0.052 s, total time 0.203 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

```

Conditions:

T=900, P=100000, N=1, W(C)=1E-2, W(MN)=2.5E-2

DEGREES OF FREEDOM 0

Temperature 900.00 K (626.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.38780E+01

Total Gibbs energy -3.55310E+04, Enthalpy 2.03102E+04, Volume 7.05497E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	4.4413E-02	1.0000E-02	2.8388E-01	-9.4226E+03	SER
FE	9.3131E-01	9.7500E-01	8.2599E-03	-3.5891E+04	SER
MN	2.4275E-02	2.5000E-02	9.2895E-05	-6.9473E+04	SER

BCC_A2 Status ENTERED Driving force 0.0000E+00

Moles 8.2303E-01, Mass 4.5951E+01, Volume fraction 8.4971E-01 Mass fractions:

FE 9.93109E-01 MN 6.84649E-03 C 4.43634E-05

CEMENTITE_D011 Status ENTERED Driving force 0.0000E+00

Moles 1.7697E-01, Mass 7.9271E+00, Volume fraction 1.5029E-01 Mass fractions:

FE 8.04416E-01 MN 1.28547E-01 C 6.70366E-02

```

POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

```

This command calculates a paraequilibrium between two phases.

You must calculate an equilibrium with the overall composition first.

```

Name of first phase: fcc_al
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:

```

Output during stepping is:

axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,

and LNACR value(s) of interstitial(s)

Phase Region from	900.000	for:				
CEMENTITE_D011						
FCC_A1						
9.000000E+02	0.932	0.068	2.565452E-02	3.333333E-01	-1.153986E+00	
8.900000E+02	0.929	0.071	2.464593E-02	3.333333E-01	-1.126044E+00	
8.800000E+02	0.926	0.074	2.365344E-02	3.333333E-01	-1.097675E+00	
8.700000E+02	0.923	0.077	2.267732E-02	3.333333E-01	-1.068873E+00	
8.600000E+02	0.921	0.079	2.171789E-02	3.333333E-01	-1.039635E+00	
8.500000E+02	0.918	0.082	2.077544E-02	3.333333E-01	-1.009954E+00	
8.400000E+02	0.915	0.085	1.985030E-02	3.333333E-01	-9.798261E-01	
8.300000E+02	0.912	0.088	1.894282E-02	3.333333E-01	-9.492462E-01	
8.200000E+02	0.910	0.090	1.805335E-02	3.333333E-01	-9.182089E-01	
8.100000E+02	0.907	0.093	1.718224E-02	3.333333E-01	-8.867094E-01	
8.000000E+02	0.905	0.095	1.632989E-02	3.333333E-01	-8.547425E-01	


```

Phase Region from      900.000      for:
CEMENTITE_D011
FCC A1
9.000000E+02  0.932  0.068  2.565452E-02  3.333333E-01 -1.153986E+00
9.100000E+02  0.935  0.065  2.667894E-02  3.333333E-01 -1.181505E+00
9.200000E+02  0.939  0.061  2.771894E-02  3.333333E-01 -1.208606E+00
9.300000E+02  0.942  0.058  2.877430E-02  3.333333E-01 -1.235294E+00
9.400000E+02  0.945  0.055  2.984478E-02  3.333333E-01 -1.261573E+00
9.500000E+02  0.949  0.051  3.093020E-02  3.333333E-01 -1.287447E+00
9.600000E+02  0.952  0.048  3.203036E-02  3.333333E-01 -1.312922E+00
9.700000E+02  0.956  0.044  3.314510E-02  3.333333E-01 -1.338000E+00
9.800000E+02  0.959  0.041  3.427427E-02  3.333333E-01 -1.362687E+00
9.900000E+02  0.963  0.037  3.541772E-02  3.333333E-01 -1.386986E+00
1.000000E+03  0.967  0.033  3.657534E-02  3.333333E-01 -1.410901E+00
1.010000E+03  0.970  0.030  3.774702E-02  3.333333E-01 -1.434437E+00
1.020000E+03  0.974  0.026  3.893267E-02  3.333333E-01 -1.457595E+00
1.030000E+03  0.978  0.022  4.013222E-02  3.333333E-01 -1.480381E+00
1.040000E+03  0.982  0.018  4.134560E-02  3.333333E-01 -1.502798E+00
1.050000E+03  0.987  0.013  4.257278E-02  3.333333E-01 -1.524849E+00
1.060000E+03  0.991  0.009  4.381372E-02  3.333333E-01 -1.546537E+00
1.070000E+03  0.995  0.005  4.506840E-02  3.333333E-01 -1.567865E+00
1.080000E+03  1.000  0.000  4.633683E-02  3.333333E-01 -1.588837E+00
1.090000E+03  1.004 -0.004  4.761902E-02  3.333333E-01 -1.609455E+00
1.100000E+03  1.009 -0.009  4.891500E-02  3.333333E-01 -1.629722E+00
1.110000E+03  1.013 -0.013  5.022480E-02  3.333333E-01 -1.649641E+00
1.120000E+03  1.018 -0.018  5.154847E-02  3.333333E-01 -1.669214E+00
1.130000E+03  1.023 -0.023  5.288611E-02  3.333333E-01 -1.688443E+00
1.140000E+03  1.028 -0.028  5.423778E-02  3.333333E-01 -1.707332E+00
1.150000E+03  1.033 -0.033  5.560358E-02  3.333333E-01 -1.725881E+00
1.160000E+03  1.038 -0.038  5.698363E-02  3.333333E-01 -1.744093E+00
1.170000E+03  1.043 -0.043  5.837804E-02  3.333333E-01 -1.761970E+00
1.180000E+03  1.049 -0.049  5.978696E-02  3.333333E-01 -1.779514E+00
1.190000E+03  1.054 -0.054  6.121053E-02  3.333333E-01 -1.796726E+00
1.200000E+03  1.060 -0.060  6.264893E-02  3.333333E-01 -1.813608E+00
*** Buffer savend on file c:\jenkins\WORKSP~1\DEV_PI-1\GENERA~1\examples\tcex42\TCEX42~2.POL

```

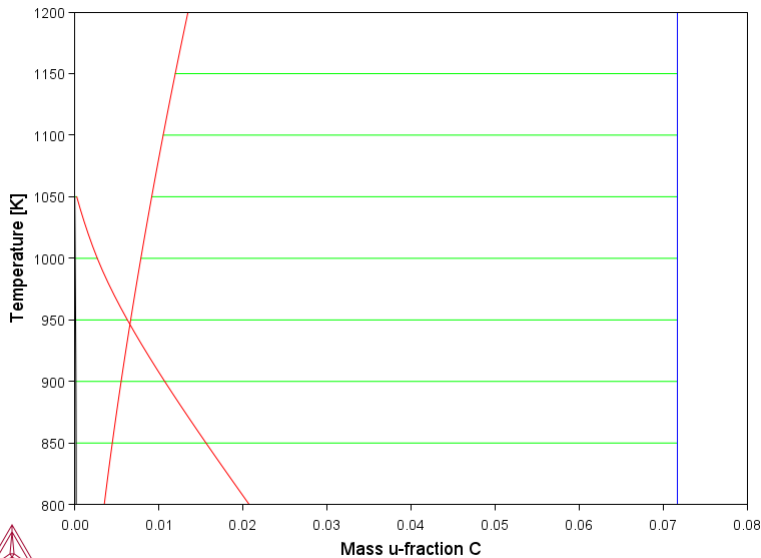
```

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-tit example 42d
... the command in full is SET_TITLE
POST: app-e n
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

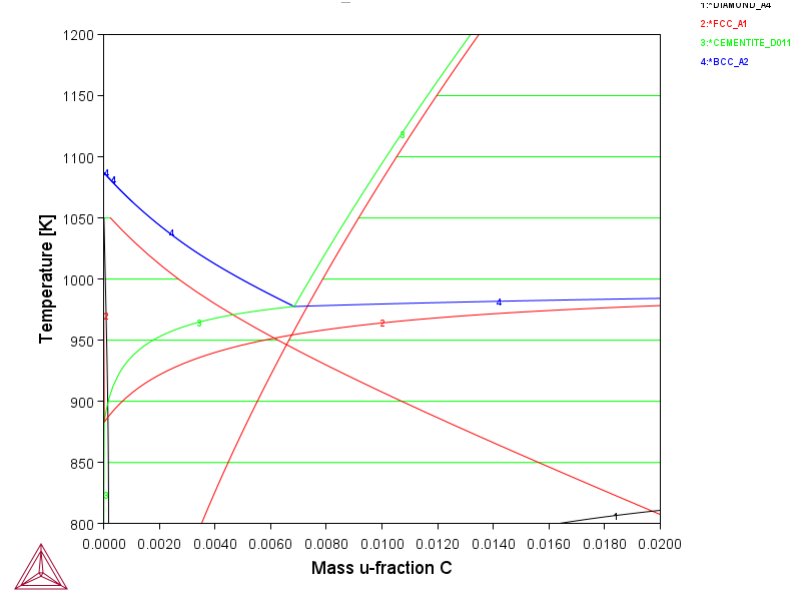


```

POST:
POST:Hit RETURN to continue
POST:
POST: app-e y tcex42
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
... the command in full is SET_SCALING_STATUS
POST: set-title example 42e
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5

```

```
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex43

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex43\tcex43.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Paraequilibrium calculation - Formation of

SYS: @@ Para-pearlite - Isothermal

SYS:

SYS: @@ This example uses an Fe-Mn-C system at 700 C to show a

SYS: @@ paraequilibrium calculation where there is formation of

SYS: @@ para-pearlite. It is an isothermal calculation and shows

SYS: @@ the Step_with_Options command.

SYS:

SYS: @@ Note that a TCFE database license is required to run

SYS: @@ the example.

SYS:

SYS: set-log ex43,,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-mater

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfell

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: c 0.1

2nd alloying element: mn 2

Next alloying element:

Temperature (C) /1000/: 700

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
GRAPHITE_A9	CEMENTITE_D011	M23C6_D84
M7C3_D101	M5C2	KSI_CARBIIDE
FE4N_LP1	C14_LAVES	C15_LAVES
G_PHASE	NBNI3_D0A	CUZN_EPSILON
AL5FE4		

Reject phase(s) /NONE/: graphite m5c2

GRAPHITE_A9 M5C2 REJECTED

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
A2_BCC	BCC_B2	FCC_A1
A1_FCC	FCC_L12	HCP_A3
CBCC_A12	CUB_A13	DIAMOND_A4
CEMENTITE_D011	M23C6_D84	M7C3_D101
KSI_CARBIIDE	FE4N_LP1	C14_LAVES
C15_LAVES	G_PHASE	NBNI3_D0A
CUZN_EPSILON	AL5FE4	

.....

OK? /Y/: Y

09:53:16,033 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 23045 grid points in 0.588 s
Found the set of lowest grid points in 0.004 s
Calculated POLY solution 0.288 s, total time 0.880 s

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=973.15, W(C)=1E-3, W(MN)=2E-2, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 973.15 K (700.00 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.56256E+01
Total Gibbs energy -4.11743E+04, Enthalpy 2.45990E+04, Volume 7.28130E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	4.6312E-03	1.0000E-03	1.2685E-01	-1.6706E+04	SER
FE	9.7512E-01	9.7900E-01	6.6201E-03	-4.0599E+04	SER
MN	2.0250E-02	2.0000E-02	1.0065E-04	-7.4471E+04	SER

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 7.8411E-01, Mass 4.3770E+01, Volume fraction 7.8786E-01 Mass fractions:
FE 9.87020E-01 MN 1.29127E-02 C 6.70791E-05

FCC_A1 Status ENTERED Driving force 0.0000E+00
Moles 2.1589E-01, Mass 1.1855E+01, Volume fraction 2.1214E-01 Mass fractions:
FE 9.49389E-01 MN 4.61663E-02 C 4.44436E-03

POLY:

POLY: @@ Change the status of component C to SPECIAL and work

POLY: @@ with u-fractions

POLY: c-s comp c

... the command in full is CHANGE_STATUS

Status: /ENTERED/: spec

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Found the set of lowest grid points in 0.005 s
Calculated POLY solution 0.153 s, total time 0.159 s

POLY:

POLY: s-a-v 1 w(c) 0 0.08

... the command in full is SET_AXIS_VARIABLE

Increment /0.002/: 2.5E-04

POLY: s-a-v 2 w(mn) 0 0.1

... the command in full is SET_AXIS_VARIABLE

Increment /0.0025/: .0025

POLY: l-a-v

... the command in full is LIST_AXIS_VARIABLE

Axis No 1: W(C)	Min: 0	Max: 8E-2	Inc: 2.5E-4
Axis No 2: W(MN)	Min: 0	Max: 0.1	Inc: 2.5E-3

POLY: save tcex43a y

... the command in full is SAVE_WORKSPACES

POLY: map

Version S mapping is selected

Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Working hard

Working hard

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10

Working hard

Working hard

Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20

Working hard

Phase region boundary 1 at: 3.082E-02 1.597E-02
BCC_A2
** CEMENTITE_D011
Calculated 17 equilibria

Phase region boundary 2 at: 3.082E-02 1.597E-02
BCC_A2
** CEMENTITE_D011
Calculated. 12 equilibria

Phase region boundary 3 at: 3.082E-02 4.346E-02

```

    BCC_A2
    ** CEMENTITE_D011
    ** FCC_A1

Phase region boundary 4 at: 3.349E-03 1.844E-02
    BCC_A2
    ** FCC_A1
Calculated 33 equilibria

Phase region boundary 5 at: 3.506E-02 5.674E-02
    CEMENTITE_D011
    ** FCC_A1
Calculated.. 48 equilibria
Terminating at axis limit.

Phase region boundary 6 at: 3.082E-02 4.346E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated 31 equilibria

Phase region boundary 7 at: 3.082E-02 1.597E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated 17 equilibria

Phase region boundary 8 at: 3.082E-02 1.597E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 9 at: 3.082E-02 2.819E-03
    BCC_A2
    ** CEMENTITE_D011
Calculated 12 equilibria

Phase region boundary 10 at: 3.082E-02 2.819E-03
    BCC_A2
    ** CEMENTITE_D011
Calculated. 18 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 3.082E-02 1.539E-03
    BCC_A2
    ** CEMENTITE_D011
Calculated 13 equilibria

Phase region boundary 12 at: 3.082E-02 1.539E-03
    BCC_A2
    ** CEMENTITE_D011
Calculated. 18 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 4.555E-04 4.440E-02
    BCC_A2
    ** FCC_A1
Calculated. 18 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 4.555E-04 4.440E-02
    BCC_A2
    ** FCC_A1
Calculated 15 equilibria

Phase region boundary 15 at: 1.376E-04 4.678E-02
    ** BCC_A2
    FCC_A1
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 1.376E-04 4.678E-02
    ** BCC_A2
    FCC_A1
Calculated 16 equilibria

Phase region boundary 17 at: 3.479E-02 1.686E-01
    ** CEMENTITE_D011
    FCC_A1
Calculated. 46 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 3.479E-02 1.686E-01
    ** CEMENTITE_D011
    FCC_A1
Calculated.. 3 equilibria
Terminating at axis limit.

Phase region boundary 19 at: 3.478E-02 1.711E-01
    ** CEMENTITE_D011
    FCC_A1
Calculated. 47 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: 1.264E-04 4.686E-02
    ** BCC_A2
    FCC_A1
Calculated 9 equilibria

Phase region boundary 21 at: 1.264E-04 4.686E-02
    ** BCC_A2
    FCC_A1
Calculated. 14 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 3.491E-02 1.118E-01
    ** CEMENTITE_D011
    FCC_A1
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 3.491E-02 1.118E-01
    ** CEMENTITE_D011
    FCC_A1
Calculated.. 26 equilibria
Terminating at axis limit.

```

Phase region boundary 24 at: 3.478E-02 1.718E-01
 ** CEMENTITE_D011
 FCC_A1
 Calculated. 48 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.501E-02 7.506E-02
 ** CEMENTITE_D011
 FCC_A1
 Calculated. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 26 at: 3.501E-02 7.506E-02
 ** CEMENTITE_D011
 FCC_A1
 Calculated.. 40 equilibria
 Terminating at axis limit.

Phase region boundary 27 at: 3.478E-02 1.701E-01
 ** CEMENTITE_D011
 FCC_A1
 Calculated. 47 equilibria
 Terminating at known equilibrium

*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex43\tcex43a.POLY3
 CPU time for mapping 10 seconds

POLY:
 POST: post
 POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-lab e
 ... the command in full is SET_LABEL_CURVE_OPTION

POST: set-title example 43a

POST: s-ax-text x N Mass u-fraction C
 ... the command in full is SET_AXIS_TEXT_STATUS

POST: s-ax-text y N Mass u-fraction Mn
 ... the command in full is SET_AXIS_TEXT_STATUS

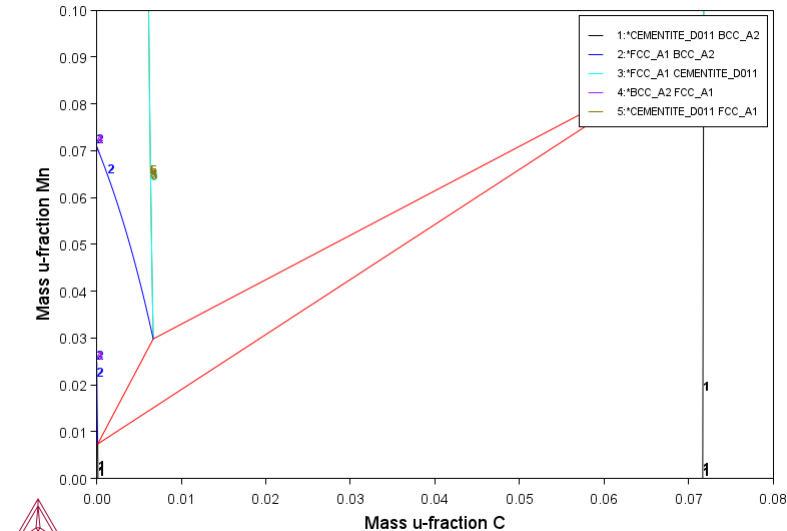
POST:
 POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 ... the command in full is MAKE_EXPERIMENTAL_DATAFI

POST: SET_EXP_FILE_FORMAT 10

POST:
 POST: plot
 ... the command in full is PLOT_DIAGRAM

example 43a



POST:
 POST:Hit RETURN to continue

POST:
 POST: make tcex43 y
 ... the command in full is MAKE_EXPERIMENTAL_DATAFI

POST: b
 ... the command in full is BACK

POLY: read tcex43a
 ... the command in full is READ_WORKSPACES

POLY: s-a-v 1 w(mn) 0 0.1
 ... the command in full is SET_AXIS_VARIABLE

Increment /.0025/ : .0025

POLY: s-a-v 2 none
 ... the command in full is SET_AXIS_VARIABLE

POLY: save tcex43b y
 ... the command in full is SAVE_WORKSPACES

POLY: step
 ... the command in full is STEP_WITH_OPTIONS

Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
 You must calculate an equilibrium with the overall composition first.

Name of first phase: fcc_a1
 Name of second phase: bcc_a2
 Fast diffusing component: /C/: C
 Fast diffusing component: /NONE/:

Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

Phase Region from 0.200000E-01 for:

	BCC_A2	FCC_A1				
2.000000E-02	0.165	0.835	2.571891E-02	4.926050E-04	-1.658137E+00	
1.750000E-02	0.148	0.852	2.818409E-02	5.501102E-04	-1.529404E+00	

1.500000E-02	0.134	0.866	3.064279E-02	6.094293E-04	-1.408661E+00
1.250000E-02	0.123	0.877	3.309442E-02	6.705749E-04	-1.294692E+00
1.000000E-02	0.112	0.888	3.553901E-02	7.335731E-04	-1.186526E+00
7.500000E-03	0.104	0.896	3.797641E-02	7.984452E-04	-1.083396E+00
5.000000E-03	0.096	0.904	4.040649E-02	8.652122E-04	-9.846802E-01
2.500000E-03	0.089	0.911	4.282917E-02	9.338953E-04	-8.898660E-01
2.500000E-09	0.082	0.918	4.524437E-02	1.004515E-03	-7.985285E-01

Phase Region from 0.200000E-01 for:

```

BCC_A2
FCC_A1
2.000000E-02 0.165 0.835 2.571891E-02 4.926050E-04 -1.658137E+00
2.250000E-02 0.185 0.815 2.324733E-02 4.368885E-04 -1.796470E+00
2.500000E-02 0.209 0.791 2.076966E-02 3.829392E-04 -1.946558E+00
2.750000E-02 0.240 0.760 1.828626E-02 3.307359E-04 -2.111382E+00
3.000000E-02 0.281 0.719 1.579754E-02 2.802573E-04 -2.295244E+00
3.250000E-02 0.338 0.662 1.330400E-02 2.314820E-04 -2.504681E+00
3.500000E-02 0.420 0.580 1.080620E-02 1.843887E-04 -2.750349E+00
3.750000E-02 0.552 0.448 8.304797E-03 1.389562E-04 -3.051429E+00
4.000000E-02 0.798 0.202 5.800548E-03 9.516350E-05 -3.448165E+00
4.250000E-02 1.418 -0.418 3.294329E-03 5.298938E-05 -4.051824E+00
4.500000E-02 5.984 -4.984 7.871532E-04 1.241291E-05 -5.521312E+00
*** Buffer savend on file c:\jenkins\WORKSP~1\DEV_PI~1\GENERA~1\examples\tcex43\TCEX43~2.POL
*** ERROR 3 IN NS01AD: Numerical error

```

POLY: po

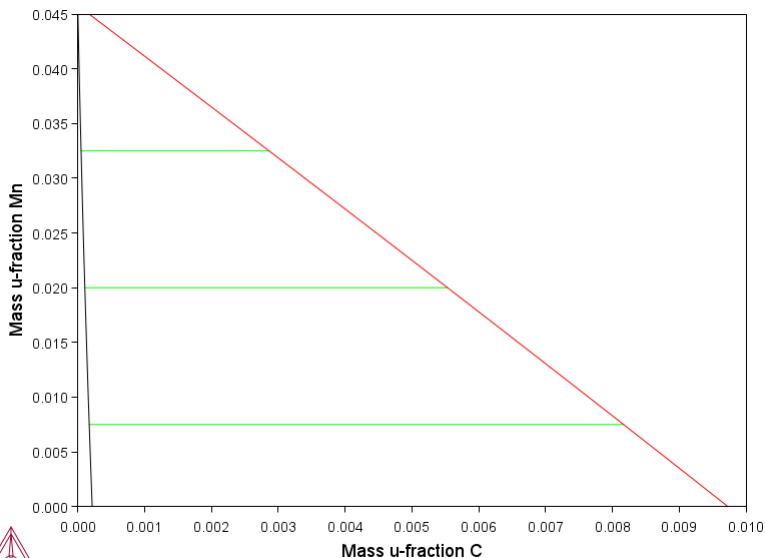
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y w(*,mn)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-title example 43b
POST: s-ax-text x N Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N Mass u-fraction Mn
... the command in full is SET_AXIS_TEXT_STATUS
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

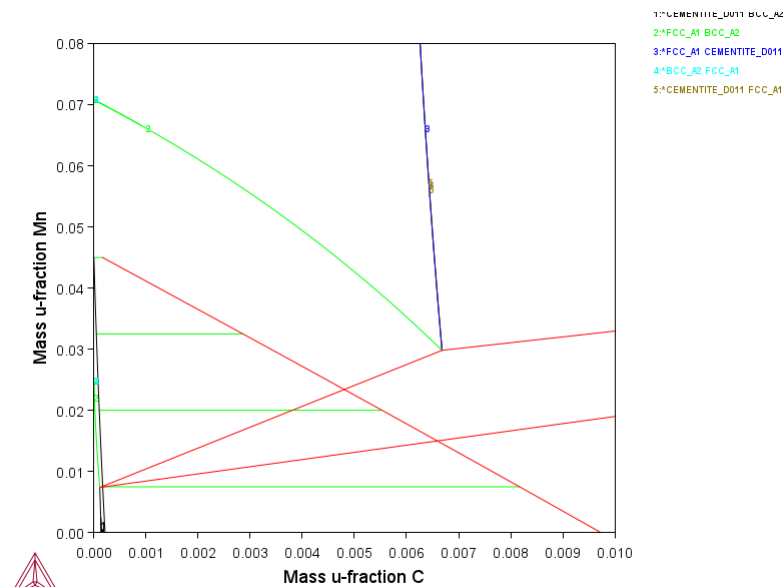
```



```

POST:
POST:Hit RETURN to continue
POST:
POST: app y tcex43
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.01
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.08
... the command in full is SET_SCALING_STATUS
POST: set-title example 43c
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



```

POST:
POST:Hit RETURN to continue
POST:
POST: b
... the command in full is BACK
POLY: read tcex43b
... the command in full is READ_WORKSPACES
POLY: l-c
... the command in full is LIST_CONDITIONS
T=973.15, W(C)=1E-3, W(MN)=2E-2, P=100000, N=1
DEGREES OF FREEDOM 0
POLY: s-c w(c)=0.008 w(mn)=0.07
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 23045 grid points in 0.162 s
Found the set of lowest grid points in 0.004 s
Calculated POLY solution 0.063 s, total time 0.229 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1, label A0 , database: TCFe11

Conditions:
T=973.15, W(C)=8E-3, W(MN)=7E-2, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 973.15 K ( 700.00 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.42144E+01
Total Gibbs energy -4.19930E+04, Enthalpy 2.75209E+04, Volume 7.10745E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C               3.5823E-02  8.0000E-03  1.7546E-01 -1.4082E+04 SER
FE              8.9565E-01  9.3000E-01  6.4327E-03 -4.0831E+04 SER
MN              6.8530E-02  7.0000E-02  1.4062E-04 -7.1765E+04 SER

FCC_A1          Status ENTERED   Driving force 0.0000E+00
Moles 9.6765E-01, Mass 5.2767E+01, Volume fraction 9.7259E-01 Mass fractions:
FE 9.27196E-01 MN 6.6490E-02 C 6.31349E-03

CEMENTITE_D011  Status ENTERED   Driving force 0.0000E+00
Moles 3.2348E-02, Mass 1.4478E+00, Volume fraction 2.7412E-02 Mass fractions:
FE 7.55790E-01 MN 1.77119E-01 C 6.70903E-02
POLY: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
NP(FCC_A1) = 0.9930 with U-fractions C = 3.50635E-02
NP(CEMENTITE) = 0.0070 with U-fractions C = 3.33333E-01
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

Phase Region from 0.700000E-01 for:
CEMENTITE_D011
FCC_A1
7.000000E-02 0.993 0.007 3.506346E-02 3.333333E-01 -1.531026E+00
6.750000E-02 0.993 0.007 3.497293E-02 3.333333E-01 -1.520657E+00
6.500000E-02 0.992 0.008 3.488283E-02 3.333333E-01 -1.510297E+00
6.250000E-02 0.992 0.008 3.479317E-02 3.333333E-01 -1.499947E+00
6.000000E-02 0.992 0.008 3.470394E-02 3.333333E-01 -1.489605E+00

```


5.750000E-02	0.992	0.008	3.461515E-02	3.333333E-01	-1.479273E+00
5.500000E-02	0.991	0.009	3.452678E-02	3.333333E-01	-1.468950E+00
5.250000E-02	0.991	0.009	3.443884E-02	3.333333E-01	-1.458637E+00
5.000000E-02	0.991	0.009	3.435133E-02	3.333333E-01	-1.448333E+00
4.750000E-02	0.990	0.010	3.426425E-02	3.333333E-01	-1.438038E+00
4.500000E-02	0.990	0.010	3.417758E-02	3.333333E-01	-1.427753E+00
4.250000E-02	0.990	0.010	3.409134E-02	3.333333E-01	-1.417478E+00
4.000000E-02	0.989	0.011	3.400552E-02	3.333333E-01	-1.407212E+00
3.750000E-02	0.989	0.011	3.392011E-02	3.333333E-01	-1.396955E+00
3.500000E-02	0.989	0.011	3.383511E-02	3.333333E-01	-1.386709E+00
3.250000E-02	0.989	0.011	3.375053E-02	3.333333E-01	-1.376471E+00
3.000000E-02	0.988	0.012	3.366636E-02	3.333333E-01	-1.366244E+00
2.750000E-02	0.988	0.012	3.358260E-02	3.333333E-01	-1.356026E+00
2.500000E-02	0.988	0.012	3.349924E-02	3.333333E-01	-1.345819E+00
2.250000E-02	0.988	0.012	3.341629E-02	3.333333E-01	-1.335621E+00
2.000000E-02	0.987	0.013	3.333374E-02	3.333333E-01	-1.325433E+00
1.750000E-02	0.987	0.013	3.325159E-02	3.333333E-01	-1.315254E+00
1.500000E-02	0.987	0.013	3.316983E-02	3.333333E-01	-1.305087E+00
1.250000E-02	0.986	0.014	3.308848E-02	3.333333E-01	-1.294928E+00
1.000000E-02	0.986	0.014	3.300753E-02	3.333333E-01	-1.284780E+00
7.500000E-03	0.986	0.014	3.292696E-02	3.333333E-01	-1.274642E+00
5.000000E-03	0.986	0.014	3.284679E-02	3.333333E-01	-1.264514E+00
2.500000E-03	0.985	0.015	3.276701E-02	3.333333E-01	-1.254396E+00
2.500000E-09	0.985	0.015	3.268761E-02	3.333333E-01	-1.244288E+00

Phase Region from 0.700000E-01 for:

CEMENTITE_D011

FCC A1

7.000000E-02	0.993	0.007	3.506346E-02	3.333333E-01	-1.531026E+00
7.250000E-02	0.993	0.007	3.515444E-02	3.333333E-01	-1.541404E+00
7.500000E-02	0.994	0.006	3.524586E-02	3.333333E-01	-1.551791E+00
7.750000E-02	0.994	0.006	3.533773E-02	3.333333E-01	-1.562187E+00
8.000000E-02	0.994	0.006	3.543004E-02	3.333333E-01	-1.572592E+00
8.250000E-02	0.995	0.005	3.552280E-02	3.333333E-01	-1.583006E+00
8.500000E-02	0.995	0.005	3.561601E-02	3.333333E-01	-1.593429E+00
8.750000E-02	0.995	0.005	3.570967E-02	3.333333E-01	-1.603861E+00
9.000000E-02	0.995	0.005	3.580380E-02	3.333333E-01	-1.614302E+00
9.250000E-02	0.996	0.004	3.589837E-02	3.333333E-01	-1.624751E+00
9.500000E-02	0.996	0.004	3.599341E-02	3.333333E-01	-1.635209E+00
9.750000E-02	0.996	0.004	3.608891E-02	3.333333E-01	-1.645676E+00
1.000000E-01	0.997	0.003	3.618487E-02	3.333333E-01	-1.656152E+00

*** Buffer savend on file c:\jenkins\WORKSP~1\DEV_PI~1\GENERA~1\examples\tcex43\TCEx43~2.POL

POLY: po

... the command in full is POST

POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x w(*,c)

... the command in full is SET_DIAGRAM_AXIS

COLUMN NUMBER /*/: *

POST: s-d-a y w(*,mn)

... the command in full is SET_DIAGRAM_AXIS

COLUMN NUMBER /*/: *

POST: set-tie 5

... the command in full is SET_TIELINE_STATUS

POST: set-title example 43d

POST: s-ax-text x N Mass u-fraction C

... the command in full is SET_AXIS_TEXT_STATUS

POST: s-ax-text y N Mass u-fraction Mn

... the command in full is SET_AXIS_TEXT_STATUS

POST: app-e n

... the command in full is APPEND_EXPERIMENTAL_DATA

POST: sel-plot new

... the command in full is SELECT_PLOT

POST:

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

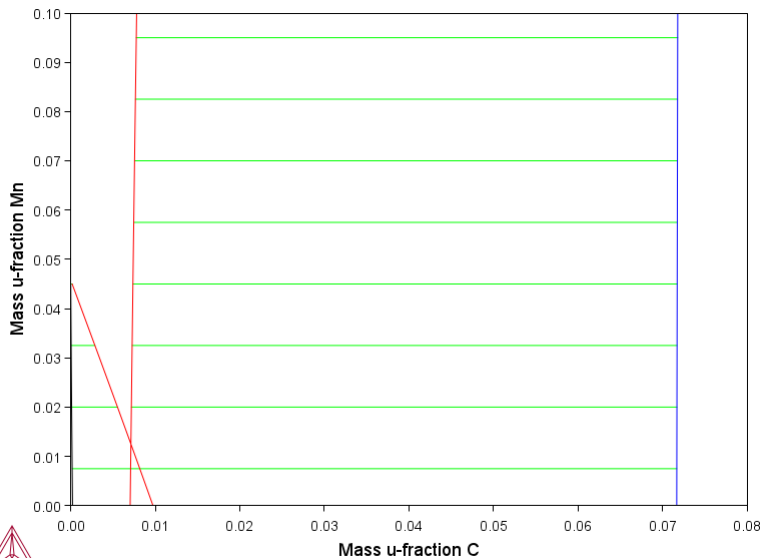
... the command in full is MAKE_EXPERIMENTAL_DATAFI

POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM



POST:

POST:

POST:Hit RETURN to continue

POST:

POST: s-s x n 0 0.01

... the command in full is SET_SCALING_STATUS

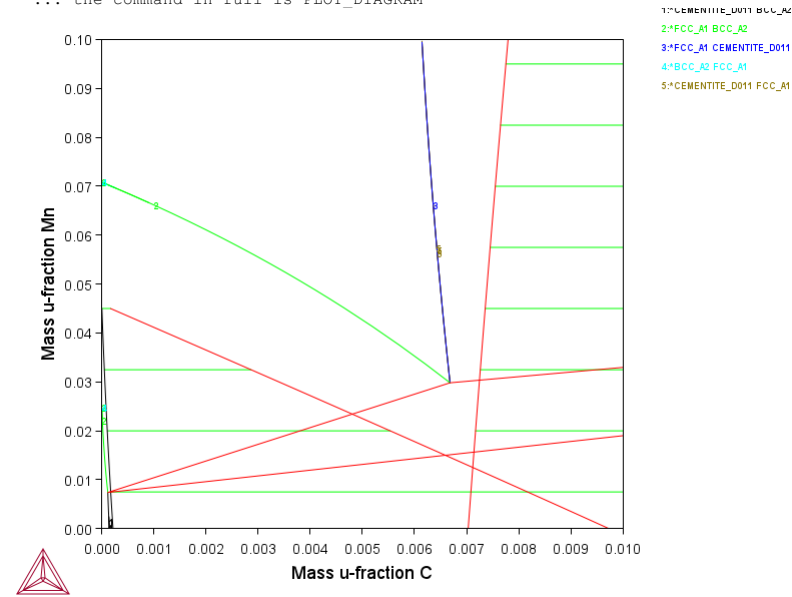
POST: s-s y n 0 0.10

... the command in full is SET_SCALING_STATUS

POST: app-e y tcex43

... the command in full is APPEND_EXPERIMENTAL_DATA

```
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 43e
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics, Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex44\tcex44.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Exploring variables and functions.

SYS:

SYS: @@ This example uses variables and functions to predict

SYS: @@ properties e.g. proof strength for an austenitic

SYS: @@ stainless steel at elevated temperatures (20-550 C).

SYS: @@ The example was created using an expression from

SYS: @@ Eliasson, J., and Sandstr m, R. (2000). 'Proof

SYS: @@ strength values for austenitic stainless steels at

SYS: @@ elevated temperatures', Steel Research, 71(6  7), 249  254.

SYS: @@ Note that a TCFE database license is required to run

SYS: @@ the example.

SYS:

SYS: @@ Note that in Graphical Mode there is a Yield Strength

SYS: @@ Property Model that does not require user input of

SYS: @@ empirical functions.

SYS:

SYS: go da

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw tcfell

TDB_TCFE11: def-sys

ELEMENTS: fe c si mn cr ni mo cu n

FE C SI

MN CR NI

MO CU N

DEFINED

TDB_TCFE11: get

09:54:33,853 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

Creating a new composition set FCC_A1#2

Creating a new composition set HCP_A3#2

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_TCFE11:

TDB_TCFE11: go p-3

POLY version 3.32

POLY:

POLY: s-c p=1e5,n=1,t=1353

POLY: s-c w(c)=0.0009,w(n)=0.0007,w(cr)=.246,w(ni)=0.2,w(mn)=0.013

POLY: s-c w(si)=0.013,w(cu)=0.0024,w(mo)=0.003

POLY: l-c

P=100000, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,

W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3

DEGREES OF FREEDOM 0

POLY: c-e

Using global minimization procedure

Calculated 51488 grid points in 1.112 s

Found the set of lowest grid points in 0.062 s

Calculated POLY solution 0.927 s, total time 2.101 s

POLY: l-e

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

P=100000, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,

W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3

DEGREES OF FREEDOM 0

Temperature 1353.00 K (1079.85 C), Pressure 1.000000E+05

Number of moles of components 1.000000E+00, Mass in grams 5.44621E+01

Total Gibbs energy -8.15441E+04, Enthalpy 3.59780E+04, Volume 7.33732E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	4.0809E-03	9.0000E-04	1.0130E-03	-7.7563E+04	SER
CR	2.5767E-01	2.4600E-01	2.9911E-03	-6.5384E+04	SER
CU	2.0569E-03	2.4000E-03	7.8672E-05	-1.0631E+05	SER
FE	5.0808E-01	5.2100E-01	1.1694E-03	-7.5948E+04	SER
MN	1.2887E-02	1.3000E-02	8.8491E-06	-1.3089E+05	SER
MO	1.7030E-03	3.0000E-03	6.5792E-05	-1.0832E+05	SER
N	2.7217E-03	7.0000E-04	1.4555E-07	-1.7710E+05	SER
NI	1.8559E-01	2.0000E-01	1.8375E-04	-9.6768E+04	SER
SI	2.5209E-02	1.3000E-02	8.7752E-09	-2.0869E+05	SER

FCC A1#1 Status ENTERED Driving force 0.0000E+00

Moles 9.8834E-01, Mass 5.3940E+01, Volume fraction 9.8975E-01 Mass fractions:

FE 5.24602E-01 NI 2.01793E-01 MN 1.30628E-02 CU 2.42325E-03 C 3.71539E-04

CR 2.41136E-01 SI 1.31259E-02 MO 2.77863E-03 N 7.06780E-04

M23C6_D84 Status ENTERED Driving force 0.0000E+00

Moles 1.1660E-02, Mass 5.2244E-01, Volume fraction 1.0249E-02 Mass fractions:

```

CR 7.48151E-01 C 5.54617E-02 NI 1.48568E-02 N 0.00000E+00 SI 0.00000E+00
FE 1.49155E-01 MO 2.58555E-02 MN 6.52026E-03 CU 0.00000E+00
POLY:
POLY: @@ Define some variables
POLY: enter-symb
Constant, variable, function or table? /FUNCTION/: variable
Name: cc
Function: 100*w(fcc_al,c)
&
POLY: ent var csi=100*w(fcc_al,si);
POLY: ent var cmn=100*w(fcc_al,mn);
POLY: ent var ccr=100*w(fcc_al,cr);
POLY: ent var cni=100*w(fcc_al,ni);
POLY: ent var cmo=100*w(fcc_al,mo);
POLY: ent var ccu=100*w(fcc_al,cu);
POLY: ent var cn=100*w(fcc_al,n);
POLY: ent var cfe=100*w(fcc_al,fe);
POLY: ent var cm23=100*bpw(m23c6);
POLY:
POLY: li-sy
DEFINED FUNCTIONS AND VARIABLES%
CC%=100*W(FCC_A1#1,C)
CSI%=100*W(FCC_A1#1,SI)
CMN%=100*W(FCC_A1#1,MN)
CCR%=100*W(FCC_A1#1,CR)
CNI%=100*W(FCC_A1#1,NI)
CMO%=100*W(FCC_A1#1,MO)
CCU%=100*W(FCC_A1#1,CU)
CN%=100*W(FCC_A1#1,N)
CFE%=100*W(FCC_A1#1,FE)
CM23%=100*BPW(M23C6_D84)
POLY:
POLY: eval
Name(s): *
CC=3.7153906E-2
CSI=1.3125912
CMN=1.306276
CCR=24.113639
CNI=20.179322
CMO=0.27786319
CCU=0.24232453
CN=7.0677989E-2
CFE=52.460153
CM23=0.95926481
POLY:
POLY: enter-symb
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: tc=t-273.15;
POLY:
POLY: @@ Enter empirical parameters as function of temperature
POLY: ent func bc=575-0.3686*tc;
POLY: ent func bsi=24.76+1.129e-4*tc*tc-0.09*tc;
POLY: ent func bmn=-1.4-0.007*tc;
POLY: ent func bcr=0.3-tc*7e-4;
POLY: ent func bni=5.3-tc*3.3e-3;
POLY: ent func bmo=6-tc*3.3e-3;
POLY: ent func bcu=-14+0.0116*tc;
POLY: ent func bn=937-2.74e-6*tc*tc*tc+5.24e-3*tc*tc-3.08*tc;
POLY: ent func bm23=48+0.0135*tc;
POLY: ent func at=1.68+4.248e-6*tc*tc-4.33e-3*tc;
POLY:
POLY: li-symb *
DEFINED FUNCTIONS AND VARIABLES%
CC%=100*W(FCC_A1#1,C)
CSI%=100*W(FCC_A1#1,SI)
CMN%=100*W(FCC_A1#1,MN)
CCR%=100*W(FCC_A1#1,CR)
CNI%=100*W(FCC_A1#1,NI)
CMO%=100*W(FCC_A1#1,MO)
CCU%=100*W(FCC_A1#1,CU)
CN%=100*W(FCC_A1#1,N)
CFE%=100*W(FCC_A1#1,FE)
CM23%=100*BPW(M23C6_D84)
TC=T-273.15
BC=575-.3686*TC
BSI=24.76+1.129E-04*TC*TC-.09*TC
BMN=-1.4-.007*TC
BCR=.3-TC*7E-04
BNI=5.3-TC*.0033
BMO=6-TC*.0033
BCU=-14+.0116*TC
BN=937-2.74E-06*TC*TC*TC+.00524*TC*TC-3.08*TC
BM23=48+.0135*TC
AT=1.68+4.248E-06*TC*TC-.00433*TC
POLY:
POLY: eval
Name(s): *
CC=3.7153906E-2
CSI=1.3125912
CMN=1.306276
CCR=24.113639
CNI=20.179322
CMO=0.27786319
CCU=0.24232453
CN=7.0677989E-2
CFE=52.460153
CM23=0.95926481
TC=1079.85
BC=176.96729
BSI=59.223483
BMN=-8.95895
BCR=-0.455895
BNI=1.736495
BMO=2.436495
BCU=-1.47374
BN=271.12745
BM23=62.577975
AT=1.9577404
POLY:
POLY: @@ Enter an empirical expression for the proof strength
POLY: @@ combining the variables and function parameters
POLY: @@ previously entered.
POLY: ent

```

```

Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp1
Function: at+bc*cc+bsi*csi+bm*cmn+bni*cn;
POLY:
POLY: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp2
Function: bcr*ccr+bmo*cmo+bcu*ccu+bn*cn+bm23*cm23;
POLY:
POLY: ent func rp02=rp1+rp2;
POLY:
POLY: eval
Name(s): *
CC=3.7153906E-2
CSI=1.3125912
CMN=1.306276
CCR=24.113639
CNI=20.179322
CMO=0.27786319
CCU=0.24232453
CN=7.0677989E-2
CFE=52.460153
CM23=0.95926481
TC=1079.85
BC=176.96729
BSI=59.223483
BMN=-8.95895
BCR=-0.455895
BNI=1.736495
BMO=2.436495
BCU=-1.47374
BN=271.12745
BM23=62.577975
AT=1.9577404
RP1=109.60742
RP2=68.518193
RP02=178.12561
POLY:
POLY: @@ Turn off the global minimization calculation and suspend
POLY: @@ all phases except fcc_al#1. This speeds up the calculation,
POLY: @@ and allows us to consider only single-phase FCC at all T.
POLY:
POLY: advanced
Which option? /STEP_AND_MAP/: glo
Settings for global minimization:
Use global minimization as much as possible /Y/: n,,,,
POLY:
POLY: c-s phase
Phase name(s): *
Status: /ENTERED/: sus
POLY:
POLY: ch-st phase fcc_al#1=enter 1
POLY:
POLY: s-c t=500
POLY: c-e
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,,
7 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
P=100000, N=1, T=500, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.44621E+01
Total Gibbs energy -1.87392E+04, Enthalpy 9.55257E+03, Volume 7.01404E-06

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
C               4.0809E-03  9.0000E-04  1.2030E-01 -8.8042E+03 SER
CR              2.5767E-01  2.4600E-01  2.8885E-01 -5.1626E+03 SER
CU              2.0569E-03  2.4000E-03  3.5447E-01 -4.3117E+03 SER
FE              5.0808E-01  5.2100E-01  3.4197E-02 -1.4033E+04 SER
MN              1.2887E-02  1.3000E-02  3.8948E-05 -4.2210E+04 SER
MO              1.7030E-03  3.0000E-03  7.9503E-02 -1.0526E+04 SER
N               2.7217E-03  7.0000E-04  8.1730E-14 -1.2528E+05 SER
NI              1.8559E-01  2.0000E-01  6.7678E-04 -3.0340E+04 SER
SI              2.5209E-02  1.3000E-02  4.6361E-16 -1.4678E+05 SER

FCC_A1#1      Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4462E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 5.21000E-01 NI 2.00000E-01 MN 1.30000E-02 CU 2.40000E-03 N 7.00000E-04
CR 2.46000E-01 SI 1.30000E-02 MO 3.00000E-03 C 9.00000E-04
POLY: l-st
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)      P(Pa)
VA              ENTERED      SER
C               ENTERED      SER
CR              ENTERED      SER
CU              ENTERED      SER
FE              ENTERED      SER
MN              ENTERED      SER
MO              ENTERED      SER
N               ENTERED      SER
NI              ENTERED      SER
SI              ENTERED      SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
FCC_A1#1      ENTERED      0.000000E+00      1.000000E+00
SUSPENDED PHASES:
Z_PHASE SIGMA_D8B SIC_B3 SI3N4 R_PHASE P_PHASE PI_A13 NIZN_L10 NIZN_B2
NISI_B31 NI3TI_D024 NI3SI2 NI3ISI2 NI2ZN11_D82 NBN13_D0A NB5SI3_D8L MU_D85
MSI_B20 MSI2_C40 MOSI2_C11B MO5SI3_D8M MNP_B31 MN9SI2_MN6SI MN6N5 MN5SIC
MN3N2 MN11SI19 MC_SHP MC_ETA M7C3_D101 M6SI5 M6C_E93 M5SI3_D88 M5C2 M4SI1_G3
M3SI M3C2_D510 M2SI_TETA M2P_C22 M23C6_D84 M11SI8 KSI CARBIDE HIGH_SIGMA
HCP_A3#2 HCP_A3#1 G_PHASE GRAPHITE_A9 FESI2_L FESI2_H FE8SI2C FE4N_LP1
FCC_L12 FCC_A1#2 ETA_M5SIN DIAMOND_A4 CUZN_EPSILON_CUB_A13 CU6Y CRZN17
CR5SI3_D8M CR3SI_A15 CO2SI_C37 CHI_A12 CEMENTITE_D011 CBCC_A12 C15_LAVES
C14_LAVES BCC_B2 BCC_A2 AL5FE4 AL4C3_D71 LIQUID_GAS
*** STATUS FOR ALL SPECIES
C              ENTERED      C5              ENTERED      CU2              ENTERED      N2              ENTERED

```

C1N1	ENTERED	C5N1	ENTERED	FE	ENTERED	N3	ENTERED
C1N2_CNN	ENTERED	C60	ENTERED	FE+2	ENTERED	NI	ENTERED
C1N2_NCN	ENTERED	C6N1	ENTERED	FE+3	ENTERED	NI+2	ENTERED
C2	ENTERED	C6N2	ENTERED	FE+4	ENTERED	NI+3	ENTERED
C2N1_CCN	ENTERED	C9N1	ENTERED	MN	ENTERED	SI	ENTERED
C2N1_CNC	ENTERED	CR	ENTERED	MN+2	ENTERED	SI+4	ENTERED
C2N2	ENTERED	CR+2	ENTERED	MN+3	ENTERED	SI3N4	ENTERED
C3	ENTERED	CR+3	ENTERED	MN+4	ENTERED	SIN4/3	ENTERED
C3N1	ENTERED	CU	ENTERED	MO	ENTERED	VA	ENTERED
C4	ENTERED	CU+1	ENTERED	MO+2	ENTERED		
C4N1	ENTERED	CU+2	ENTERED	N	ENTERED		
C4N2	ENTERED	CU+3	ENTERED	N-3	ENTERED		

POLY:Hit RETURN to continue

POLY: s-a-v 1 t

Min value /0/: 200

Max value /1/: 1000

Increment /20/: 10

POLY:

POLY: save tcex44 y

POLY:

POLY: @@ Step in temperature in order to evaluate proof strength

POLY: @@ as a function of temperature.

POLY:

POLY: step normal

No initial equilibrium, using default

Step will start from axis value 500.000

POLY has calculated initial equilibrium

Phase Region from 500.000 for:

FCC_A1#1

Terminating at 1000.00

Calculated 53 equilibria

Phase Region from 500.000 for:

FCC_A1#1

Terminating at 200.000

Calculated 33 equilibria

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex44\tcex44.POLY3

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a y rp02

POST: s-d-a x t-c

POST:

POST: set-title example 44a

POST:

POST: SET_EXP_FILE_FORMAT 5

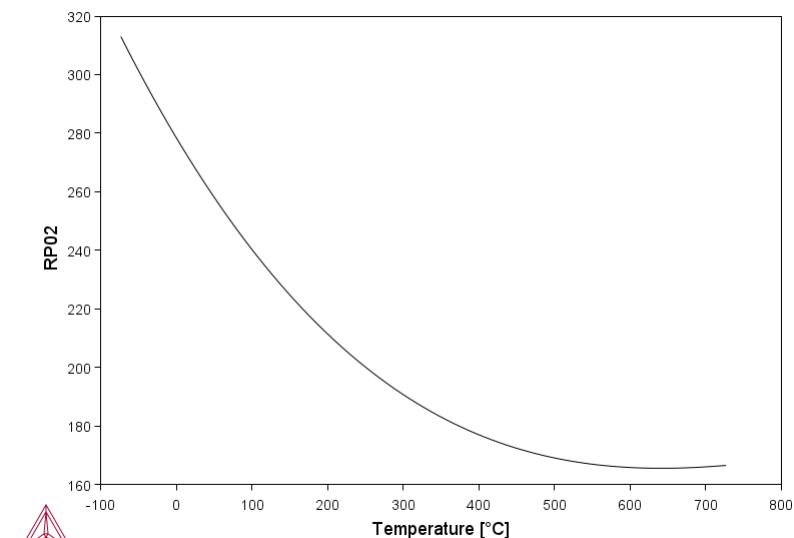
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

example 44a



POST:Hit RETURN to continue

POST:

POST: s-s-s x n 0 500

POST:

POST: set-ras y

POST:

POST: set-title example 44b

POST:

POST: SET_EXP_FILE_FORMAT 5

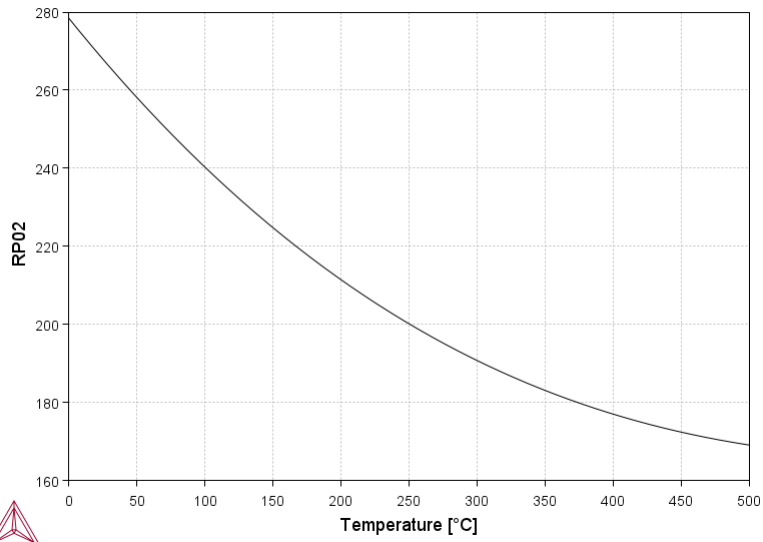
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

POST: SET_EXP_FILE_FORMAT 10

POST:

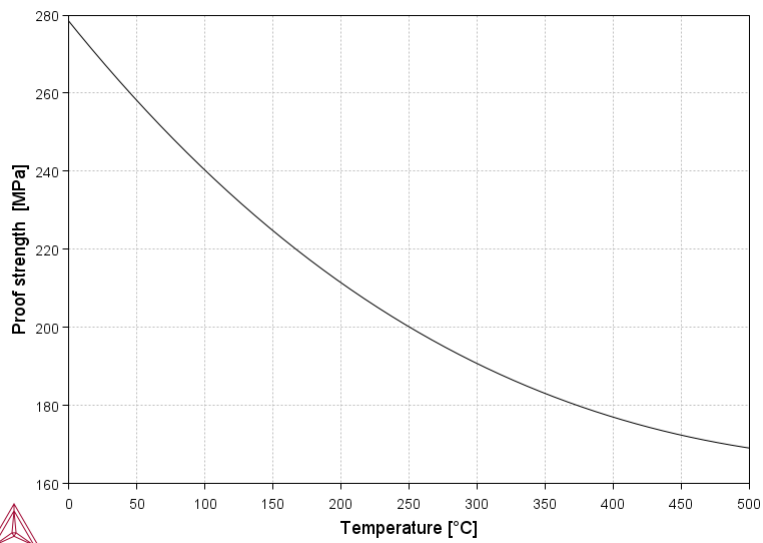
POST: plot

example 44b



```
POST:
POST:Hit RETURN to continue
POST:
POST: set-axis-text-status
POST: AXIS (X, Y OR Z) : y
POST: AUTOMATIC AXIS TEXT (Y OR N) /N/: n
POST: AXIS TEXT : Proof strength [MPa]
POST:
POST: set-title example 44c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

example 44c



```
POST:
POST: set-inter
POST:
```

tcex48

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex48\tcex48.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Scheil solidification with C "back diffusion"

SYS:

SYS: @@ This is an example of Scheil solidification with

SYS: @@ simulated back diffusion of carbon in solid phases.

SYS: @@ The results are compared between a simple Scheil and

SYS: @@ equilibrium calculation.

SYS:

SYS: @@ First perform a Partial Equilibrium Scheil by assigning

SYS: @@ carbon as a fast diffusing element.

SYS: @@ Plot solidification curve and a microsegregation

SYS: @@ diagram and save to file (so called .exp files).

SYS:

SYS: @@ The "back diffusion" of C in solid phases is not from

SYS: @@ any calculation involving kinetics, but comes from the

SYS: @@ equilibration of chemical potential of C at each step

SYS: @@ in temperature, thus allowing each already solidified

SYS: @@ part of the system to change its C concentration.

SYS:

SYS: @@ Note that there is a calculation type that calculates

SYS: @@ "real" back diffusion. See Console Mode example tcex54.

SYS: @@ This model requires a kinetic (mobility) database

SYS: @@ in addition to the thermodynamic one.

SYS:

SYS:

SYS: go scheil

SCHEIL: save-file-name tcex48a

SCHEIL: start

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: FEDEMO

Current database: Iron Demo Database v6.0

VA /- DEFINED

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: c 1

2nd alloying element: cr 10

Next alloying element:

Temperature (C) /2000/: 2000

VA /- DEFINED

REINITIATING GES

FE DEFINED

C DEFINED

CR DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
C14_LAVES	CBCC_A12	CEMENTITE_D011
CHI_A12	CUB_A13	DIAMOND_A4
FCC_A1	GRAPHITE_A9	HCP_A3
KSI_CARBIDE	M23C6_D84	M3C2_D510
M5C2	M7C3_D101	SIGMA_D8B

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
C14_LAVES	CBCC_A12	CEMENTITE_D011
CHI_A12	CUB_A13	DIAMOND_A4
FCC_A1	GRAPHITE_A9	HCP_A3
KSI_CARBIDE	M23C6_D84	M3C2_D510
M5C2	M7C3_D101	SIGMA_D8B

.....

OK? /Y/: Y

09:55:44,815 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

Creating a new composition set FCC_A1#2

Creating a new composition set HCP_A3#2

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/: C

This command is a combination of CHANGE_STATUS and SET_CONDITION

to calculate directly when a phase may form by releasing one condition.


```

You must release one of these conditions
T=2273.15, W(C)=1E-2, W(CR)=0.1, P=100000, N=1    DEGREES OF FREEDOM 0
PHASE CHANGE AT 1715.05468788
FCC_A1#1 forms
Testing POLY result by global minimization procedure
Calculated      20164 grid points in      0.071 s
    CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

Phase Region from      1715.14      for:
    LIQUID
Terminating at      1715.24
Calculated      4 equilibria

Phase Region from      1715.14      for:
    LIQUID
Global check of adding phase at      1.71505E+03
Calculated      3 equilibria

Phase Region from      1715.05      for:
    LIQUID
    FCC_A1#2
Global test at      1.70714E+03 .... OK
Global test at      1.69714E+03 .... OK
Global test at      1.68714E+03 .... OK
Global test at      1.67714E+03 .... OK
Global test at      1.66714E+03 .... OK
Global test at      1.65714E+03 .... OK
Global test at      1.64714E+03 .... OK
Global test at      1.63714E+03 .... OK
Global test at      1.62714E+03 .... OK
Global test at      1.61714E+03 .... OK
Global test at      1.60714E+03 .... OK
Global check of removing phase at      1.59813E+03
Calculated      120 equilibria

Phase Region from      1598.13      for:
    FCC_A1#2
Calculated      4 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex48\tcex48a.POLY3
    POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

    POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file c:\jenkins\WORKSP~1\DEV_PI~1\GENERA~1\examples\tcex48\tcex48a_EQ.EXP
has been created to store the equilibrium solidification results.
    CALCULATING SCHEIL SOLIDIFICATION
    T(C)      fraction solid
    1441.995      0.000000
PHASE REGION:LIQUID + FCC_A1#1
    T(C)      fraction solid
    1441.899      0.1329022E-03
    1440.899      0.2342642E-01
    1439.899      0.4585953E-01
    1438.899      0.6763138E-01
    1437.899      0.8876763E-01
    1436.899      0.1092937
    1435.899      0.1292335
    1434.899      0.1486098
    1433.899      0.1674443
    1432.899      0.1857574
    1431.899      0.2035686
    1430.899      0.2208963
    1429.899      0.2377580
    1428.899      0.2541705
    1427.899      0.2701497
    1426.899      0.2857107
    1425.899      0.3008678
    1424.899      0.3156350
    1423.899      0.3300252
    1422.899      0.3440509
    1421.899      0.3577242
    1420.899      0.3710564
    1419.899      0.3840585
    1418.899      0.3967408
    1417.899      0.4091133
    1416.899      0.4211856
    1415.899      0.4329668
    1414.899      0.4444657
    1413.899      0.4556908
    1412.899      0.4666499
    1411.899      0.4773509
    1410.899      0.4878012
    1409.899      0.4980079
    1408.899      0.5079779
    1407.899      0.5177177
    1406.899      0.5272337
    1405.899      0.5365319
    1404.899      0.5456182
    1403.899      0.5544983
    1402.899      0.5631775
    1401.899      0.5716612
    1400.899      0.5799544
    1399.899      0.5880619
    1398.899      0.5959884
    1397.899      0.6037386
    1396.899      0.6113168
    1395.899      0.6187271
    1394.899      0.6259739
    1393.899      0.6330609
    1392.899      0.6399920
    1391.899      0.6467711
    1390.899      0.6534016
    1389.899      0.6598870
    1388.899      0.6662309
    1387.899      0.6724363
    1386.899      0.6785066
    1385.899      0.6844448
    1384.899      0.6902539
    1383.899      0.6959369
    1382.899      0.7014966
    1381.899      0.7069357

```

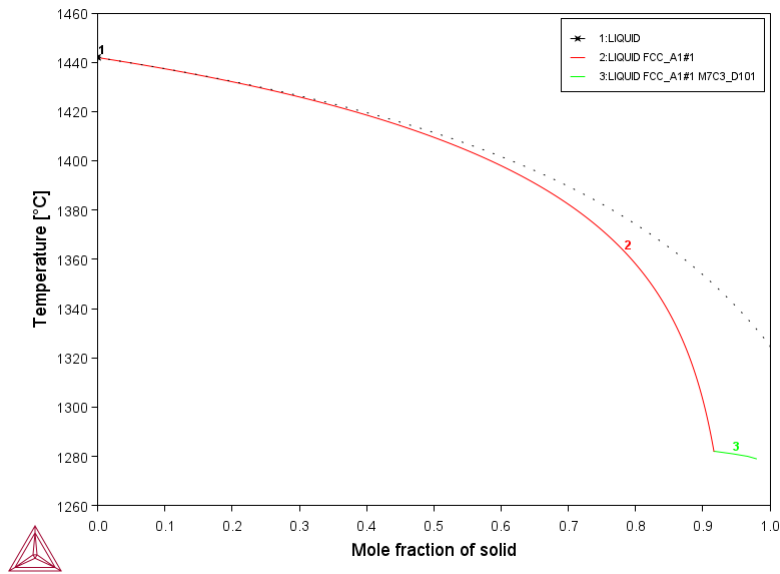
1380.899	0.7122570
1379.899	0.7174630
1378.899	0.7225564
1377.899	0.7275396
1376.899	0.7324150
1375.899	0.7371850
1374.899	0.7418519
1373.899	0.7464180
1372.899	0.7508854
1371.899	0.7552562
1370.899	0.7595327
1369.899	0.7637168
1368.899	0.7678105
1367.899	0.7718157
1366.899	0.7757345
1365.899	0.7795686
1364.899	0.7833198
1363.899	0.7869901
1362.899	0.7905810
1361.899	0.7940944
1360.899	0.7975319
1359.899	0.8008952
1358.899	0.8041858
1357.899	0.8074053
1356.899	0.8105553
1355.899	0.8136373
1354.899	0.8166528
1353.899	0.8196031
1352.899	0.8224898
1351.899	0.8253143
1350.899	0.8280778
1349.899	0.8307818
1348.899	0.8334275
1347.899	0.8360162
1346.899	0.8385492
1345.899	0.8410277
1344.899	0.8434529
1343.899	0.8458260
1342.899	0.8481482
1341.899	0.8504206
1340.899	0.8526443
1339.899	0.8548203
1338.899	0.8569498
1337.899	0.8590339
1336.899	0.8610734
1335.899	0.8630695
1334.899	0.8650231
1333.899	0.8669352
1332.899	0.8688067
1331.899	0.8706385
1330.899	0.8724315
1329.899	0.8741866
1328.899	0.8759047
1327.899	0.8775867
1326.899	0.8792332
1325.899	0.8808453
1324.899	0.8824235
1323.899	0.8839688
1322.899	0.8854819
1321.899	0.8869634
1320.899	0.8884142
1319.899	0.8898350
1318.899	0.8912264
1317.899	0.8925891
1316.899	0.8939237
1315.899	0.8952310
1314.899	0.8965116
1313.899	0.8977660
1312.899	0.8989948
1311.899	0.9001988
1310.899	0.9013784
1309.899	0.9025342
1308.899	0.9036667
1307.899	0.9047766
1306.899	0.9058642
1305.899	0.9069302
1304.899	0.9079750
1303.899	0.9089992
1302.899	0.9100032
1301.899	0.9109874
1300.899	0.9119524
1299.899	0.9128985
1298.899	0.9138263
1297.899	0.9147361
1296.899	0.9156283
1295.899	0.9165035
1294.899	0.9173618
1293.899	0.9182039
1292.899	0.9190299
1291.899	0.9198404
1290.899	0.9206356
1289.899	0.9214159
1288.899	0.9221816
1287.899	0.9229331
1286.899	0.9236708
1285.899	0.9243949
1284.899	0.9251057
1283.899	0.9258036
1282.899	0.9264888
1282.038	0.9271048

PHASE REGION: LIQUID + FCC A1#1 + M7C3_D101

T(C)	fraction solid
1282.007	0.9294371
1281.007	0.9559108
1280.007	0.9776565
1279.007	0.9907091

Calculating properties ...

Liquidus temperature: 1715.055 K



.....

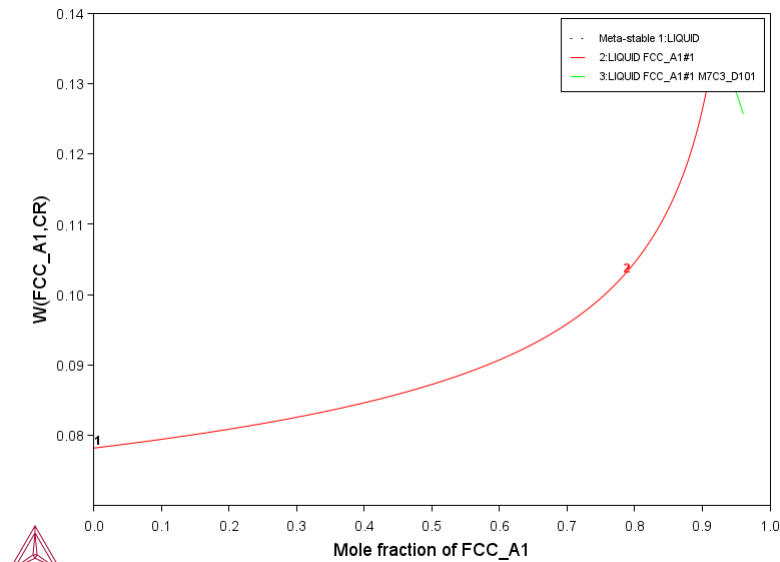
The following axis variables are available

T - Temperature in Celsius
 NL/BL/VL - Mole/mass/volume fraction of liquid
 NS/BS/VS - Mole/mass/volume fraction of all solid phases
 NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
 VS(ph) - Volume fraction of a solid phase
 W(ph,el) - Weight fraction of an element in a phase
 X(ph,el) - Mole fraction of an element in a phase
 Y(ph,el) - Site fraction of an element in a phase
 NN(ph,el) - Distribution of an element in a phase
 NH/BH - Heat release and Latent heat per mole/gram
 CP/BCP - Apparent heat capacity per mole/gram
 NV/NV(ph) - Molar volume of the system or a phase
 DS/DS(ph) - Average density of the system or a phase
 BT - Apparent volumetric TEC of the system
 DVIS(ph) - Dynamic viscosity of a phase
 KVIS(ph) - Kinematic viscosity of a phase
 SURF(ph) - Surface tension of a liquid phase
 ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
 ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
 THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
 "*" can be used as a wild character for "el" and "ph"

.....

POST:Hit RETURN to continue
 POST: make tcex48a.exp y
 POST:
 POST: set-dia-ax x ns(fcc_al)
 POST: set-dia-ax y w(fcc_al,cr)
 POST: sel-plot new
 POST:
 POST: SET_EXP_FILE_FORMAT 5
 POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 POST: SET_EXP_FILE_FORMAT 10
 POST:
 POST: plot,,,,,



POST:Hit RETURN to continue

POST:

POST:

POST: make tcex48b.exp y

POST:

POST: back

SCHEIL:

SCHEIL: @@ Ignore back diffusion of C in solids and do Scheil

SCHEIL: @@ with the same alloy by choosing option 3 from the

SCHEIL: @@ Scheil simulation option list.

SCHEIL: @@ Also plot solidification and microsegregation

SCHEIL: @@ diagrams and save to files

SCHEIL:

SCHEIL: save-file-name tcex48b

SCHEIL: start

Database /TCFE11/: FEDEMO

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: c 1

2nd alloying element: cr 10

Next alloying element:

Temperature (C) /2000/: 1700

VA /- DEFINED

REINITIATING GES

FE DEFINED

C DEFINED

CR DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC A2
C14_LAVES	CBCC_A12	CEMENTITE_D011
CHI_A12	CUB_A13	DIAMOND_A4
FCC_A1	GRAPHITE_A9	HCP_A3
KSI_CARBIIDE	M23C6_D84	M3C2_D510
M5C2	M7C3_D101	SIGMA_D8B

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC A2
C14_LAVES	CBCC_A12	CEMENTITE_D011
CHI_A12	CUB_A13	DIAMOND_A4
FCC_A1	GRAPHITE_A9	HCP_A3
KSI_CARBIIDE	M23C6_D84	M3C2_D510
M5C2	M7C3_D101	SIGMA_D8B

OK? /Y/: Y

ELEMENTS

SPECIES

PHASES

Creating a new composition set FCC_A1#2

Creating a new composition set HCP_A3#2

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/: NONE

This command is a combination of CHANGE_STATUS and SET_CONDITION

to calculate directly when a phase may form by releasing one condition.

You must release one of these conditions

T=1793.15, W(C)=1E-2, W(CR)=0.1, P=100000, N=1 DEGREES OF FREEDOM 0

PHASE CHANGE AT 1715.05468788

FCC_A1#1 forms

Testing POLY result by global minimization procedure

Calculated 20164 grid points in 0.068 s

CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS

...OK

Phase Region from 1715.14 for:

LIQUID

Terminating at 1715.24
Calculated 4 equilibria

Phase Region from 1715.14 for:
LIQUID
Global check of adding phase at 1.71505E+03
Calculated 3 equilibria

Phase Region from 1715.05 for:
LIQUID
FCC A1#2
Global test at 1.70714E+03 OK
Global test at 1.69714E+03 OK
Global test at 1.68714E+03 OK
Global test at 1.67714E+03 OK
Global test at 1.66714E+03 OK
Global test at 1.65714E+03 OK
Global test at 1.64714E+03 OK
Global test at 1.63714E+03 OK
Global test at 1.62714E+03 OK
Global test at 1.61714E+03 OK
Global test at 1.60714E+03 OK
Global check of removing phase at 1.59813E+03
Calculated 120 equilibria

Phase Region from 1598.13 for:
FCC A1#2
Calculated 4 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex48\tcex48b.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file c:\jenkins\WORKSP~1\DEV_PI~1\GENERA~1\examples\tcex48\tcex48b_EQ.EXP
has been created to store the equilibrium solidification results.

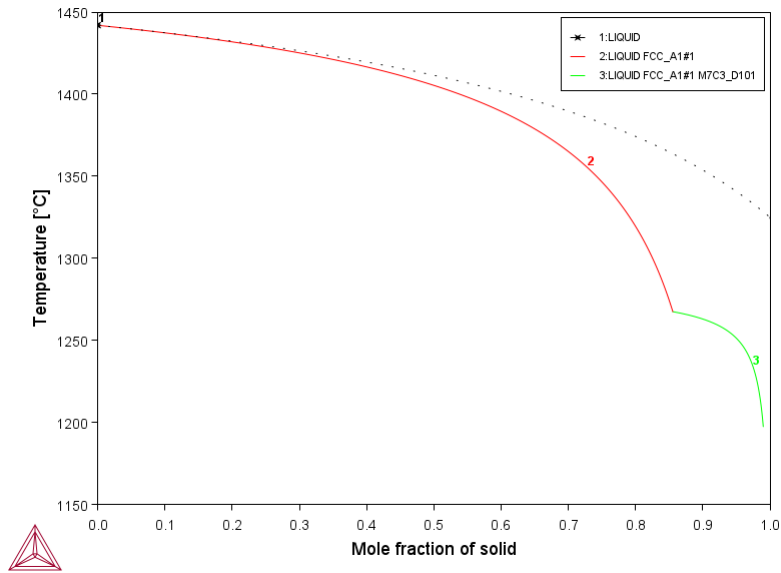
CALCULATING SCHEIL SOLIDIFICATION

T(C)	fraction solid
1441.995	0.000000
PHASE REGION: LIQUID + FCC A1#1	
T(C)	fraction solid
1441.899	0.1329022E-03
1440.899	0.2342642E-01
1439.899	0.4585862E-01
1438.899	0.6747197E-01
1437.899	0.8830633E-01
1436.899	0.1083992
1435.899	0.1277857
1434.899	0.1464991
1433.899	0.1645706
1432.899	0.1820295
1431.899	0.1989037
1430.899	0.2152193
1429.899	0.2310011
1428.899	0.2462723
1427.899	0.2610552
1426.899	0.2753706
1425.899	0.2892383
1424.899	0.3026771
1423.899	0.3157047
1422.899	0.3283380
1421.899	0.3405930
1420.899	0.3524849
1419.899	0.3640280
1418.899	0.3752362
1417.899	0.3861225
1416.899	0.3966992
1415.899	0.4069781
1414.899	0.4169706
1413.899	0.4266874
1412.899	0.4361386
1411.899	0.4453340
1410.899	0.4542829
1409.899	0.4629942
1408.899	0.4714763
1407.899	0.4797374
1406.899	0.4877852
1405.899	0.4956271
1404.899	0.5032702
1403.899	0.5107212
1402.899	0.5179866
1401.899	0.5250727
1400.899	0.5319853
1399.899	0.5387303
1398.899	0.5453131
1397.899	0.5517388
1396.899	0.5580126
1395.899	0.5641393
1394.899	0.5701234
1393.899	0.5759695
1392.899	0.5816819
1391.899	0.5872646
1390.899	0.5927217
1389.899	0.5980568
1388.899	0.6032737
1387.899	0.6083758
1386.899	0.6133667
1385.899	0.6182494
1384.899	0.6230272
1383.899	0.6277031
1382.899	0.6322800
1381.899	0.6367608
1380.899	0.6411480
1379.899	0.6454444
1378.899	0.6496525
1377.899	0.6537746
1376.899	0.6578132
1375.899	0.6617705
1374.899	0.6656487
1373.899	0.6694499
1372.899	0.6731762
1371.899	0.6768295
1370.899	0.6804118
1369.899	0.6839248
1368.899	0.6873704
1367.899	0.6907503
1366.899	0.6940662

1365.899	0.6973196
1364.899	0.7005122
1363.899	0.7036455
1362.899	0.7067209
1361.899	0.7097399
1360.899	0.7127038
1359.899	0.7156140
1358.899	0.7184717
1357.899	0.7212783
1356.899	0.7240349
1355.899	0.7267427
1354.899	0.7294029
1353.899	0.7320165
1352.899	0.7345847
1351.899	0.7371085
1350.899	0.7395889
1349.899	0.7420270
1348.899	0.7444235
1347.899	0.7467796
1346.899	0.7490960
1345.899	0.7513737
1344.899	0.7536136
1343.899	0.7558163
1342.899	0.7579829
1341.899	0.7601140
1340.899	0.7622104
1339.899	0.7642728
1338.899	0.7663021
1337.899	0.7682988
1336.899	0.7702636
1335.899	0.7721973
1334.899	0.7741005
1333.899	0.7759738
1332.899	0.7778178
1331.899	0.7796331
1330.899	0.7814204
1329.899	0.7831801
1328.899	0.7849129
1327.899	0.7866192
1326.899	0.7882996
1325.899	0.7899547
1324.899	0.7915848
1323.899	0.7931906
1322.899	0.7947724
1321.899	0.7963308
1320.899	0.7978662
1319.899	0.7993790
1318.899	0.8008697
1317.899	0.8023387
1316.899	0.8037865
1315.899	0.8052133
1314.899	0.8066196
1313.899	0.8080059
1312.899	0.8093723
1311.899	0.8107195
1310.899	0.8120476
1309.899	0.8133570
1308.899	0.8146482
1307.899	0.8159213
1306.899	0.8171768
1305.899	0.8184150
1304.899	0.8196361
1303.899	0.8208405
1302.899	0.8220285
1301.899	0.8232004
1300.899	0.8243564
1299.899	0.8254969
1298.899	0.8266221
1297.899	0.8277323
1296.899	0.8288277
1295.899	0.8299086
1294.899	0.8309753
1293.899	0.8320279
1292.899	0.8330668
1291.899	0.8340922
1290.899	0.8351043
1289.899	0.8361033
1288.899	0.8370895
1287.899	0.8380631
1286.899	0.8390242
1285.899	0.8399732
1284.899	0.8409101
1283.899	0.8418353
1282.899	0.8427488
1281.899	0.8436510
1280.899	0.8445419
1279.899	0.8454218
1278.899	0.8462908
1277.899	0.8471492
1276.899	0.8479970
1275.899	0.8488346
1274.899	0.8496620
1273.899	0.8504794
1272.899	0.8512869
1271.899	0.8520848
1270.899	0.8528732
1269.899	0.8536522
1268.899	0.8544220
1267.899	0.8551827
1267.548	0.8554471
PHASE REGION:LIQUID + FCC A1#1 + M7C3_D101	
T(C)	fraction solid
1267.517	0.8556564
1266.517	0.8680204
1265.517	0.8787644
1264.517	0.8881677
1263.517	0.8964509
1262.517	0.9037902
1261.517	0.9103282
1260.517	0.9161808
1259.517	0.9214436
1258.517	0.9261957
1257.517	0.9305032
1256.517	0.9344216
1255.517	0.9379979
1254.517	0.9412722

1253.517	0.9442785
1252.517	0.9470463
1251.517	0.9496011
1250.517	0.9519649
1249.517	0.9541568
1248.517	0.9561939
1247.517	0.9580907
1246.517	0.9598604
1245.517	0.9615144
1244.517	0.9630630
1243.517	0.9645153
1242.517	0.9658794
1241.517	0.9671625
1240.517	0.9683712
1239.517	0.9695113
1238.517	0.9705881
1237.517	0.9716065
1236.517	0.9725706
1235.517	0.9734845
1234.517	0.9743516
1233.517	0.9751754
1232.517	0.9759587
1231.517	0.9767042
1230.517	0.9774144
1229.517	0.9780917
1228.517	0.9787380
1227.517	0.9793554
1226.517	0.9799457
1225.517	0.9805103
1224.517	0.9810510
1223.517	0.9815690
1222.517	0.9820657
1221.517	0.9825423
1220.517	0.9829999
1219.517	0.9834395
1218.517	0.9838622
1217.517	0.9842688
1216.517	0.9846601
1215.517	0.9850370
1214.517	0.9854002
1213.517	0.9857504
1212.517	0.9860882
1211.517	0.9864142
1210.517	0.9867291
1209.517	0.9870333
1208.517	0.9873273
1207.517	0.9876116
1206.517	0.9878867
1205.517	0.9881530
1204.517	0.9884108
1203.517	0.9886606
1202.517	0.9889027
1201.517	0.9891375
1200.517	0.9893652
1199.517	0.9895861
1198.517	0.9898005
1197.517	0.9900088

Calculating properties ...
 Liquidus temperature: 1715.055 K



.....

The following axis variables are available

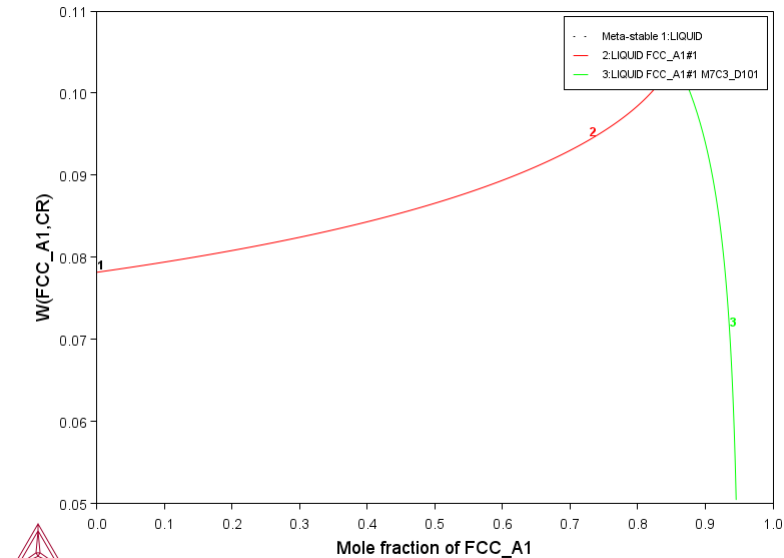
- T - Temperature in Celsius
- NL/BL/VL - Mole/mass/volume fraction of liquid
- NS/BS/VS - Mole/mass/volume fraction of all solid phases
- NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
- VS(ph) - Volume fraction of a solid phase
- W(ph,el) - Weight fraction of an element in a phase
- X(ph,el) - Mole fraction of an element in a phase
- Y(ph,el) - Site fraction of an element in a phase
- NN(ph,el) - Distribution of an element in a phase
- NH/BH - Heat release and Latent heat per mole/gram
- CP/BCP - Apparent heat capacity per mole/gram
- NV/NV(ph) - Molar volume of the system or a phase
- DS/DS(ph) - Average density of the system or a phase
- BT - Apparent volumetric TEC of the system
- DVIS(ph) - Dynamic viscosity of a phase
- KVIS(ph) - Kinematic viscosity of a phase
- SURF(ph) - Surface tension of a liquid phase
- ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
- ELCD/ELCD(ph) - Electrical conductivity of the system or a phase

THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
 "*" can be used as a wild character for "el" and "ph"

.....

POST:Hit RETURN to continue
 POST: make tcex48c.exp y
 POST: set-dia-ax x ns(fcc_al)
 POST: set-dia-ax y w(fcc_al,cr)
 POST: sel-plot new
 POST:
 POST:
 POST: SET_EXP_FILE_FORMAT 5
 POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
 POST: SET_EXP_FILE_FORMAT 10
 POST:
 POST: plot,,,,,



POST: make tcex48d.exp y
 POST: back
 SCHEIL:Hit RETURN to continue
 SCHEIL: @@ Calculate simple equilibrium solidification of the
 SCHEIL: @@ same alloy and compare the results with those of
 SCHEIL: @@ Scheil and ScheilC
 SCHEIL: go p-3
 POLY: read tcex48b
 POLY: list-condition
 T=1470.666563, P=100000, N(C)=1.712684108E-3, N(CR)=8.722253348E-4,
 N(FE)=7.614559498E-3
 DEGREES OF FREEDOM 0
 POLY: list-equilibrium
 OUTPUT TO SCREEN OR FILE /SCREEN/:
 Options /VWCS/: VWCS
 Output from POLY-3, equilibrium = 1, label A0 , database: FEDEMO
 Conditions:
 T=1470.666563, P=100000, N(C)=1.712684108E-3, N(CR)=8.722253348E-4,
 N(FE)=7.614559498E-3
 DEGREES OF FREEDOM 0
 Temperature 1470.67 K (1197.52 C), Pressure 1.000000E+05
 Number of moles of components 1.01995E-02, Mass in grams 4.91174E-01
 Total Gibbs energy -7.59430E+02, Enthalpy 5.56424E+02, Volume 7.04651E-08

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	1.7127E-03	4.1881E-02	5.7244E-02	-3.4977E+04	SER
CR	8.7223E-04	9.2334E-02	2.0297E-04	-1.0397E+05	SER
FE	7.6146E-03	8.6578E-01	1.4460E-03	-7.9958E+04	SER

LIQUID Status ENTERED Driving force 0.0000E+00
 Moles 9.9912E-03, Mass 4.8105E-01, Volume fraction 9.8002E-01 Mass fractions:
 FE 8.66596E-01 CR 9.14436E-02 C 4.19606E-02

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
 Moles 1.3784E-04, Mass 7.1889E-03, Volume fraction 1.4059E-02 Mass fractions:
 FE 9.31133E-01 CR 5.04939E-02 C 1.83727E-02

M7C3_D101 Status ENTERED Driving force 0.0000E+00
 Moles 7.0414E-05, Mass 2.9323E-03, Volume fraction 5.9217E-03 Mass fractions:
 FE 5.72418E-01 CR 3.41056E-01 C 8.65257E-02

POLY:Hit RETURN to continue
 POLY:
 POLY: reinit
 POLY: set-condition t=1717.15 w(cr)=0.1 w(c)=0.01 p=1e5 n=1
 POLY: c-e
 Using global minimization procedure
 Calculated 20919 grid points in 0.122 s
 Found the set of lowest grid points in 0.004 s
 Calculated POLY solution 0.033 s, total time 0.159 s
 POLY: set-ax-var 1 t 500 1717.15 10
 POLY: advanced
 Which option? /STEP_AND_MAP/: break-condition
 Break condition: np(liquid)=0


```

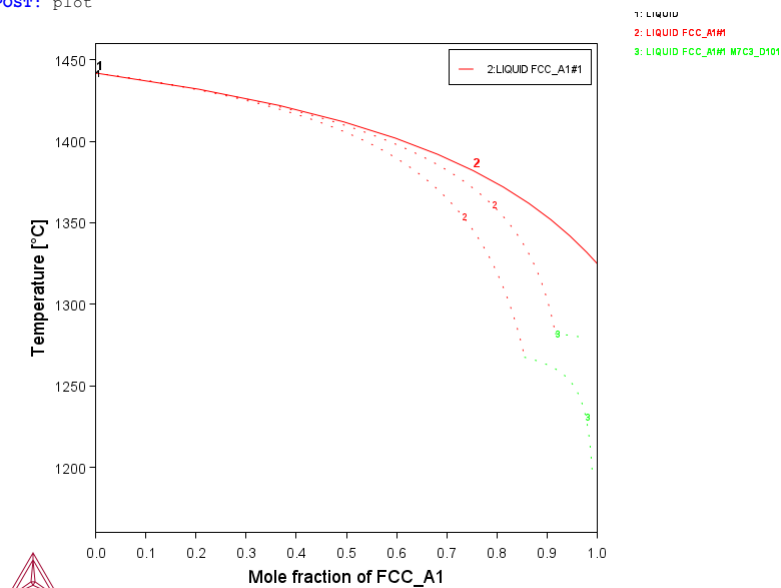
POLY: save tcex48c y
POLY: step normal
No initial equilibrium, trying to add one
Step will start from axis value 1717.15

Phase Region from 1717.15 for:
LIQUID
Calculated 4 equilibria

Phase Region from 1715.05 for:
LIQUID
FCC_A1#1
Calculated 14 equilibria

Phase Region from 1598.13 for:
FCC_A1#1
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex48\tcex48c.POLY3
POLY: post
POST: @@ Define a function to get the amount of solids
POST: ent fun fs=1-np(liquid);
POST: @@ Plot a solidification diagram
POST: set-dia-ax x fs
POST: set-dia-ax y t-c
POST: append-exp y tcex48a tcex48c 0; 1; 0; 1;
POST: set-ax-text x n
AXIS TEXT : Mole fraction of FCC_A1
POST: set-scaling-status y n 1160 1460
POST: set-title example 48e
POST: sel-plot new
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

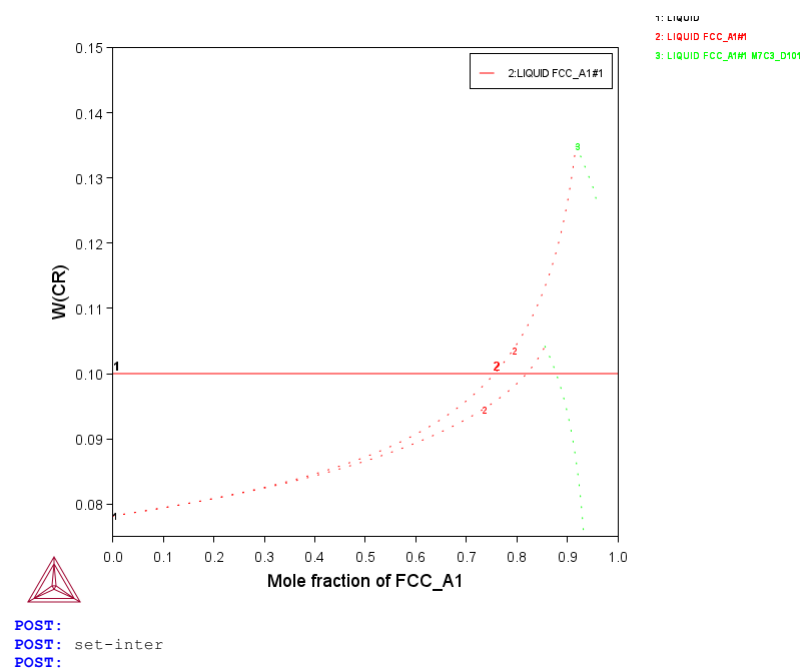
```



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ Plot microsegregation, which represents the composition
POST: @@ profile of the solid. For equilibrium solidification
POST: @@ there is no solute segregation and the composition of
POST: @@ solidified solid is uniform.
POST:
POST: set-dia-ax x fs
POST: set-dia-ax y w(cr)
POST: append-exp y tcex48b tcex48d 0; 1; 0; 1;
POST: set-ax-text x n
AXIS TEXT : Mole fraction of FCC_A1
POST: set-scaling y n 0.075 0.15
POST: set-title example 48f
POST: sel-plot new
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



tcex49

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex49\tcex49.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Quasichemical model using the GES module

SYS:

SYS: @@ This example shows how to enter parameters

SYS: @@ for a FACT quasichemical liquid model and

SYS: @@ how to calculate the sulfur activity using

SYS: @@ the Gibbs energy system (GES) module commands.

SYS:

SYS: @@ This example uses some GES commands that are not yet

SYS: @@ supported by GES6. Therefore, we enforce the use of GES5.

SYS:

SYS: set-ges-version 5

SYS:

SYS: set-log ex49,,,

SYS:

SYS: go gibbs

... the command in full is GOTO_MODULE

GIBBS ENERGY SYSTEM

GES5: ent-el /- VA CU S

... the command in full is ENTER_ELEMENT

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

GES5: am_el_d /- ELECTRON_GAS 0.0000E+00 0.0000E+00 0.0000E+00 1

... the command in full is AMEND_ELEMENT_DATA

GES5: am_el_d VA VACUUM 0.0000E+00 0.0000E+00 0.0000E+00 1

... the command in full is AMEND_ELEMENT_DATA

GES5: am_el_d CU FCC_A1 6.3546E+01 5.0041E+03 3.3150E+01 1

... the command in full is AMEND_ELEMENT_DATA

GES5: am_el_d S FC_ORTHORHOMBIC 3.2066E+01 0.0000E+00 0.0000E+00 1

... the command in full is AMEND_ELEMENT_DATA

GES5:

GES5:

GES5: @@ The quasichemical model requires species entered with the

GES5: @@ stoichiometry. The factor 2/ZZ is needed

GES5: @@ for the pure elements and 1/ZZ for the compounds.

GES5: @@ For Cu ZZ=0.9294 and 2/ZZ_Cu=2.15193

GES5: @@ For S ZZ=1.8366 and 2/ZZ_S=1.08897

GES5: @@ For CuS the stoichiometries are thus 1/ZZ_Cu=1.07596 and

GES5: @@ 1/ZZ_S=0.54448

GES5:

GES5: enter-specie CUQ CU2.15193

... the command in full is ENTER_SPECIES

GES5: enter-specie CUQS CU1.07596S0.54448

... the command in full is ENTER_SPECIES

GES5: enter-specie S2 S2

... the command in full is ENTER_SPECIES

GES5: enter-specie SQ S1.08897

... the command in full is ENTER_SPECIES

GES5:

GES5:

GES5: @@ The Gibbs energy difference between FCC-Cu

GES5: @@ and quasichemical liquid-Cu

GES5:

GES5: ent-sym fun GQCU 2.98150E+02 +16547-7.6815*T; 6.00000E+03 N

... the command in full is ENTER_SYMBOL

GES5:

GES5:

GES5: @@ The Gibbs energy difference between GAS-S and

GES5: @@ quasichemical liquid-S

GES5:

GES5: ent-sym fun GQS 2.98150E+02 -65357+165.396*T-13.513*T*LN(T);

... the command in full is ENTER_SYMBOL

HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N

GES5:

GES5:

GES5:

GES5: @@ Gibbs energies for the pure elements and gases referred to SER

GES5: ent-sym fun GHSERCU 2.98150E+02 -7770.458+130.485403*T

... the command in full is ENTER_SYMBOL

& -24.112392*T*LN(T)-.00265684*T**2+1.29223E

& -07*T**3+52478*T**(-1); 1.35802E+03 Y

FUNCTION: -13542.33+183.804197*T-31.38*T*LN(T)+3.64643E+29*T**(-9);

HIGH TEMPERATURE LIMIT /6000/: 3.20000E+03 N

GES5: ent-sym fun GS2GAS 2.98150E+02 +117374.548+2.98629558*T

... the command in full is ENTER_SYMBOL

& -34.09678*T*LN(T)-.002325464*T**2+1.85480167E-07*T**3

& +128593.6*T**(-1); 1.00000E+03 Y

FUNCTION: +117352.438+2.50383258*T-34.04744*T*LN(T)-.0021150245*T**2

& +9.16602333E-08*T**3+175718.45*T**(-1); 3.40000E+03 Y

FUNCTION: +124361.091+14.5182895*T-36.1923*T*LN(T)-5.930925E-04*T**2

& -7.54259333E-09*T**3-7484105*T**(-1); 6.00000E+03 N

GES5: ent-sym fun GSSLIQ 2.98150E+02 -4001.549+77.889686*T

... the command in full is ENTER_SYMBOL

& -15.504*T*LN(T)-.018629*T**2-2.4942E-07*T**3

& -113945*T**(-1); 3.88360E+02 Y

FUNCTION: -5285183.35+118449.585*T-19762.4*T*LN(T)+32.79275*T**2

& -.0102214167*T**3+2.646735E+08*T**(-1); 4.28150E+02 Y

FUNCTION: -8174995.23+319914.078*T-57607.3*T*LN(T)+135.3045*T**2

```

& -.0529973333*T**3; 4.32250E+02 Y
FUNCTION: -219408.801+7758.83993*T-1371.85*LN(T)+2.845035*T**2
& -.00101380333*T**3; 4.53150E+02 Y
FUNCTION: +92539.872-1336.36627*T+202.958*LN(T)-.2531915*T**2
& +5.18835E-05*T**3-8202200*T*(-1); 7.17000E+02 Y
FUNCTION: -6889.972+176.35482*T-32*LN(T); 1.30000E+03 N
GES5: ent-sym fun GCULIQ 2.98150E+02 +12964.84-9.510243*T
... the command in full is ENTER_SYMBOL
& -5.83932E-21*T**7+GHSERCU ; 1.35802E+03 Y
FUNCTION: +13495.4-9.920463*T-3.64643E+29*T*(-9)+GHSERCU ;
HIGH TEMPERATURE LIMIT /6000/: 3.20000E+03 N
GES5:
GES5:
GES5:
GES5: ent-phase GAS G, 1 S2 ; N N
... the command in full is ENTER_PHASE
GES5:
GES5:
GES5: ent-param G(GAS,S2;0) 2.98150E+02 +GS2GAS +RTLNP ;
... the command in full is ENTER_PARAMETER
G(GAS,S2;0)- 2 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES5:
GES5:
GES5:
GES5: ent-phase FCC_A1 , 1 CU ; N N
... the command in full is ENTER_PHASE
GES5: amend_phase FCC_A1 magnetic -3.0 2.80000E-01
... the command in full is AMEND_PHASE_DESCRIPTION
GES5:
GES5:
GES5: ent-param G(FCC_A1,CU;0) 2.98150E+02 +GHSERCU; 3.20000E+03 N
... the command in full is ENTER_PARAMETER
G(FCC_A1,CU;0)-G(FCC_A1,CU;0)
GES5:
GES5:
GES5:
GES5: ent-phase QUASI L, 1 CUQ,CUQS,SQ ; N N
... the command in full is ENTER_PHASE
GES5:
GES5:
GES5: @@ The stoichiometry parameter for pure Cu is 2/ZZ,
GES5: @@ the stoichiometry ratio
GES5:
GES5: ent-param VK(QUASI,CUQ;0) 2.98150E+02 .9294; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
VK(QUASI,CUQ;0)
GES5:
GES5: @@ The energy parameter for pure Cu (factor is 2/VK)
GES5:
GES5: ent-param G(QUASI,CUQ;0) 2.98150E+02 +2.15193*GCULIQ
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ;0)-2.15193 G(FCC_A1,CU;0)
& +2.15193*GQCU ; 6.00000E+03 N
GES5:
GES5: @@ The Gibbs energy parameter for the molecule CUQS
GES5: @@ (factors 1/ZZ_cu and 1/ZZ_s)
GES5:
GES5: ent-param G(QUASI,CUQS;0) 2.98150E+02 +1.07596*GCULIQ
... the command in full is ENTER_PARAMETER
G(QUASI,CUQS;0)-1.07596 G(FCC_A1,CU;0)-0.54448 G(FC_ORTHORHOMBIC,S;0)
& +1.075963*GQCU+.54448*GSSLIQ ; 6.00000E+03 N
GES5:
GES5:
GES5: @@ The stoichiometry parameter for pure S is 2/ZZ
GES5:
GES5: ent-param VK(QUASI,SQ;0) 2.98150E+02 1.8366; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
VK(QUASI,SQ;0)
GES5:
GES5: @@ The energy parameter for pure S (factor is 2/VK)
GES5:
GES5: ent-param G(QUASI,SQ;0) 2.98150E+02 +1.08897*GSSLIQ ;
... the command in full is ENTER_PARAMETER
G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES5:
GES5: @@ The mixing terms
GES5:
GES5: ent-param G(QUASI,CUQ,CUQS;0) 2.98150E+02 -82768; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;0)
GES5: ent-param G(QUASI,CUQ,CUQS;1) 2.98150E+02 -32070; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;1)
GES5: ent-param G(QUASI,CUQ,CUQS;2) 2.98150E+02 68734; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;2)
GES5: ent-param G(QUASI,CUQ,CUQS;3) 2.98150E+02 -84194+50*T;
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;3)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES5: ent-param G(QUASI,CUQ,CUQS;4) 2.98150E+02 -43638; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;4)
GES5: ent-param G(QUASI,CUQ,CUQS;5) 2.98150E+02 +20*T; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;5)
GES5:
GES5:
GES5: @@ This command makes the entropy calculation according
GES5: @@ to FACT quasichemical model
GES5:
GES5: amend-phase-description QUASI quasi-fact00
GES5:
GES5: @@ Binary excess Legendre with 1 as independent
GES5: @@ Note that the order of the species are important.
GES5:
GES5: amend-phase-description QUASI excess
MODEL NAME /REDLICH-KISTER MUGGIANU/: mixed
First (the independent) constituent: CUQ

```

Second (the dependent) constituent: CUQS
Excess model type: /LEGENDRE/: Legendre

Any other non-Redlich-Kister binary excess parameters?

First (the independent) constituent: NONE

GES5:

GES5:

GES5:

GES5: list-data

OUTPUT TO SCREEN OR FILE /SCREEN/:

OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT DATE 2025- 5-12
FROM DATABASE: User data 2025.05.12

ALL DATA IN SI UNITS

FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON_GAS		0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	CU	FCC_A1		6.3546E+01	5.0041E+03	3.3150E+01
2	S	FC_ORTHORHOMBIC		3.2066E+01	0.0000E+00	0.0000E+00

SPECIES	STOICHIOMETRY
1 CU	CU
2 CUQ	CU2.15193
3 CUQS	CU1.07596S0.54448
4 S	S
5 S2	S2
6 SQ	S1.08897
7 VA	VA

GAS

CONSTITUENTS: S2

G(GAS,S2;0) - 2 G(FC_ORTHORHOMBIC,S;0) = +GS2GAS+RTLNP

QUASI

\$ QUASICHEMICAL-FACT00 ENTROPY CONTRIBUTION

CONSTITUENTS: CUQ,CUQS,SQ

VK(QUASI,CUQ;0) = +.9294
G(QUASI,CUQ;0)-2.15193 G(FCC_A1,CU;0) = +2.15193*GCULIQ+2.15193*GQCU
G(QUASI,CUQS;0)-1.07596 G(FCC_A1,CU;0)-0.54448 G(FC_ORTHORHOMBIC,S;0) =
+1.07596*GCULIQ+1.075963*GQCU+.54448*GSSLIQ
VK(QUASI,SQ;0) = +1.8366
G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0) = +1.08897*GSSLIQ

\$ Binary excess model Legendre with CUQ as independent

L(QUASI,CUQ,CUQS;0) = -82768
L(QUASI,CUQ,CUQS;1) = -32070
L(QUASI,CUQ,CUQS;2) = +68734
L(QUASI,CUQ,CUQS;3) = -84194+50*T
L(QUASI,CUQ,CUQS;4) = -43638
L(QUASI,CUQ,CUQS;5) = +20*T

FCC_A1

ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING

Magnetic function below Curie Temperature
+1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
-.0017449124*TAO**15
Magnetic function above Curie Temperature
-.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
-2.84601512E-04*TAO**(-25)

CONSTITUENTS: CU

G(FCC_A1,CU;0)-G(FCC_A1,CU;0) = 298.15<T< 3200.00: +GHSERCU

SYMBOL STATUS VALUE/FUNCTION

FUNCTION R 298.15 8.31451000000000 ; 6000 N REFO !
2 RTLNP 20000000 +R*T*LN(1E-05*P)
103 GQCU 20000000 +16547-7.6815*T
104 GQS 20000000 -65357+165.396*T-13.513*T*LN(T)
105 GHSERCU 20000000
 298.15<T< 1358.02: -7770.458+130.485403*T-24.112392*T*LN(T)
 -.00265684*T**2+1.29223E-07*T**3+52478*T**(-1)
 1358.02<T< 3200.00: -13542.33+183.804197*T-31.38*T*LN(T)
 +3.64643E+29*T**(-9)
106 GS2GAS 20000000
 298.15<T< 1000.00: +117374.548+2.98629558*T-34.09678*T*LN(T)
 -.002325464*T**2+1.85480167E-07*T**3+128593.6*T**(-1)
 1000.00<T< 3400.00: +117352.438+2.50383258*T-34.04744*T*LN(T)
 -.0021150245*T**2+9.16602333E-08*T**3+175718.45*T**(-1)
 3400.00<T< 6000.00: +124361.091+14.5182895*T-36.1923*T*LN(T)
 -5.930925E-04*T**2-7.54259333E-09*T**3-7484105*T**(-1)
107 GSSLIQ 20000000
 298.15<T< 388.36: -4001.549+77.889686*T-15.504*T*LN(T)-.018629*T**2
 -2.4942E-07*T**3-113945*T**(-1)
 388.36<T< 428.15: -5285183.35+118449.585*T-19762.4*T*LN(T)
 +32.79275*T**2-.0102214167*T**3+2.646735E+08*T**(-1)
 428.15<T< 432.25: -8174995.23+319914.078*T-57607.3*T*LN(T)
 +135.3045*T**2-.0529973333*T**3
 432.25<T< 453.15: -219408.801+7758.83993*T-1371.85*T*LN(T)
 +2.845035*T**2-.00101380333*T**3
 453.15<T< 717.00: +92539.872-1336.36627*T+202.958*T*LN(T)
 -.2531915*T**2+5.18835E-05*T**3-8202200*T**(-1)
 717.00<T< 1300.00: -6889.972+176.35482*T-32*T*LN(T)
108 GCULIQ 20000000
 298.15<T< 1358.02: +12964.84-9.510243*T-5.83932E-21*T**7+GHSERCU
 1358.02<T< 3200.00: +13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU

GES5:

GES5:Hit RETURN to continue

GES5: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

```

POLY:
POLY:
POLY: l-st ph
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS          DRIVING FORCE    MOLES
FCC_A1          ENTERED          0.000000E+00    0.000000E+00
QUASI           ENTERED          0.000000E+00    0.000000E+00
GAS             ENTERED          0.000000E+00    0.000000E+00
POLY: c-st p *=sus
... the command in full is CHANGE_STATUS
POLY: c-st p q gas
... the command in full is CHANGE_STATUS
Status: /ENTERED/: ENTERED
Start value, number of mole formula units /0/: 0
POLY:
POLY:
POLY: s-c t=1473 p=1e5 n=1 x(s)=.33
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1966 grid points in      0.097 s
Found the set of lowest grid points in    0.001 s
Calculated POLY solution      0.091 s, total time    0.189 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: User dat

Conditions:
T=1473, P=100000, N=1, X(S)=0.33
DEGREES OF FREEDOM 0

Temperature  1473.00 K ( 1199.85 C), Pressure  1.000000E+05
Number of moles of components  1.00000E+00, Mass in grams  5.31576E+01
Total Gibbs energy -1.24169E+05, Enthalpy  1.52783E+04, Volume  0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CU              6.7000E-01  8.0094E-01  8.2231E-04 -8.6997E+04 SER
S              3.3000E-01  1.9906E-01  8.3318E-08 -1.9964E+05 SER

QUASI              Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 5.3158E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 8.00936E-01 S 1.99064E-01
POLY:Hit RETURN to continue
POLY: s-r-s s gas
... the command in full is SET_REFERENCE_STATE
Temperature /*/: *
Pressure /1E5/: 1E5
POLY: sh acr(s)
... the command in full is SHOW_VALUE
ACR(S)=2.1652884E-3
POLY:Hit RETURN to continue
POLY: s-a-v l x(s)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: .3
Max value /1/: .4
Increment /.0025/: .0025
POLY: save tcex49 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value  0.330000
...OK

Phase Region from  0.330000      for:
QUASI
Global test at  3.50000E-01 .... OK
Global check of adding phase at  3.61133E-01
Calculated      15 equilibria

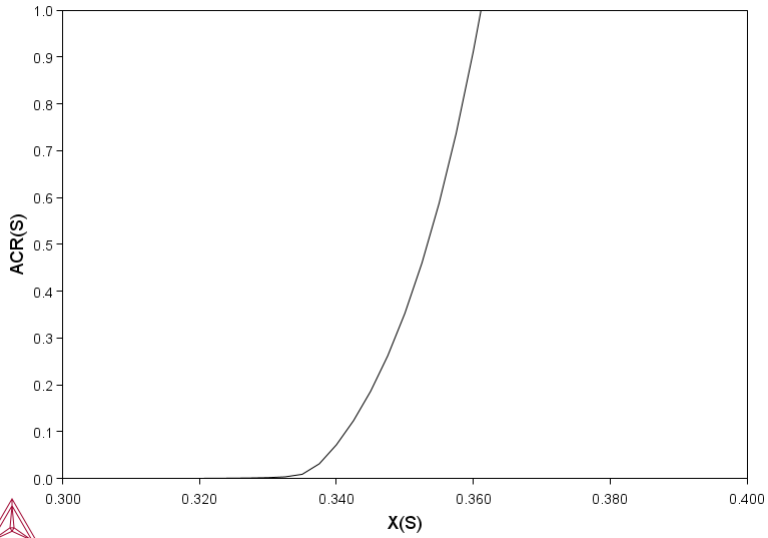
Phase Region from  0.361133      for:
GAS
QUASI
Global test at  3.80000E-01 .... OK
Terminating at  0.400000
Calculated      19 equilibria

Phase Region from  0.330000      for:
QUASI
Global test at  3.10000E-01 .. Creating a new composition set QUASI#2
Backtracking to find phase change for QUASI#2
Global test at  3.27500E-01 .... OK
Global test at  3.22500E-01 .... OK
Global test at  3.17500E-01 .... OK
Global test at  3.12500E-01 .... OK
Global check of adding phase at  3.11581E-01
Calculated      11 equilibria

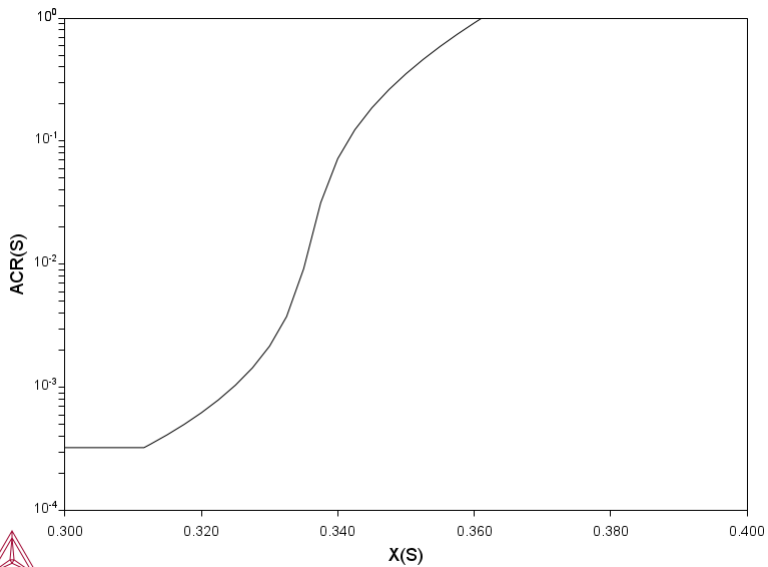
Phase Region from  0.311581      for:
QUASI#1
QUASI#2
Terminating at  0.300000
Calculated      8 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex49\tcex49.POLY3
POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x x(s)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y acr(s)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

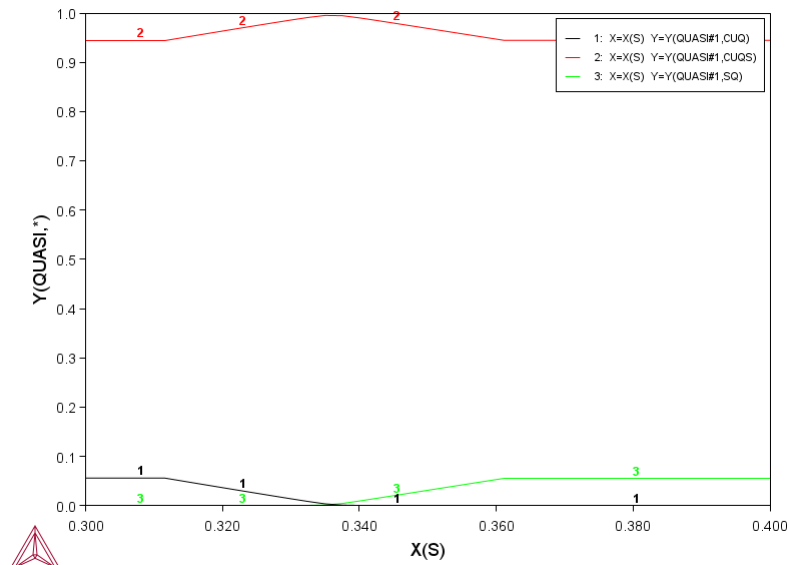
example 49a



```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: set-title example 49b
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-d-a y y(quasi,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-a-ty y lin
... the command in full is SET_AXIS_TYPE
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 49c
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```



```

POST:
POST:
POST:@?
POST: back
POLY: read tcex49
... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: s-c t=1573
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1966 grid points in      0.096 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.195 s, total time      0.291 s
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value  0.300000
...OK

Phase Region from  0.300000      for:
  QUASI#1
  QUASI#2
Global check of removing phase at  3.06778E-01
Calculated      5 equilibria

Phase Region from  0.306778      for:
  QUASI#1
Global test at  3.25000E-01 .... OK
Global test at  3.50000E-01 .... OK
Global check of adding phase at  3.56605E-01
Calculated      23 equilibria

Phase Region from  0.356605      for:
  GAS
  QUASI#1
Global test at  3.75000E-01 .... OK
Global test at  4.00000E-01 .... OK
Terminating at  0.400000
Calculated      21 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex49\tcex49.POLY3
POLY:
POLY: read tcex49
... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: s-c t=1673
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1966 grid points in      0.096 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.015 s, total time      0.111 s
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value  0.400000
...OK

Phase Region from  0.400000      for:
  GAS
  QUASI#1
Global test at  3.80000E-01 .... OK
Global test at  3.55000E-01 .... OK
Global check of removing phase at  3.52789E-01
Calculated      21 equilibria

Phase Region from  0.352789      for:
  QUASI#1
Global test at  3.35000E-01 .... OK
Global test at  3.10000E-01 .... OK
Global check of adding phase at  3.01642E-01
Calculated      24 equilibria

Phase Region from  0.301642      for:
  QUASI#1
  QUASI#2
Terminating at  0.300000
Calculated      4 equilibria

```

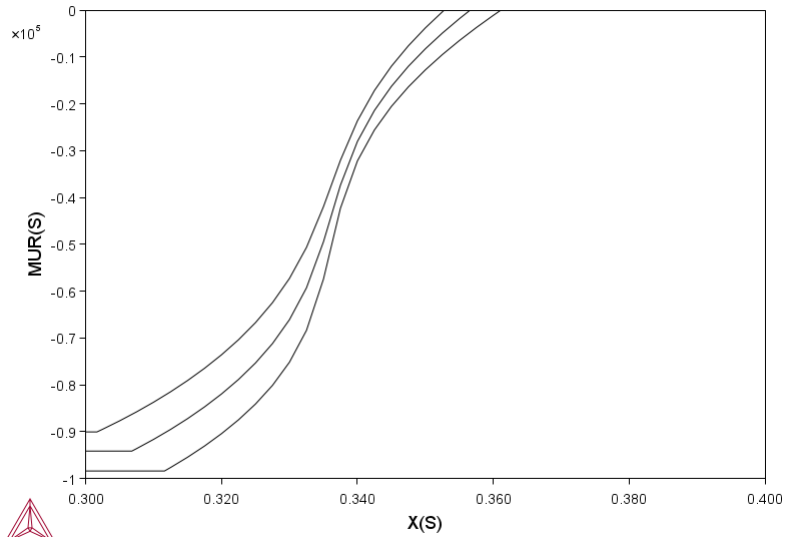


```

*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex49\tcex49.POLY3
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a y mur(s)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x x(s)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49d
POST: sel.plot new
... the command in full is SELECT_PLOT
*** ERROR 1037 IN GETINT: NO DIGIT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 49d



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tcex51

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex51\tcex51.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculation of molar volume,

SYS: @@ thermal expansivity, and density.

SYS:

SYS: @@ This example uses the POLY3 module to calculate

SYS: @@ the molar volume, thermal expansivity, and density

SYS: @@ of the FCC_A1, BCC_A2 LIQUID, and liquid phases of C-Fe.

SYS:

SYS: set-log ex51,,

SYS:

SYS: go data

... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw FEDEMO

... the command in full is SWITCH_DATABASE

Current database: Iron Demo Database v6.0

VA /- DEFINED

TDB_FEDEMO:

TDB_FEDEMO: @@ Volume of a unary system

TDB_FEDEMO: d-sys fe

... the command in full is DEFINE_SYSTEM

FE DEFINED

TDB_FEDEMO: rej-ph * all

... the command in full is REJECT

GAS:G LIQUID:L BCC_A2

C14 LAVES CBCC_A12 CUB_A13

FCC_A1 HCP_A3 REJECTED

TDB_FEDEMO: rest-ph fcc_a1,bcc_a2,liquid

... the command in full is RESTORE

FCC_A1 BCC_A2 LIQUID:L

RESTORED

TDB_FEDEMO: get

... the command in full is GET_DATA

09:59:01,656 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_FEDEMO:

TDB_FEDEMO: go poly

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: s-c t=400, n=1, p=1e5

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 3 grid points in 0.174 s

POLY: s-a-v 1 t 298 2000,,

... the command in full is SET_AXIS_VARIABLE

POLY:

POLY: save tcex51 y

... the command in full is SAVE_WORKSPACES

POLY: step normal

... the command in full is STEP_WITH_OPTIONS

No initial equilibrium, using default

Step will start from axis value 400.000

...OK

Phase Region from 400.000 for:

BCC_A2

Global test at 4.80000E+02 OK

Global test at 5.80000E+02 OK

Global test at 6.80000E+02 OK

Global test at 7.80000E+02 OK

Global test at 8.80000E+02 OK

Global test at 9.80000E+02 OK

Global test at 1.08000E+03 OK

Global test at 1.18000E+03 OK

Global check of adding phase at 1.18481E+03

Calculated 81 equilibria

Phase Region from 1184.81 for:

BCC_A2

FCC_A1

Calculated 2 equilibria

Phase Region from 1184.81 for:

FCC_A1

```

Global test at 1.26000E+03 .... OK
Global test at 1.36000E+03 .... OK
Global test at 1.46000E+03 .... OK
Global test at 1.56000E+03 .... OK
Global test at 1.66000E+03 .... OK
Global check of adding phase at 1.66747E+03
Calculated 51 equilibria

Phase Region from 1667.47 for:
  BCC_A2
  FCC_A1
Calculated 2 equilibria

Phase Region from 1667.47 for:
  BCC_A2
Global test at 1.74000E+03 .... OK
Global check of adding phase at 1.81095E+03
Calculated 18 equilibria

Phase Region from 1810.95 for:
  LIQUID
  BCC_A2
Calculated 2 equilibria

Phase Region from 1810.95 for:
  LIQUID
Global test at 1.89000E+03 .... OK
Global test at 1.99000E+03 .... OK
Terminating at 2000.00
Calculated 22 equilibria

Phase Region from 400.000 for:
  BCC_A2
Global test at 3.20000E+02 .... OK
Terminating at 298.000
Calculated 14 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex51\tcex51.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

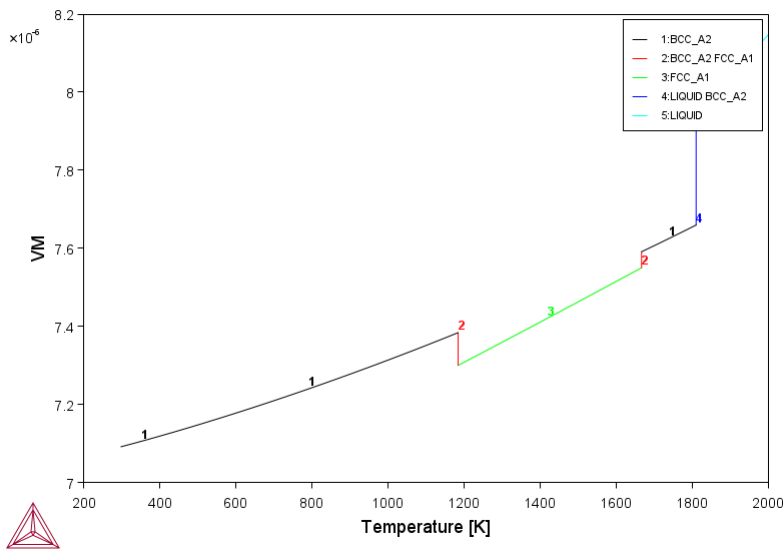
Setting automatic diagram axes

```

POST: s-d-a x t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51a
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 51a

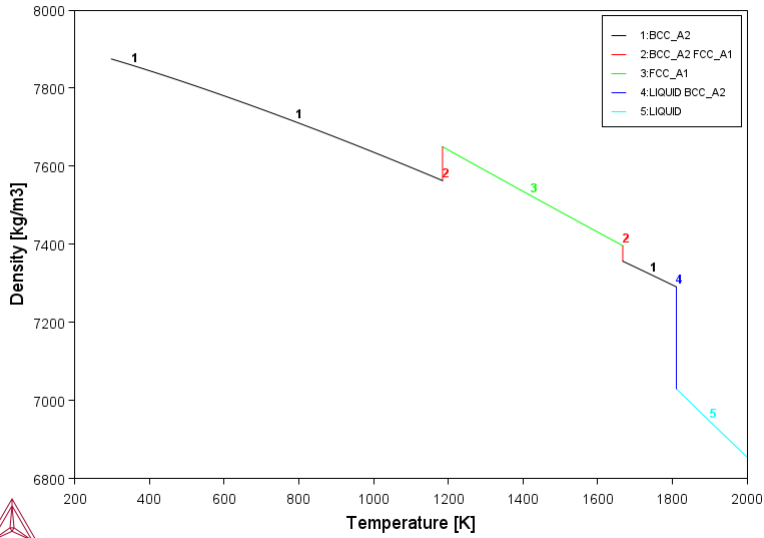


```

POST:
POST: Hit RETURN to continue
POST: @@ Define and plot density
POST: ent fun density=b*1e-3/vm;
... the command in full is ENTER_SYMBOL
POST: s-d-a y density
... the command in full is SET_DIAGRAM_AXIS
POST: set-axis-text y n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Density [kg/m3]
POST: set-title example 51b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 51b

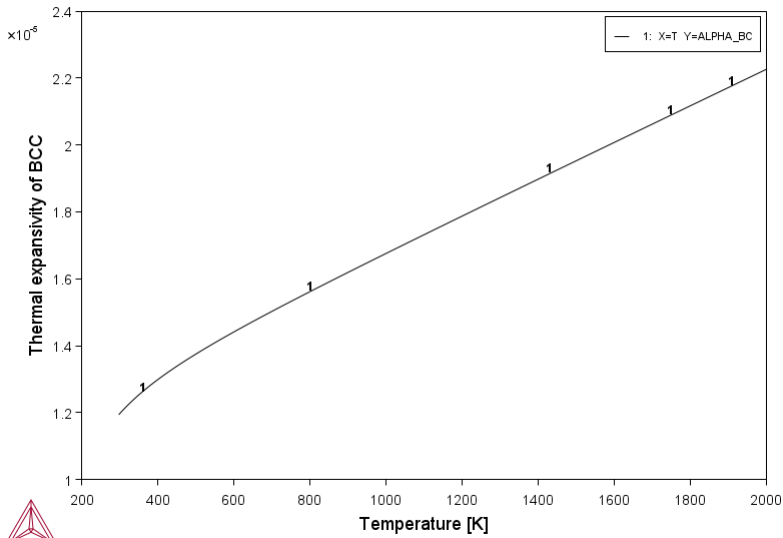


```

POST:
POST:Hit RETURN to continue
POST: @@ Define and plot coefficient of linear
POST: @@ thermal expansion
POST: ent fun alpha_bcc_a2=vm(bcc_a2).t/vm(bcc_a2)/3;
... the command in full is ENTER_SYMBOL
POST: s-d-a y alpha_bcc_a2
... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-axis-text y n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Thermal expansivity of BCC
POST: set-title example 51c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 51c



```

POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Volume of Fe-C binary system
POLY: go da
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej sys
... the command in full is REJECT
VA /- DEFINED
REINITIATING GES .....
TDB_FEDEMO: de-sys fe c
... the command in full is DEFINE_SYSTEM
FE C DEFINED
TDB_FEDEMO: rej-ph * all
... the command in full is REJECT
GAS:G LIQUID:L BCC_A2
C14 LAVES CBCC_A12 CEMENTITE_D011
CUB_A13 DIAMOND_A4 FCC_A1
GRAPHITE_A9 HCP_A3 KSI_CARBIIDE
M23C6_D84 M5C2 M7C3_D101
REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,cementite,liquid
... the command in full is RESTORE
FCC_A1 BCC_A2 CEMENTITE_D011
LIQUID:L RESTORED

```

```

TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: s-c t=400, n=1, p=1e5
... the command in full is SET_CONDITION
POLY: s-c w(c)=.6e-2
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      628 grid points in      0.083 s
Found the set of lowest grid points in      0.003 s
Calculated POLY solution      0.103 s, total time      0.189 s
POLY: s-a-v l t 298 2000,,
... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: save tcex51 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value      400.000
...OK

Phase Region from      400.000      for:
  BCC_A2
  CEMENTITE_D011
Global test at 4.80000E+02 .... OK
Global test at 5.80000E+02 .... OK
Global test at 6.80000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 9.80000E+02 .... OK
Global check of adding phase at 9.99685E+02
Calculated      62 equilibria

Phase Region from      999.685      for:
  BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated      2 equilibria

Phase Region from      999.685      for:
  BCC_A2
  FCC_A1
Global check of removing phase at 1.02363E+03
Calculated      6 equilibria

Phase Region from      1023.63      for:
  FCC_A1
Global test at 1.10000E+03 .... OK
Global test at 1.20000E+03 .... OK
Global test at 1.30000E+03 .... OK
Global test at 1.40000E+03 .... OK
Global test at 1.50000E+03 .... OK
Global test at 1.60000E+03 .... OK
Global check of adding phase at 1.69090E+03
Calculated      70 equilibria

Phase Region from      1690.90      for:
  LIQUID
  FCC_A1
Global check of removing phase at 1.76294E+03
Calculated      10 equilibria

Phase Region from      1762.94      for:
  LIQUID
Global test at 1.84000E+03 .... OK
Global test at 1.94000E+03 .... OK
Terminating at      2000.00
Calculated      27 equilibria

Phase Region from      400.000      for:
  BCC_A2
  CEMENTITE_D011
Global test at 3.20000E+02 .... OK
Terminating at      298.000
Calculated      14 equilibria
*** Buffer saved on file: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex51\tcex51.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

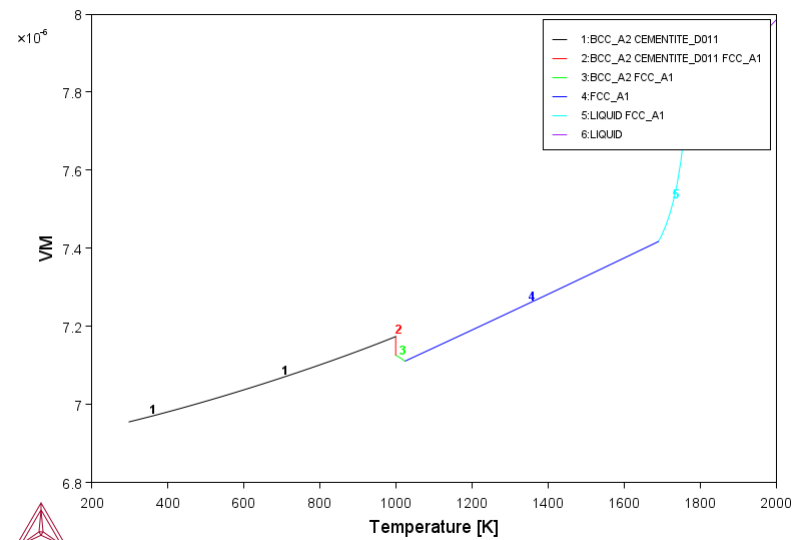
Setting automatic diagram axes

POST: s-d-a x t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51d
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST:

```

```
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 51d



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex52\tcex52.TCM.test"

SYS: set-echo

SYS:

SYS:

SYS: @@ Changing the excess models for interaction

SYS: @@ parameters in a solution phase

SYS:

SYS:

SYS: @@ This example shows how to change the excess models for binary

SYS: @@ and ternary interactions in a solution phase, either through

SYS: @@ direct interactive amendments of phase descriptions within

SYS: @@ the GES module, or enforced by specific type-definitions

SYS: @@ given in a database file retrieved by the TDB module.

SYS: @@ -----

SYS: @@ For Binary Excess Model: from the default R-K model to

SYS: @@ Mixed-Excess-Model (the phase has to be a substitutional phase)

SYS: @@ -----

SYS: @@ For Ternary Extrapolation Model: from the default R-K-M model to

SYS: @@ Toop_Kohler model

SYS: @@ -----

SYS: set-log TCEX52.LOG

Heading: Example showing how to enter a TOOP binary extrapolation model

SYS:

SYS:

SYS: @@ This example uses features not supported by GES6.

SYS: @@ Therefore, we enforce the use of GES5.

SYS: set-ges-version 5

SYS:

SYS: go gibbs

... the command in full is GOTO_MODULE

GIBBS ENERGY SYSTEM

GES5: reinitiate ,,,

Default element reference state symbol index /1/:

GES5: ent-el /- VA A B C

... the command in full is ENTER_ELEMENT

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

GES5:

GES5: am_el_d /- ELECTRON GAS 0.0000E+00 0.0000E+00 0.0000E+00 1

... the command in full is AMEND_ELEMENT_DATA

GES5: am_el_d VA VACUUM 0.0000E+00 0.0000E+00 0.0000E+00 1

... the command in full is AMEND_ELEMENT_DATA

GES5: am_el_d A UNKNOWN 1.0000E+01 0.0000E+00 0.0000E+00 2

... the command in full is AMEND_ELEMENT_DATA

GES5: am_el_d B BETA_RHOMBO_B 1.0811E+01 1.2220E+00 5.9000E+00 2

... the command in full is AMEND_ELEMENT_DATA

GES5: am_el_d C GRAPHITE 1.2011E+01 1.0540E+00 5.7400E+00 2

... the command in full is AMEND_ELEMENT_DATA

GES5:

GES5: ent-phase LIQUID L, 1 A,B,C ; N N

... the command in full is ENTER_PHASE

GES5:

GES5: ent-param G(LIQUID,A;0) 298.15 0; 6000 N!

... the command in full is ENTER_PARAMETER

G(LIQUID,A;0)-H298(UNKNOWN,A;0)

GES5: ent-param G(LIQUID,B;0) 298.15 0; 6000 N!

... the command in full is ENTER_PARAMETER

G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0)

GES5: ent-param G(LIQUID,C;0) 298.15 0; 6000 N!

... the command in full is ENTER_PARAMETER

G(LIQUID,C;0)-H298(GRAPHITE,C;0)

GES5:

GES5: ent-param L(LIQUID,A,B;0) 298.15 10000; 6000 N

... the command in full is ENTER_PARAMETER

L(LIQUID,A,B;0)

GES5: ent-param L(LIQUID,A,B;1) 298.15 -10000; 6000 N

... the command in full is ENTER_PARAMETER

L(LIQUID,A,B;1)

GES5:

GES5: list-data ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT DATE 2025- 5-12
FROM DATABASE: User data 2025.05.12

ALL DATA IN SI UNITS

FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON	GAS	0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	A	UNKNOWN		1.0000E+01	0.0000E+00	0.0000E+00
2	B	BETA_RHOMBO_B		1.0811E+01	1.2220E+00	5.9000E+00
3	C	GRAPHITE		1.2011E+01	1.0540E+00	5.7400E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 C	C
4 VA	VA

```
LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000

SYMBOL      STATUS  VALUE/FUNCTION
FUNCTION R   298.15  8.314510000000000    ; 6000 N REFO !
  2 RTLNP    20000000 +R*T*LN(1E-05*P)
```

GES5:Hit RETURN to continue

```
GES5:
GES5: @@ =====
GES5: @@ Step 1: Amending the binary excess model:
GES5: @@ =====
GES5: @@ The default binary excess model is the Redlich-Kister Model
GES5: @@ for all the three associated binary interaction pairs
GES5: @@ (A-B, A-C and B-C) in the substitutional LIQUID solution
GES5: @@ phase (without sublattice) that consists of three elements
GES5: @@ (A, B and C).
GES5:
GES5: @@ Before changing this default binary excess model for the
GES5: @@ ternary LIQUID solution phase, one must have already entered
GES5: @@ the G parameters (for standard Gibbs energies of all pure
GES5: @@ end-members) and L parameters (for binary R-K excess
GES5: @@ interaction energies), as shown here.
GES5:
GES5: @@ In this particular example, we want to change from the
GES5: @@ default R-K binary excess model to the Mixed-Excess-Model
GES5: @@ (with three different binary excess models, namely Legendre,
GES5: @@ Polynom and Redlich-Kister models, applied to the A-B,
GES5: @@ A-C and B-C binaries, respectively), as demonstrated below:
GES5:
GES5: @@ For the A-B interaction, the Legendre binary excess model
GES5: @@ should be used (rather than the default Redlich-Kister
GES5: @@ Model), with the first species (i.e. A) as the independent constituent
GES5: @@ and the second species (i.e. B) as the dependent constituent,
GES5: @@ while the L parameters for the A-B interaction shall remain
GES5: @@ the same as those handled by the R-K model.
GES5: amend-phase-description liquid
AMEND WHAT /COMPOSITION_SETS/: ?
```

```
You can amend
EXCESS_MODEL
MAGNETIC_ORDERING
DEBYE_HUCKEL
STATUS_BITS
NEW_CONSTITUENT
RENAME_PHASE
COMPOSITION_SETS
GLASS_TRANSITION
DISORDERED_PART
MAJOR_CONSTITUENT
ZRO2_TRANSITION
REMOVE_ADDITIONS
QUASICHEM_IONIC
QUASICHEM_FACT00
QUASICHEM_IRSID
TERNARY_EXTRAPOLAT
HKF_ELECTROSTATIC
DEFAULT_STABLE
SITE_RATIOS
FRACTION_LIMITS
NEVER_DISORDER_PAR
```

AMEND WHAT /COMPOSITION_SETS/: excess

MODEL NAME /REDLICH-KISTER_MUGGIANU/: ?

```
REDLICH-KISTER_MUGGIANU
REDLICH-KISTER_KOHLER
FLORY-HUGGINS POLYMER MODEL
MIXED-EXCESS-MODELS (R-K default)
HKF
PITZER
CENTRAL_ATOM_MODEL
```

MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed

First (the independent) constituent: ?

```
FILE SYSTEM ERROR IN FILHLP
ERROR          1717  READING HELP FILE
```

First (the independent) constituent: A

Second (the dependent) constituent: B

Excess model type: /LEGENDRE/: ?

Legal choices are: LEGENDRE, POLYNOM or REDLICH-KISTER

Excess model type: /LEGENDRE/: legendre

Any other non-Redlich-Kister binary excess parameters?

First (the independent) constituent: NONE

GES5:

GES5: list-data , ,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT DATE 2025- 5-12
FROM DATABASE: User data 2025.05.12

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON_GAS		0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	A	UNKNOWN		1.0000E+01	0.0000E+00	0.0000E+00
2	B	BETA_RHOMBO_B		1.0811E+01	1.2220E+00	5.9000E+00
3	C	GRAPHITE		1.2011E+01	1.0540E+00	5.7400E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B


```

3 C
4 VA

C
VA

LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
$ Binary excess model Legendre with A as independent
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000

SYMBOL      STATUS      VALUE/FUNCTION
FUNCTION R      298.15      8.314510000000000      ; 6000 N REF0 !
2 RTLNP      20000000 +R*T*LN(1E-05*P)

GES5:Hit RETURN to continue
GES5:
GES5: @@ For the A-C interaction, the Polynom binary excess model
GES5: @@ should be used (rather than the default Redlich-Kister
GES5: @@ Model), with the second species (i.e. C) as the
GES5: @@ independent constituent and the first species (i.e. A)
GES5: @@ as the dependent constituent, while the L parameters for
GES5: @@ the A-C interaction shall remain the same as those
GES5: @@ handled by the R-K model.
GES5:
GES5: ent-param G(LIQUID,A,C;0) 298.15 10000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,A,C;0)
GES5: ent-param G(LIQUID,A,C;1) 298.15 5000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,A,C;1)
GES5:
GES5: amend-phase-des LIQUID excess mixed C A polynom
... the command in full is AMEND_PHASE_DESCRIPTION

Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent:
GES5: list-data ,,

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT      DATE 2025- 5-12
FROM DATABASE: User data 2025.05.12

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT STABLE ELEMENT REFERENCE MASS      H298-H0      S298
-1 /- ELECTRON_GAS      0.0000E+00 0.0000E+00 0.0000E+00
0 VA VACUUM      0.0000E+00 0.0000E+00 0.0000E+00
1 A UNKNOWN      1.0000E+01 0.0000E+00 0.0000E+00
2 B BETA RHOMBO_B      1.0811E+01 1.2220E+00 5.9000E+00
3 C GRAPHITE      1.2011E+01 1.0540E+00 5.7400E+00

SPECIES      STOICHIOMETRY
1 A      A
2 B      B
3 C      C
4 VA      VA

LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
$ Binary excess model Legendre with A as independent
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000
$ Binary excess model Polynom with C as independent
L(LIQUID,A,C;0) = +10000
L(LIQUID,A,C;1) = +5000

SYMBOL      STATUS      VALUE/FUNCTION
FUNCTION R      298.15      8.314510000000000      ; 6000 N REF0 !
2 RTLNP      20000000 +R*T*LN(1E-05*P)

GES5:Hit RETURN to continue
GES5:
GES5: @@ For the B-C interaction, the default Redlich-Kister binary
GES5: @@ excess model shall still be used; so we do not need to
GES5: @@ amend anything regarding that.
GES5:
GES5: ent-param G(LIQUID,B,C;0) 298.15 10000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,B,C;0)
GES5: ent-param G(LIQUID,B,C;1) 298.15 -2000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,B,C;1)
GES5:
GES5: list-data ,,

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC / WINDOWS NT      DATE 2025- 5-12
FROM DATABASE: User data 2025.05.12

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT STABLE ELEMENT REFERENCE MASS      H298-H0      S298
-1 /- ELECTRON_GAS      0.0000E+00 0.0000E+00 0.0000E+00
0 VA VACUUM      0.0000E+00 0.0000E+00 0.0000E+00
1 A UNKNOWN      1.0000E+01 0.0000E+00 0.0000E+00
2 B BETA RHOMBO_B      1.0811E+01 1.2220E+00 5.9000E+00
3 C GRAPHITE      1.2011E+01 1.0540E+00 5.7400E+00

```

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 C	C
4 VA	VA

LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0

\$ Binary excess model Legendre with A as independent

L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000

\$ Binary excess model Polynom with C as independent

L(LIQUID,A,C;0) = +10000
L(LIQUID,A,C;1) = +5000
L(LIQUID,B,C;0) = +10000
L(LIQUID,B,C;1) = -2000

SYMBOL	STATUS	VALUE/FUNCTION	
FUNCTION R	298.15	8.314510000000000	; 6000 N REF0 !
2 RTLN	20000000	+R*T*LN(1E-05*P)	

GES5:Hit RETURN to continue

GES5:

GES5: @@ =====

GES5: @@ Step 2: Amending the ternary extrapolation model:

GES5: @@ =====

GES5: @@ The default ternary excess model is the

GES5: @@ Redlich-Kister_Muggianu Model (i.e., the MUGGIANU_RESTOR

GES5: @@ method for ternary extrapolation based on binary parameters)

GES5: @@ for the associated ternary interaction terms; when no

GES5: @@ ternary L parameter is entered for that, such a default

GES5: @@ Redlich-Kister_Muggianu Model is thus to be used for

GES5: @@ extrapolation from binary excess energies to ternary

GES5: @@ interactions in the substitutional LIQUID solution phase

GES5: @@ (without sublattice) that consists of three elements

GES5: @@ (A, B and C).

GES5:

GES5: @@ However, in this particular example as follows.

GES5: @@ We shall change from this default R-K-M ternary excess

GES5: @@ model to the TOOP-KOHLER method for the ternary extrapolation

GES5: @@ method, with the species C as the Toop constituent, while

GES5: @@ the species A and B as the Kohler constituents (entering A

GES5: @@ and B, or B and A, as the basis constituent and first

GES5: @@ interacting constituent). This implicitly enforces that,

GES5: @@ during the ternary extrapolation, only the A-B binary

GES5: @@ interaction parameters are utilized in accordance with the

GES5: @@ Kohler ternary extrapolation formula for A-B-C ternary

GES5: @@ interaction, while any other binary interaction parameters

GES5: @@ involving the Toop species C (i.e., of A-C and B-C binaries)

GES5: @@ are used in line with the Toop-Kohler ternary extrapolation

GES5: @@ formula (for the A-C-B and B-C-A ternary interactions). This

GES5: @@ makes the extrapolated ternary excess interaction terms

GES5: @@ different from those handled either by the default

GES5: @@ MUGGIANU_RESTOR method or by the alternative KOHLER-ALL

GES5: @@ method.

GES5:

GES5: @@ Note that only when all the relevant binary excess energies

GES5: @@ in a ternary system are treated by the default Redlich-Kister

GES5: @@ Model (i.e., the Mixed-Excess-Model should have not been

GES5: @@ used), the MUGGIANU_RESTOR method for ternary extrapolations

GES5: @@ is equivalent to the Redlich-Kister_Muggianu Model, or the

GES5: @@ KOHLER-ALL method to the Redlich-Kister_Kohler Model.

GES5:

GES5: amend_phase-des LIQUID

... the Command in full is AMEND_PHASE_DESCRIPTION

AMEND WHAT /COMPOSITION_SETS/: ?

You can amend

EXCESS_MODEL

MAGNETIC_ORDERING

DEBYE_HUCKEL

STATUS_BITS

NEW_CONSTITUENT

RENAME_PHASE

COMPOSITION_SETS

GLASS_TRANSITION

DISORDERED_PART

MAJOR_CONSTITUENT

ZRO2_TRANSITION

REMOVE_ADDITIONS

QUASICHEM_IONIC

QUASICHEM_FACT00

QUASICHEM_IRSID

TERNARY_EXTRAPOLAT

HKF_ELECTROSTATIC

DEFAULT_STABLE

SITE_RATIOS

FRACTION_LIMITS

NEVER_DISORDER_PAR

AMEND WHAT /COMPOSITION_SETS/: TERN-EXT

Extrapolation method: /TOOP-KOHLER/: ?

Default method is Muggianu, you can use

TOOP-KOHLER

KOHLER-ALL

MUGGIANU_RESTOR

Extrapolation method: /TOOP-KOHLER/: TOOP-KOHLER

Constituent in sublattice 1: A

First interaction constituent: B

Toop constituent: C

GES5:

GES5: list-data , ,

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON_GAS	0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM	0.0000E+00	0.0000E+00	0.0000E+00
1	A	UNKNOWN	1.0000E+01	0.0000E+00	0.0000E+00
2	B	BETA RHOMBO_B	1.0811E+01	1.2220E+00	5.9000E+00
3	C	GRAPHITE	1.2011E+01	1.0540E+00	5.7400E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 C	C
4 VA	VA

LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
\$ Binary excess model Legendre with A as independent
\$ Ternary extrapolation for LIQUID using KOHLER A B C
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000
\$ Binary excess model Polynom with C as independent
\$ Ternary extrapolation for LIQUID using TOOP-KOHLER A C B
L(LIQUID,A,C;0) = +10000
L(LIQUID,A,C;1) = +5000
\$ Ternary extrapolation for LIQUID using TOOP-KOHLER B C A
L(LIQUID,B,C;0) = +10000
L(LIQUID,B,C;1) = -2000

SYMBOL STATUS VALUE/FUNCTION
FUNCTION R 298.15 8.314510000000000 ; 6000 N REFO !
2 RTLNP 20000000 +R*T*LN(1E-05*P)

GES5:Hit RETURN to continue

GES5: @@ =====

GES5: @@ Step 3: Performing an equilibrium calculation using the

GES5: @@ entered and amended descriptions.

GES5: @@ =====

GES5:

GES5: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 1965 grid points in 0.002 s

Found the set of lowest grid points in 0.000 s

Calculated POLY solution 0.007 s, total time 0.009 s

POLY: l-e , X

... the command in full is LIST_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:

T=1500, P=100000, N=1, X(B)=0.2, X(C)=0.3

DEGREES OF FREEDOM 0

Temperature 1500.00 K (1226.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 1.07655E+01

Total Gibbs energy -1.08432E+04, Enthalpy 1.99843E+03, Volume 0.00000E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
A	5.0000E-01	5.0000E-01	4.7833E-01	-9.1973E+03	SER
B	2.0000E-01	2.0000E-01	1.9875E-01	-2.0151E+04	SER
C	3.0000E-01	3.0000E-01	5.5332E-01	-7.3811E+03	SER

LIQUID Status ENTERED Driving force 0.0000E+00

Moles 1.0000E+00, Mass 1.0766E+01, Volume fraction 0.0000E+00 Mole fractions:

A 5.00000E-01 C 3.00000E-01 B 2.00000E-01

POLY: sh qf(*)

... the command in full is SHOW_VALUE

QF(LIQUID)=0.52168269

POLY: sh gm(*) dgm(*)

... the command in full is SHOW_VALUE

GM(LIQUID)=-10843.162

DGM(LIQUID)=0

POLY:

POLY: save TCEX52a.POLY3 y

... the command in full is SAVE_WORKSPACES

POLY:Hit RETURN to continue

POLY: @@ =====

POLY: @@ Step 4: Reading the same data from a small database and

POLY: @@ Performing the same equilibrium calculation.

POLY: @@ =====

POLY:

POLY: go data

... the command in full is GOTO_MODULE

TDB_TCFE11: rej sys

... the command in full is REJECT

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

TDB_TCFE11:

TDB_TCFE11: sw user TCEX52-TOOP.TDB

... the command in full is SWITCH_DATABASE

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

TDB_USER: d-sys /all

... the command in full is DEFINE_SYSTEM

```

A                               B                               C
DEFINED
TDB_USER: l-sys const
... the command in full is LIST_SYSTEM
LIQUID:L      :A B C:
TDB_USER: get
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

AFTER ...
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
-OK-
TDB_USER:
TDB_USER:Hit RETURN to continue
TDB_USER: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:
POLY: s-c t=1500 p=1e5 n=1 x(b)=-.2 x(c)=-.3
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1965 grid points in      0.002 s
Found the set of lowest grid points in      0.000 s
Calculated POLY solution      0.006 s, total time      0.008 s
POLY: l-e , X
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: USER

Conditions:
T=1500, P=100000, N=1, X(B)=0.2, X(C)=0.3
DEGREES OF FREEDOM 0

Temperature  1500.00 K ( 1226.85 C), Pressure  1.000000E+05
Number of moles of components  1.000000E+00, Mass in grams  1.07655E+01
Total Gibbs energy -1.08432E+04, Enthalpy  1.99843E+03, Volume  0.000000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
A                5.0000E-01  5.0000E-01  4.7833E-01 -9.1973E+03 SER
B                2.0000E-01  2.0000E-01  1.9875E-01 -2.0151E+04 SER
C                3.0000E-01  3.0000E-01  5.5332E-01 -7.3811E+03 SER

LIQUID                      Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 1.0766E+01, Volume fraction 0.0000E+00 Mole fractions:
A 5.000000E-01 C 3.000000E-01 B 2.000000E-01
POLY: sh qf(*)
... the command in full is SHOW_VALUE
QF(LIQUID)=0.52168269
POLY: sh gm(*) dgm(*)
... the command in full is SHOW_VALUE
GM(LIQUID)=-10843.162
DGM(LIQUID)=0
POLY:
POLY: save TCEX52b.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY:
POLY:
POLY: @@ As you have noticed, the calculated equilibrium (using the
POLY: @@ small database) is exactly the same as the first
POLY: @@ calculation (with data amended in the GES module
POLY: @@ step-by-step, for the binary/ternary excess models).
POLY:
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```

tcex53

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex53\tcex53.TCM.test"

SYS: go sys

SYS: set-echo

SYS:

SYS: set-log TCEX53.LOG

Heading: Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine

SYS:

SYS: @@ Some Pourbaix diagrams

SYS:

SYS:

SYS: @@ =====

SYS: @@ Copyright: Thermo-Calc Software AB, Stockholm, Sweden

SYS: @@ Developer: Dr. Pingfang Shi, Thermo-Calc Software AB

SYS: @@ Date: 2014-05-26 (revision)

SYS: @@ Text updated July 2017 (AJW)

SYS:

SYS: @@ =====

SYS: @@ Example description:

SYS: @@ =====

SYS: @@ TCEX53 uses the PAQ2 database to calculate some Pourbaix

SYS: @@ diagrams. The DATABASE_RETRIEVAL (TDB),

SYS: @@ GIBBS ENERGY_SYSTEM (GES), POLY3, and POSTA modules are

SYS: @@ used for the Fe-X-H2O-NaCl heterogeneous interaction

SYS: @@ system, where X = Cr-Ni-Co.

SYS:

SYS: @@ Note: The initial bulk composition of Fe-based alloy in

SYS: @@ this calculation is only preliminarily assigned, in which

SYS: @@ the BCC_A2 and/or FCC_A1 solution phase(s) are considered

SYS: @@ as of primarily interest. For practical calculations,

SYS: @@ you need more precise inputs for the initial bulk

SYS: @@ compositions of alloys.

SYS:

SYS: @@ =====

SYS: @@ Notes about the example and the PAQ2 database:

SYS: @@ =====

SYS: @@ The so-called Pourbaix diagram is actually a phase diagram

SYS: @@ with independently-varied electropotential (Eh) and

SYS: @@ acidity (pH), for an heterogeneous interaction system at a

SYS: @@ certain bulk composition (that is by default always set as

SYS: @@ 1 kg of water solving a specified amount of metals and

SYS: @@ other solutes), under defined temperature and pressure

SYS: @@ conditions.

SYS:

SYS: @@ The PAQ2 database is specially designed for Pourbaix

SYS: @@ diagram calculations (i.e., Eh-pH plots). It contains an

SYS: @@ AQUEOUS solution phase and REF_ELECTRODE phase (as a

SYS: @@ reference for electron in aqueous electrolyte systems),

SYS: @@ as well as some data for various solid phases (solution

SYS: @@ or stoichiometric) and a gaseous mixture phase.

SYS:

SYS: @@ For more Pourbaix diagram exercises, see TCEX40 and the

SYS: @@ extended examples TCEX40A to TCEX40E.

SYS:

SYS: @@ =====

SYS: @@ Step 1: Single-Point Calculations for H2O-NaCl system

SYS: @@ =====

SYS: @@ To demonstrate how to define the molality of NaCl

SYS: @@ in an aqueous-bearing heterogeneous interaction system

SYS:

SYS: @@ Retrieve data from the PAQ2 database:

SYS: go data

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: rej sys

... the command in full is REJECT

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

TDB_TCFE11: @@ Switch to the PAQ2 database

TDB_TCFE11: sw PAQ2

... the command in full is SWITCH_DATABASE

Current database: Public Aqueous Solution (SIT) v2.5

H	O	ZE
VA DEFINED		
LIQUID:L REJECTED		
GRAPHITE	DIAMOND_A4	FC_ORTHORHOMBIC
MONOCLINIC REJECTED		
CBCC_A12	CUB_A13	CHI_A12
FE4N	FECN_CHI REJECTED	
CEMENTITE	M23C6	M7C3
M5C2	M3C2	KSI_CARBIDE
PI REJECTED		
FE3C	NI3C	CR3C2
CR7C3	CR23C6 REJECTED	
COCO3	FECO3	NAHCO3
NA2CO3_S1	NA2CO3_S2	NICO3
CRC6O6 REJECTED		
CO3N	CRN	CR2N

```

FE2N          NI3N REJECTED
NANO2_S1      NANO2_S2          NANO3
REJECTED
COCL2         CRCL2             CRCL3
FECL2         FECL3             NICL2
REJECTED
FECLO         NACLO4_S1         NACLO4_S2
REJECTED
TDB_PAQ2: data
... the command in full is DATABASE INFORMATION
Current database: Public Aqueous Solution (SIT) v2.5

```

```

                PAQ2
Thermo-Calc PUBLIC AQUEOUS DATABASE FOR POURBAIX MODULE
(based on and replacing AQ in TCC/TCW & PAQ in TCC-Demo/TCW-Demo)
*****
                (Version 2.5, Feb. 2021)
Copyright © 1997-2008: Thermo-Calc Software AB, Sweden
This public aqueous solution database contains aqueous solution species,
and gaseous mixture species and solid/liquid (pure and solution) phases
in an 11-element system (Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl). As a demo version
of the complete TCAQ2 Aqueous Solution Database, it is specially designed
for uses with the special POURBAIX module which allows easy and automatic
calculations of the so-called Pourbaix diagrams (i.e., Eh-pH plots) and
many types of property diagrams. It can also be used in normal TCC/TCW
calculations for aqueous involved heterogeneous interaction systems.
The TCAQ2 Aqueous Solution Database covers 83 elements (compatible with
the SGTE PURE/SSUB/SSOL and other databases), and can be used together
with the SIT (Specific Interaction Theory) Model for complex aqueous
solution that has already implemented in Thermo-Calc.
PAQ has been developed since 1996, and gradually modified and expanded
later on. PAQ2.4 combines 4 files from its previous version PAQ2 [i.e.,
PAQ2setup.TDB for defining elements, species and phases; PAQ2param.TDB
for assigning various functions and parameters for standard properties
of various phases; PAQ2inter.TDB for assigning binary or higher-order
interaction parameters for non-ideal properties of aqueous solution
phase; and PAQ2funct.TDB for entering extra functions referred in
PAQ2param.TDB].
The AQUEOUS solution phase can be treated by the SIT Model, using the
TCAQ2 (or PAQ2) database that can be applied to low PTX conditions (up
to 100 bar, 350 C and 3 molality). However, if investigated heterogeneous
interaction processes occur at high PTX (up to 5 kbar, 1000 C and 10
molality), the other aqueous solution database, called AQS2, which
implies the complete Revised HKF (Helgeson-Kirkham-Flowers) Model, is
required.
Data for pure elements are taken from the SGTE unary database (PURE) with
explicit magnetic and pressure dependencies. The reference state is
298.15 K and 1 bar. All data follow the new temperature scale ITPS 90.
For calculations of the so-called Pourbaix-diagrams (pH-Eh) and related
property diagrams within either the POURBAIX-module or through normal
TDB-GES-POLY-POST routines, following types of phases must be defined
in the heterogeneous interaction systems:
    AQUEOUS:      from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
    REF ELECTRODE: from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
    GAS:          from PAQ2 (or PAQS2) or SSUB4 (or TCMP2);
    Various Solids: from PAQ2 (or PAQS2) or SSOL4 (or TCFE6, TCMP2, etc.).
There are many solid phases (stoichiometric or solution) and a metallic
liquid mixture phase which are included in the public PAQ2 and PAQS2
databases. By default, however, many such phases have been rejected
automatically. Of course, if one wishes to consider any of such phases
(such as Cementite or M23C6) into a defined interaction system, they
can be appropriately restored in the POURBAIX or TDB modules.
Either TCAQ2 or AQS2 databases can be used by the advanced, easy-to-use
POURBAIX Module via its multiple-database option, or be utilized along
with ordinary Thermo-Calc routines. For a gaseous mixture phase, one
could append from the SSUB (SGTE PURE SUBSTANCES DATABASE, which treats
the gas phase as an ideal mixture at all temperatures, pressures and
compositions), or from some non-ideal gaseous/fluid mixture models
implemented in the Thermo-Calc GES system (such as the SUPERFLUID model,
i.e., the non-ideal EOS and non-ideal mixing for the C-H-O-S-N-Ar fluids;
Shi and Saxena, 1992). For other condensed materials except for aqueous
solution species, one could append data (of stoichiometric and solution
solid phases) from any compatible Thermo-Calc database(s) [e.g., PURE,
SSUB, SSOL, TCFE, TCNI, TCNF, CCCL, TTNi, TTTi, TTAl, TTMg, TTZr, NSLD,
SEMC, TCMP, TCES, SALT, ION, SLAG, NOX, NUOX, SNUX, NUMT, GCE, and other
substances/solutions databases), depending upon application systems and
investigated aqueous-bearing heterogeneous interaction processes.
In a normal POLY calculation (single points, stepping, and/or mapping),
one should always remember as the first step to appropriately redefine
the components as follows:
    DEF-COMP H2O H+1 Ze Fe Ni NaCl Cl-1 S <= other components> ;
Then, one can appropriately define the equilibrium conditions, e.g.,
    SET-COND P=1e5 T=300 B=1000 N(H+1)=0 N(Ze)=0 N(Fe)=1e-6 N(NaCl)=3...;
and set the necessary reference states for some components, e.g.,
    SET-REFERENCE-STATE H2O AQUEOUS * 1E5 ;
    SET-REFERENCE-STATE Ze REF_ELEC * 1E5 ;
    SET-REFERENCE-STATE NaCl HALITE * 1E5 ;
    SET-REFERENCE-STATE Fe BCC * 1E5 ;
The pH and Eh are thus defined by entering the following functions:
    ENT-SYM FUNC pH=-log10(ACR(H+1)) ;
    ENT-SYM FUNC Eh=MUR(Ze)/RNF ;
However, if the reference state for H+1 component has been defined by
    SET-REFERENCE-STATE H+1 AQUEOUS * 1E5 ;
then the pH quantity should be alternatively entered as:
    ENT-SYM FUNC pH=-log10(ACR(H+1,AQUEOUS)) ;
For defining activity and activity coefficients of the solvent, use:
    ENT-SYM FUNC ACRH2O=ACR(H2O,AQUEOUS) ;
    ENT-SYM FUNC RCH2O=ACR(H2O,AQUEOUS) ;
while for defining activity, activity coefficients and molality of
a specific solute species "i", use:
    ENT-SYM FUNC AII=ACR(i,AQUEOUS)*AH2O ;
    ENT-SYM FUNC Rci=ACR(i,AQUEOUS)*YH2O/Y(AQUEOUS,i) ;
    ENT-SYM FUNC Mli=Y(AQUEOUS,i)*AH2O/YH2O ;
where RNF=96485.309, AH2O=55.508435 and YH2O=Y(AQUEOUS,H2O) as
predefined functions, and i=Fe+2 (for instance) as species name.
Important Note: The REF ELECTRODE phase is the reference electrode which
should always be included in a defined system involving aqueous solution
for the purpose of calculating electron potential [MUR(Ze)], while this
phase should always be SUSPENDED in all the POLY calculations.
For further information, please contact Dr. Pingfang Shi at TCSAB.
Release History: Version 1.0 initial release (as AQ),          1997
                  Version 1.1 with minor improvements (as AQ), 1998
                  Version 1.2 with minor improvements (as AQ), 2000
                  Version 2.0 with major improvements (as PAQ2.0), 2002
                  Version 2.1 with minor improvements (as PAQ2.1), 2003
                  Version 2.2 with minor improvements (as PAQ2.2), 2006

```

Version 2.3 with minor improvements (as PAQ2.3), 2007
Version 2.4 with major improvements (as PAQ2.4), 2008
Edited by: Dr. Pingfang Shi (Thermo-Calc Software, 1997-2008).

```
=====
TDB_PAQ2: d-sys H O Na Cl
... the command in full is DEFINE_SYSTEM
NA                                CL    DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
AQUEOUS:A      :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CL2 CL-1 CLO2 CLO-1 CLO2-1
CLO3-1 CLO4-1 HClO HClO2 NA+1:
> Aqueous Solution: using the SIT Model (from TCAQ2 database)
REF ELECTRODE :ZE:
> Reference Electrode for ZE potential; always SUSPENDED in POLY.
GAS:G          :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1NA1 CL2NA2 CL3NA3 H
H1NA1 H1NA1O1 H1O1 H1O2 H2 H2NA2O2 H2O1 H2O2 NA NA1O1 NA2 NA2O1 NA2O2 O O2
O3:
> Gaseous Mixture, using the ideal gas model
FCC_A1         :NA O:VA:
> This is also the MX (X=C,N) solution phase.
BCC_A2         :NA O:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP_A3         :NA:VA:
> This is also the M2X (X=C,N) solution phase.
HALITE         :NA1CL1:
NAO2           :NA1O2:
NA2O_S1        :NA2O1:
NA2O_S2        :NA2O1:
NA2O_S3        :NA2O1:
NA2O2_S1       :NA2O2:
NA2O2_S2       :NA2O2:
NAOH_S1        :H1NA1O1:
NAOH_S2        :H1NA1O1:
TDB_PAQ2: get
... the command in full is GET_DATA
10:01:05,032 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data
```

```
-OK-
10:01:05,489 [Thread-0] WARN  MacroProcessingContext: The handling of the excess model command is not yet supported in GES6.
10:01:05,489 [Thread-0] WARN  MacroProcessingContext: The handling of the add contribution command is not yet supported in GES6.
10:01:05,491 [Thread-0] WARN  MacroProcessingContext: The handling of the fraction limits command is not yet supported in GES6.
```

TDB_PAQ2:Hit RETURN to continue

TDB_PAQ2:

TDB_PAQ2: @@ Define the system-components and the reference states:

TDB_PAQ2: go p-3

... the command in full is GOTO_MODULE

```
POLY version 3.32
POLY: d-com H2O H+1 ZE Na Cl
... the command in full is DEFINE_COMPONENTS
POLY: s-r-s H2O AQUEOUS * 1e5
... the command in full is SET_REFERENCE_STATE
POLY: s-r-s ZE REF_ELE * 1e5
... the command in full is SET_REFERENCE_STATE
POLY: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS    REF. STATE    T(K)          P(Pa)
VA              ENTERED    SER
H2O             ENTERED    AQUEOUS      *              100000
H+1             ENTERED    SER
ZE              ENTERED    REF_ELECTRODE *              100000
NA              ENTERED    SER
CL              ENTERED    SER
POLY:
POLY: @@ Define the equilibrium conditions
POLY: @@ -----
POLY: @@ Define P-T and bulk composition in the interaction system
POLY: @@ for the calculations of initial equilibria:
POLY:
POLY: s-c P=1e5 T=298.15 b(H2O)=1000
... the command in full is SET_CONDITION
POLY: s-in-am b(NaCl1)=5
... the command in full is SET_INPUT_AMOUNTS
POLY: s-c n(H+1)=0 n(ZE)=0
... the command in full is SET_CONDITION
Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, T=298.15, B(H2O)=1000, B(NA)=1.966861769, B(CL)=3.033138231,
N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0
POLY:
POLY: @@ Calculate an equilibrium with only AQUEOUS:
POLY: c-st p *-sus
... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS    DRIVING FORCE    MOLES
AQUEOUS        ENTERED    0.000000E+00    1.785600E+03
SUSPENDED PHASES:
REF ELECTRODE  NAOH_S2 NAOH_S1 NAO2 NA2O_S3 NA2O_S2 NA2O_S1 NA2O2_S2 NA2O2_S1
HCP_A3 HALITE FCC_A1 BCC_A2 GAS
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
```

```

Using global minimization procedure
Calculated      1212 grid points in      0.002 s
Found the set of lowest grid points in      0.000 s
Creating a new composition set AQUEOUS#2
Calculated POLY solution      0.281 s, total time      0.283 s
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, B(NA)=1.966861769, B(CL)=3.033138231,
N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0

Temperature      298.15 K (      25.00 C), Pressure      1.000000E+05
Number of moles of components      5.56795E+01, Mass in grams      1.00500E+03
Total Gibbs energy -1.70630E+07, Enthalpy -1.59010E+07, Volume      0.00000E+00

Component      Moles      M-Fraction      Activity      Potential      Ref.stat
H2O      5.5508E+01      9.9693E-01      9.9654E-01      -8.5871E+00      AQUEOUS#
H+1      -9.7239E-08      -1.7464E-09      1.0405E-07      -3.9858E+04      SER
ZE      8.6043E-08      1.5453E-09      3.4476E+12      7.1565E+04      REF_ELEC
NA      8.5554E-02      1.5365E-03      4.5046E-63      -3.5588E+05      SER
CL      8.5554E-02      1.5365E-03      4.1623E-18      -9.9210E+04      SER

AQUEOUS#1      Status ENTERED      Driving force      0.0000E+00
Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00      Mole fractions:
H2O      9.96927E-01      NA      1.53654E-03      H+1      -1.74641E-09
CL      1.53654E-03      ZE      1.54532E-09
Constitution:      SiteFraction      Molality      Activity      log10Act
H2O      9.96927E-01      5.55084E+01      9.96605E-01      -0.0015
CL-1      1.53654E-03      8.55538E-02      6.73425E-02      -1.1717
NA+1      1.53654E-03      8.55538E-02      6.73424E-02      -1.1717
H+1      2.37132E-09      1.32034E-07      1.04050E-07      -6.9828
OH-1      2.19965E-09      1.22476E-07      9.63757E-08      -7.0160
O2      4.70270E-10      2.61844E-08      2.61828E-08      -7.5820
O3      1.00000E-12      0.00000E+00      2.70935E-38      -37.5671
HClO      1.00000E-12      0.00000E+00      3.25360E-20      -19.4876
H2O2      1.00000E-12      0.00000E+00      3.68420E-21      -20.4337
HClO2      1.00000E-12      0.00000E+00      1.28717E-37      -36.8904
H2      1.00000E-12      0.00000E+00      5.39110E-43      -42.2683
HO2-1      1.00000E-12      0.00000E+00      7.49315E-26      -25.1253
ClO4-1      1.00000E-12      0.00000E+00      8.09139E-33      -32.0920
ClO3-1      1.00000E-12      0.00000E+00      1.41605E-30      -29.8489
ClO2-1      1.00000E-12      0.00000E+00      1.29472E-32      -31.8878
ClO2      1.00000E-12      0.00000E+00      4.84011E-38      -37.3151
ClO-1      1.00000E-12      0.00000E+00      6.77886E-21      -20.1688
CL2      1.00000E-12      0.00000E+00      4.80004E-25      -24.3188
Solution Properties:      pH =      6.9828      Eh =      0.7417 V      I =      0.0856
pe =      12.5375      Ah =      71.5647 kJ      m* =      0.1711
Aw =      0.9966      Os =      1.1033      pKw =      13.9973
At1= 1.0000E-12      At2= 1.2248E-07 (equiv_mol/kg_H2O)

POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
AQUEOUS#2      ENTERED      0.000000E+00      0.000000E+00
AQUEOUS#1      ENTERED      0.000000E+00      5.567954E+01
SUSPENDED PHASES:
REF_ELECTRODE      NaOH_S2      NaOH_S1      NaO2      Na2O_S3      Na2O_S2      Na2O_S1      Na2O2_S2      Na2O2_S1
HCP_A3      HALITE      FCC_A1      BCC_A2      GAS
POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.
N=55.679543
N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042554E-8,
N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY:Hit RETURN to continue
POLY:
POLY: @@ Calculate an equilibrium with all phases (except for REF_ELE)
POLY:
POLY: c-st p *=ent 0
... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY:
POLY: @@ Always set the REF_ELECTRODE phase as SUSPENDED:
POLY:
POLY: c-st p REF_ELE=sus
... the command in full is CHANGE_STATUS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
NaOH_S2      ENTERED      0.000000E+00      0.000000E+00
NaOH_S1      ENTERED      0.000000E+00      0.000000E+00
NaO2      ENTERED      0.000000E+00      0.000000E+00
Na2O_S3      ENTERED      0.000000E+00      0.000000E+00
Na2O_S2      ENTERED      0.000000E+00      0.000000E+00
Na2O_S1      ENTERED      0.000000E+00      0.000000E+00
Na2O2_S2      ENTERED      0.000000E+00      0.000000E+00
Na2O2_S1      ENTERED      0.000000E+00      0.000000E+00
HCP_A3      ENTERED      0.000000E+00      0.000000E+00
HALITE      ENTERED      0.000000E+00      0.000000E+00
FCC_A1      ENTERED      0.000000E+00      0.000000E+00
BCC_A2      ENTERED      0.000000E+00      0.000000E+00
AQUEOUS#2      ENTERED      0.000000E+00      0.000000E+00
AQUEOUS#1      ENTERED      0.000000E+00      5.580000E+01
GAS      ENTERED      0.000000E+00      0.000000E+00
SUSPENDED PHASES:
REF_ELECTRODE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      806 grid points in      0.089 s
Found the set of lowest grid points in      0.004 s
Calculated POLY solution      0.383 s, total time      0.476 s
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, B(NA)=1.966861769, B(CL)=3.033138231,
N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0

```


Temperature 298.15 K (25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56795E+01, Mass in grams 1.00500E+03
Total Gibbs energy -1.70630E+07, Enthalpy -1.59010E+07, Volume 0.00000E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
H2O	5.5508E+01	9.9693E-01	9.9654E-01	-8.5871E+00	AQUEOUS#
H+1	-9.7239E-08	-1.7464E-09	1.0405E-07	-3.9858E+04	SER
ZE	8.6043E-08	1.5453E-09	3.4476E+12	7.1565E+04	REF_ELEC
NA	8.5554E-02	1.5365E-03	4.5046E-63	-3.5588E+05	SER
CL	8.5554E-02	1.5365E-03	4.1623E-18	-9.9210E+04	SER

AQUEOUS#1 Status ENTERED Driving force 0.0000E+00
Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00 Mole fractions:
H2O 9.96927E-01 NA 1.53654E-03 H+1 -1.74641E-09
CL 1.53654E-03 ZE 1.54532E-09

Constitution:	SiteFraction	Molality	Activity	log10Act
H2O	9.96927E-01	5.55084E+01	9.96605E-01	-0.0015
CL-1	1.53654E-03	8.55538E-02	6.73425E-02	-1.1717
NA+1	1.53654E-03	8.55538E-02	6.73424E-02	-1.1717
H+1	2.37132E-09	1.32034E-07	1.04050E-07	-6.9828
OH-1	2.19965E-09	1.22476E-07	9.63757E-08	-7.0160
O2	4.70270E-10	2.61844E-08	2.61828E-08	-7.5820
O3	1.00000E-12	0.00000E+00	2.70935E-38	-37.5671
HClO	1.00000E-12	0.00000E+00	3.25360E-20	-19.4876
H2O2	1.00000E-12	0.00000E+00	3.68420E-21	-20.4337
HClO2	1.00000E-12	0.00000E+00	1.28717E-37	-36.8904
H2	1.00000E-12	0.00000E+00	5.39110E-43	-42.2683
HO2-1	1.00000E-12	0.00000E+00	7.49315E-26	-25.1253
ClO4-1	1.00000E-12	0.00000E+00	8.09139E-33	-32.0920
ClO3-1	1.00000E-12	0.00000E+00	1.41605E-30	-29.8489
ClO2-1	1.00000E-12	0.00000E+00	1.29472E-32	-31.8878
ClO2	1.00000E-12	0.00000E+00	4.84011E-38	-37.3151
ClO-1	1.00000E-12	0.00000E+00	6.77886E-21	-20.1688
CL2	1.00000E-12	0.00000E+00	4.80004E-25	-24.3188

Solution Properties: pH = 6.9828 Eh = 0.7417 V I = 0.0856
pe = 12.5375 Ah = 71.5647 kJ m* = 0.1711
Aw = 0.9966 Os = 1.1033 pKw = 13.9973
At1= 1.0000E-12 At2= 1.2248E-07 (equiv_mol/kg_H2O)

POLY: 1-st p

... the command in full is LIST_STATUS

*** STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
AQUEOUS#2	ENTERED	0.000000E+00	0.000000E+00
AQUEOUS#1	ENTERED	0.000000E+00	5.567954E+01
GAS	ENTERED	-3.453482E+00	0.000000E+00
HALITE	ENTERED	-4.519288E+00	0.000000E+00
NAOH_S1	ENTERED	-1.737487E+01	0.000000E+00
BCC_A2	ENTERED	-1.752962E+01	0.000000E+00
FCC_A1	ENTERED	-1.752962E+01	0.000000E+00
NAOH_S2	ENTERED	-1.793977E+01	0.000000E+00
NAO2	ENTERED	-1.999496E+01	0.000000E+00
NA2O2_S1	ENTERED	-2.605088E+01	0.000000E+00
NA2O2_S2	ENTERED	-2.640940E+01	0.000000E+00
NA2O_S1	ENTERED	-4.241247E+01	0.000000E+00

ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.257992E+01

NA2O_S2 NA2O_S3 HCP_A3

SUSPENDED PHASES:

REF ELECTRODE

POLY: sh b n n(*)

... the command in full is SHOW_VALUE

B=1005.

N=55.679543

N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042547E-8,

N(NA)=8.5553782E-2, N(CL)=8.5553803E-2

POLY:

POLY: @@ As shown here, 0.5wt% of NaCl (in 1 kg of H2O) is

POLY: @@ equivalent to 0.085554 molality of NaCl.

POLY:

POLY: @@ Save the workspace for the H2O-NaCl system:

POLY: save TCEX53_a.POLY3 y

... the command in full is SAVE_WORKSPACES

POLY:Hit RETURN to continue

POLY:

POLY: @@ =====

POLY: @@ Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co)

POLY: @@ =====

POLY: @@ To demonstrate how to define the initial amount of alloy

POLY: @@ in an aqueous-bearing heterogeneous interaction system:

POLY: @@ =====

POLY: @@ Note: We are only interested in the BCC_A2 and FCC_A1

POLY: @@ phases in the Fe-based alloy, in the current testing

POLY: @@ calculation. If necessary, you can consider other

POLY: @@ phases (which exist in the applied steel material).

POLY:

POLY: go data

... the command in full is GOTO_MODULE

TDB_PAQ2: rej sys

... the command in full is REJECT

H	O	ZE
VA DEFINED		
LIQUID:L REJECTED		
GRAPHITE	DIAMOND_A4	FC_ORTHORHOMBIC
MONOCLINIC REJECTED		
CBCC_A12	CUB_A13	CHI_A12
FE4N	FECN_CHI REJECTED	
CEMENTITE	M23C6	M7C3
M5C2	M3C2	KSI_CARBIIDE
PI REJECTED		
FE3C	NI3C	CR3C2
CR7C3	CR23C6 REJECTED	
COCO3	FECO3	NAHCO3
NA2CO3_S1	NA2CO3_S2	NICO3
CRC6O6 REJECTED		
CO3N	CRN	CR2N
FE2N	NI3N REJECTED	
NANO2_S1	NANO2_S2	NANO3
REJECTED		
COCL2	CRCL2	CRCL3
FECL2	FECL3	NICL2
REJECTED		
FECLO	NACLO4_S1	NACLO4_S2
REJECTED		

REINITIATING GES

TDB_PAQ2: sw PAQ2

```

... the command in full is SWITCH_DATABASE
TDB_PAQ2: rej ele H O ZE
... the command in full is REJECT
H          O          ZE
REJECTED
TDB_PAQ2: d-sys Fe Cr Ni Co
... the command in full is DEFINE_SYSTEM
FE          CR          NI
CO DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
GAS:G      :CO CR CR2 FE NI:
> Gaseous Mixture, using the ideal gas model
FCC_A1     :CO CR FE NI:VA:
> This is also the MX (X=C,N) solution phase.
BCC_A2     :CO CR FE NI:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP_A3     :CO CR FE NI:VA:
> This is also the M2X (X=C,N) solution phase.
SIGMA      :CO FE NI:CR:CO CR FE NI:
TDB_PAQ2: rej-ph *
... the command in full is REJECT
GAS:G      FCC_A1          BCC_A2
HCP_A3     SIGMA REJECTED
TDB_PAQ2: rest-ph FCC_A1 BCC_A2
... the command in full is RESTORE
FCC_A1     BCC_A2 RESTORED
TDB_PAQ2: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS ....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:
POLY: @@ You can turn on the Global Minimization:
POLY: Adv-Opt EQ_CALC Y Y !
... the command in full is ADVANCED_OPTIONS
Settings for the minimization of an equilibra:
POLY: Adv-Opt GLOBAL Y 20000 !
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY:
POLY: s-c P=1e5 T=298.15
... the command in full is SET_CONDITION
POLY:
POLY: @@ The following conditions [system-size B and initial bulk
POLY: @@ composition w(i) of Fe-alloy] corresponds to the total
POLY: @@ initial amount of Fe-based alloy in the interaction,
POLY: @@ i.e., 1 gram of steel (Fe-10Cr-5Ni-1Co wt%).
POLY:
POLY: s-c B=1 w(Cr)=.10 w(Ni)=.05 w(Co)=.01
... the command in full is SET_CONDITION
POLY:
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 39232 grid points in 0.382 s
Found the set of lowest grid points in 0.006 s
Creating a new composition set BCC_A2#2
Calculated POLY solution 0.054 s, total time 0.442 s
Creating a new composition set BCC_A2#3
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 1.79859E-02, Mass in grams 1.00000E+00
Total Gibbs energy -1.58616E+02, Enthalpy -1.09889E+01, Volume 1.20553E-07

Component      Moles      M-Fraction Activity Potential Ref.stat
CO              1.6968E-04  9.4342E-03 4.4157E-08 -4.1983E+04 SER
CR              1.9232E-03  1.0693E-01 5.8926E-02 -7.0192E+03 SER
FE              1.5041E-02  8.3627E-01 3.7073E-02 -8.1679E+03 SER
NI              8.5193E-04  4.7367E-02 7.7089E-04 -1.7769E+04 SER

BCC_A2#3              Status ENTERED      Driving force 0.0000E+00
Moles 1.4641E-02, Mass 8.1821E-01, Volume fraction 8.5170E-01 Mole fractions:
FE 9.87131E-01 CO 1.15888E-02 NI 8.17873E-04 CR 4.61992E-04

BCC_A2#1              Status ENTERED      Driving force 0.0000E+00
Moles 1.9166E-03, Mass 9.9654E-02, Volume fraction 1.1495E-01 Mole fractions:
CR 9.99946E-01 FE 5.39522E-05 CO 9.25541E-12 NI 8.81026E-12

FCC_A1              Status ENTERED      Driving force 0.0000E+00
Moles 1.4280E-03, Mass 8.2138E-02, Volume fraction 3.3346E-02 Mole fractions:
NI 5.88202E-01 FE 4.11792E-01 CO 5.30943E-06 CR 6.98908E-09
POLY: l-st cp
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)          P(Pa)
VA              ENTERED      SER
CO              ENTERED      SER

```

```

CR                ENTERED  SER
FE                ENTERED  SER
NI                ENTERED  SER
*** STATUS FOR ALL PHASES
PHASE            STATUS    DRIVING FORCE    MOLES
FCC_A1           ENTERED    0.000000E+00    1.428010E-03
BCC_A2#3         ENTERED    0.000000E+00    1.464136E-02
BCC_A2#2         ENTERED    0.000000E+00    0.000000E+00
BCC_A2#1         ENTERED    0.000000E+00    1.916564E-03
POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1.
N=1.7985937E-2
N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(Fe)=1.5041094E-2, N(NI)=8.5193389E-4
POLY:Hit RETURN to continue
POLY:
POLY: s-c T=1073.15
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          39232 grid points in          0.293 s
Found the set of lowest grid points in          0.009 s
Calculated POLY solution          0.058 s, total time          0.360 s
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =          1, label A0 , database: PAQ2

Conditions:
P=100000, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0

Temperature 1073.15 K ( 800.00 C), Pressure 1.000000E+05
Number of moles of components 1.79859E-02, Mass in grams 1.00000E+00
Total Gibbs energy -9.18150E+02, Enthalpy 5.59649E+02, Volume 1.23044E-07

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
CO              1.6968E-04    9.4342E-03  1.8364E-05 -9.7303E+04 SER
CR              1.9232E-03    1.0693E-01  3.0133E-03 -5.1794E+04 SER
FE              1.5041E-02    8.3627E-01  4.2352E-03 -4.8757E+04 SER
NI              8.5193E-04    4.7367E-02  1.1925E-04 -8.0610E+04 SER

FCC_A1          Status ENTERED    Driving force 0.0000E+00
Moles 1.7986E-02, Mass 1.0000E+00, Volume fraction 1.0000E+00 Mole fractions:
FE 8.36270E-01 CR 1.06929E-01 NI 4.73667E-02 CO 9.43424E-03
POLY: l-st cp
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS    REF. STATE    T(K)          P(Pa)
VA             ENTERED  SER
CO             ENTERED  SER
CR             ENTERED  SER
FE             ENTERED  SER
NI             ENTERED  SER
*** STATUS FOR ALL PHASES
PHASE            STATUS    DRIVING FORCE    MOLES
FCC_A1           ENTERED    0.000000E+00    1.798594E-02
BCC_A2#1         ENTERED    -1.564120E-02    0.000000E+00
BCC_A2#3         ENTERED    -1.564120E-02    0.000000E+00
BCC_A2#2         ENTERED    -1.564120E-02    0.000000E+00
POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1.
N=1.7985937E-2
N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(Fe)=1.5041094E-2, N(NI)=8.5193389E-4
POLY: @@
POLY: @@ As shown here, 1 gram of steel (Fe-10Cr-5Ni-1Co wt%)
POLY: @@ is equivalent to:
POLY: @@      n(Fe) = 1.5041094E-2
POLY: @@      n(Cr) = 1.9232249E-3
POLY: @@      n(Ni) = 8.5193389E-4
POLY: @@      n(Co) = 1.6968422E-4
POLY:
POLY: @@ Save the workspace for the Fe-Cr-Ni-Co system:
POLY: save TCEX53_b.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continue
POLY:
POLY: @@ =====
POLY: @@ Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl
POLY: @@ =====
POLY: @@ Bulk composition in the heterogeneous interaction system:
POLY: @@      b(H2O) = 1000
POLY: @@      n(NaCl) = 0.085554
POLY: @@      n(Fe) = 1.5041094E-2
POLY: @@      n(Cr) = 1.9232249E-3
POLY: @@      n(Ni) = 8.5193389E-4
POLY: @@      n(Co) = 1.6968422E-4
POLY:
POLY: @@ Retrieve data from the PAQ2 database:
POLY: go data
... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
... the command in full is REJECT
H              O              ZE
VA DEFINED
LIQUID:L REJECTED
GRAPHITE       DIAMOND_A4      FC_ORTHORHOMBIC
MONOCLINIC REJECTED
CBCC_A12       CUB_A13         CHI_A12
FE4N           FECN_CHI REJECTED M7C3
CEMENTITE      M23C6
M5C2           M3C2            KSI_CARBIIDE
PI REJECTED
FE3C           NI3C             CR3C2
CR7C3          CR23C6 REJECTED
COCO3          FECO3            NAHCO3
NA2CO3_S1      NA2CO3_S2            NICO3
CRC606 REJECTED
CO3N           CRN              CR2N

```

```

FE2N          NI3N REJECTED
NANO2_S1      NANO2_S2          NANO3
REJECTED
COCL2         CRCL2             CRCL3
FECL2         FECL3             NICL2
REJECTED
FECLO         NACLO4_S1         NACLO4_S2
REJECTED
REINITIATING GES .....
TDB_PAQ2: @@ Switch to the PAQ2 database
TDB_PAQ2: sw PAQ2
... the command in full is SWITCH_DATABASE
TDB_PAQ2: d-sys H O Na Cl Fe Cr Ni Co
... the command in full is DEFINE_SYSTEM
NA            CL                FE
CR            NI                CO
DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
AQUEOUS:A      :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CO1H2O2 CL2 CL-1 CLO2 CLO-1
CLO2-1 CLO3-1 CLO4-1 HCLO HCLO2 CO+2 CO+3 CR+2 CR+3 CROH+2 CRO+1 CRO2-1
HCRO2 HCRO4-1 CRO4-2 CR2O7-2 FE+2 FE+3 FEOH+1 FEOH+2 FEO3H3-1 FE2O2H2+4
FECL+2 NA+1 NI+2 NIOH+1:
> Aqueous Solution: using the SIT Model (from TCAQ2 database)
REF ELECTRODE :ZE:
> Reference Electrode for ZE potential; always SUSPENDED in POLY.
GAS:G          :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1CO1 CL1CR1 CL1CR1O1
CL1CR1O2 CL1FE1 CL1NA1 CL1NI1 CL2CO1 CL2CR1 CL2CR1O1 CL2CR1O2 CL2FE1
CL2NA2 CL2NI1 CL3CO1 CL3CR1 CL3CR1O1 CL3FE1 CL3NA3 CL4CO2 CL4CR1 CL4CR1O1
CL4FE2 CL5CR1 CL6CR1 CL6FE2 CO CO1H1 CO1H2O2 CO1O1 CR CR1H1 CR1H1O1
CR1H1O2 CR1H1O3 CR1H2O2 CR1H2O3 CR1H2O4 CR1H3O3 CR1H3O4 CR1H4O4 CR1H4O5
CR1O1 CR1O2 CR1O3 CR2 CR2O1 CR2O2 CR2O3 FE FE1H1O1 FE1H1O2 FE1H2O2 FE1O1
FE1O2 H H1NA1 H1NA1O1 H1NI1 H1NI1O1 H1O1 H1O2 H2 H2NA2O2 H2NI1O2 H2O1 H2O2
NA NA1O1 NA2 NA2O1 NA2O2 NI NI1O1 O O2 O3:
> Gaseous Mixture, using the ideal gas model
FCC_A1         :CO CR FE NA NI O:VA:
> This is also the MX (X=C,N) solution phase.
BCC_A2         :CO CR FE NA NI O:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP_A3         :CO CR FE NA NI:VA:
> This is also the M2X (X=C,N) solution phase.
SIGMA          :CO FE NI:CR:CO CR FE NI:
HALITE         :NA1CL1:
WUSTITE        :FE0.947O1:
MAGNETITE      :FE3O4:
HEMATITE       :FE2O3:
FE2O3_GAMMA    :FE2O3:
FE2O2H2        :FE1H2O2:
FE2O3H3        :FE1H3O3:
FEOOH          :FE1H1O2:
FE2O2O2H2      :FE2H2O4:
COO_S          :CO1O1:
CO3O4          :CO3O4:
COO2H2         :CO1H2O2:
CR02           :CR1O2:
CR03           :CR1O3:
CR2O3          :CR2O3:
CR5O12         :CR5O12:
CR8O21         :CR8O21:
NAO2           :NA1O2:
NA2O_S1        :NA2O1:
NA2O_S2        :NA2O1:
NA2O_S3        :NA2O1:
NA2O2_S1       :NA2O2:
NA2O2_S2       :NA2O2:
NAOH_S1        :H1NA1O1:
NAOH_S2        :H1NA1O1:
NIO_S1         :NI1O1:
NIO_S2         :NI1O1:
NIO2H2         :H2NI1O2:
NIOOH         :H1NI1O2:
FECR2O4        :CR2FE1O4:
COCR2O4        :CO1CR2O4:
NICR2O4        :CR2NI1O4:
NA2CR2O4       :CR2NA2O4:
COFE2O4        :CO1FE2O4:
NIFE2O4        :FE2NI1O4:
NA2CRO4_S1     :CR1NA2O4:
NA2CRO4_S2     :CR1NA2O4:
NA2FEO2        :FE1NA1O2:

```

TDB_PAQ2:Hit RETURN to continue

TDB_PAQ2:

TDB_PAQ2: rej ph HCP_A3 CBCC_A12 CUB_A13 CHI_A12 Fe4N

... the command in full is REJECT
HCP_A3 REJECTED

TDB_PAQ2: rej ph SIGMA

... the command in full is REJECT
SIGMA REJECTED

TDB_PAQ2: rej ph NaH

... the command in full is REJECT

TDB_PAQ2: get

... the command in full is GET_DATA
REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

10:01:08,428 [Thread-0] WARN MacroProcessingContext: The handling of the excess model command is not yet supported in GES6.

10:01:08,432 [Thread-0] WARN MacroProcessingContext: The handling of the add contribution command is not yet supported in GES6.

10:01:08,434 [Thread-0] WARN MacroProcessingContext: The handling of the fraction limits command is not yet supported in GES6.

TDB_PAQ2:Hit RETURN to continue

TDB_PAQ2:

TDB_PAQ2: @@ Define system-components and the reference states:

TDB_PAQ2: go p-3

```

... the command in full is GOTO_MODULE

POLY version 3.32
POLY: d-com H2O H+1 ZE Na Cl Fe Cr Ni Co
... the command in full is DEFINE_COMPONENTS
POLY: s-r-s H2O AQUEOUS * 1e5
... the command in full is SET_REFERENCE_STATE
POLY: s-r-s ZE REF_ELE * 1e5
... the command in full is SET_REFERENCE_STATE
POLY: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)      P(Pa)
VA              ENTERED      SER
H2O             ENTERED      AQUEOUS        *      100000
H+1             ENTERED      SER
ZE             ENTERED      REF ELECTRODE  *      100000
NA             ENTERED      SER
CL             ENTERED      SER
FE             ENTERED      SER
CR             ENTERED      SER
NI             ENTERED      SER
CO             ENTERED      SER
POLY:
POLY: @@ Define some symbols (constants/variables/functions/tables):
POLY: @@ You can define some important ones e.g., RNF; pH, Eh
POLY: @@ =====
POLY: @@ Important: With the default reference state (SER) used for
POLY: @@ system-component H+1, the pH condition in aqueous solution
POLY: @@ should be defined as:
POLY: @@      pH = -log10[act(H+1,aqs)] (traditional)
POLY: @@           = -log10[acr(H+1,AQUEOUS)*55.508435] (Thermo-Calc)
POLY: @@           = -ln[acr(H+1,AQUEOUS)*55.508435]*2.302585093
POLY: @@ where
POLY: @@      act(H+1,aqs) is molality based activity of
POLY: @@      H+1 species (as of the traditional concept);
POLY: @@      acr(H+1,AQ)*AH2O is site-fraction based activity of
POLY: @@      H+1 species (calculated in Thermo-Calc).
POLY: @@
POLY: @@ Such a definition not only gives correct pH values for all
POLY: @@ thermodynamic models (SIT and HKF) but also does not affect
POLY: @@ the calculation of ACR(H+1) [LNACR(H+1)] quantity that is
POLY: @@ normally used as MAPPING/STEPPING variables in all modules
POLY: @@ (POURBAIX & TDB/GES5/POLY3/POST).
POLY: @@ =====
POLY:
POLY: @@ You can also choose to define many other symbols (for
POLY: @@ plotting) on the same scope of the POURBAIX module.
POLY:
POLY: @@ A list of valid symbols for the Fe-Cr-Ni-Co-H2O-NaCl
POLY: @@ heterogeneous interaction system on the scope same as the
POLY: @@ automatically defined symbols in the POURBAIX module can be
POLY: @@ found at the end of this MACRO file (but only as a reference).
POLY: @@ -----
POLY: @@ It is important to note that:
POLY: @@ * AH2O is always a constant, and YH2O is the site fraction
POLY: @@ of the solvent H2O, i.e.,
POLY: @@      AH2O = 55.508435
POLY: @@      YH2O = Y(AQ,H2O)
POLY:
POLY: @@ * The AYT and ART quantities are on the Site-Fraction basis:
POLY: @@      AYT for AC(i,AQ)
POLY: @@      ART for ACR(i,AQ)
POLY:
POLY: @@ * The AIT (Aii), RCT (RCi) and MLT (MLi) quantities are
POLY: @@ on the Molality basis:
POLY: @@      AIT for ACR(i,AQ)*AH2O
POLY: @@      as activity based on molality
POLY: @@      RCT for ACR(i,AQ)*YH2O/Y(AQ,i)
POLY: @@      as activity coefficient based on molality
POLY: @@      MLT for Y(AQ,i)*AH2O/YH2O
POLY: @@      as molality
POLY: @@ -----
POLY: @@      Aii = RCi * MLi
POLY: @@           = ACR(i,AQ)*YH2O/Y(AQ,i) * Y(AQ,i)*AH2O/YH2O
POLY: @@           = ACR(i,AQ)*AH2O
POLY:
POLY: @@ * It is always ACR(sp,AQ) = AC(sp,AQ)
POLY:
POLY: @@ * It is always the Aii=AIT(H+1) [=ACR(H+1,AQ)*AH2O]
POLY: @@ quantity, rather than ART(H+1) [=ACR(H+1,AQ)] quantity,
POLY: @@ that is the equivalent property for the acidity
POLY: @@ condition pH.
POLY: @@ -----
POLY:
POLY: ent-sym const AH2O=55.508435
... the command in full is ENTER_SYMBOL
POLY: ent-sym const RNF =96485.309
... the command in full is ENTER_SYMBOL
POLY: ent-sym funct Eh = mur(ZE)/RNF;
... the command in full is ENTER_SYMBOL
POLY: ent-sym funct pH = -log10(acr(H+1,AQUEOUS)*AH2O);
... the command in full is ENTER_SYMBOL
POLY: l-sym
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
  AH2O=55.508435, RNF=96485.309
DEFINED FUNCTIONS AND VARIABLES%
  EH=MUR(ZE)/RNF
  PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
POLY:
POLY: @@ Define the equilibrium conditions:
POLY: @@ -----
POLY: @@ Define P-T and bulk composition in the interaction system
POLY: @@ for calculating starting point [at e.g pH=7 & Eh=0 (V)]:
POLY:
POLY: @@ P-T conditions:
POLY: s-c P=1e5 T=298.15
... the command in full is SET_CONDITION
POLY: @@
POLY: @@ Alternatively, it can be manually input as below:

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POLY: @@      s-c P=
POLY: @@ @?Pressure_in_Pascal:

POLY: @@      s-c T=
POLY: @@ @?Temperature_In_Kelvin:

POLY:
POLY: @@ For Aqueous-involving interaction systems, it is always
POLY: @@ recommended to define 1 kg of H2O, so that it is
POLY: @@ convenient to consider molality quantities and other
POLY: @@ properties in aqueous solution.
POLY:
POLY: s-c b(H2O)=1000
... the command in full is SET_CONDITION
POLY:
POLY: @@ The following is equivalent to 0.085554 mole of NaCl
POLY: @@ in 1 kg of H2O:
POLY: s-c n(Na)=0.085554  n(Cl)=0.085554
... the command in full is SET_CONDITION
POLY:
POLY: @@ For calculating Pourbaix diagrams or other diagrams in
POLY: @@ aqueous-involving interaction system, it is important
POLY: @@ to consider the so-called "effective interaction rate".
POLY:
POLY: @@ The following is equivalent to 1 gram of specified
POLY: @@ steel (Fe-10Cr-5Ni-1Co wt%) in an effective interaction
POLY: @@ with 1 kg of H2O (dissolving 0.085554 mole of NaCl):
POLY:
POLY: s-c n(Fe)=1.5041094E-2  n(Cr)=1.9232249E-3
... the command in full is SET_CONDITION
POLY: s-c n(Ni)=8.5193389E-4  n(Co)=1.6968422E-4
... the command in full is SET_CONDITION
POLY:
POLY: @@ Let's calculate initial equilibrium at pH=7 & Eh=0 (V):
POLY: s-c lnacr(H+1)=-16.11809565  mur(ZE)=0
... the command in full is SET_CONDITION
POLY:
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(Fe)=1.5041094E-2, N(Cr)=1.9232249E-3, N(Ni)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.11809565, MUR(ZE)=0
DEGREES OF FREEDOM 0
POLY:
POLY: @@ =====
POLY: @@ Turn off GLOBAL completely for aqueous calculations
POLY: @@ -----
POLY: @@ Adv-Opt GLOBAL
POLY: @@ Use global minimization as much as possible /N/: N
POLY: @@ Use global minimization for test only? /N/:      N
POLY: @@ -----
POLY: @@
POLY: Adv-Opt GLOBAL N N !
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY: @@
POLY: @@ -----
POLY: @@ Adv-Opt EQ_CALC
POLY: @@ Force positive definite phase Hessian /Y/:      N
POLY: @@ Control stepsize during minimization /Y/:      Y
POLY: @@ -----
POLY: Adv-Opt EQ_CALC N Y !
... the command in full is ADVANCED_OPTIONS
Settings for the minimization of an equilibra:
POLY:
POLY: @@ =====
POLY: @@ Set numerical limits:
POLY: @@ -----
POLY: @@ Notes:
POLY: @@ For equilibrium calculations (single-point, stepping or
POLY: @@ mapping) of complex aqueous-bearing heterogeneous
POLY: @@ interaction systems, it is recommended to modify the
POLY: @@ numerical limits.
POLY:
POLY: @@ The next command (changing the numerical limits from the
POLY: @@ default values "500 1E-6 1E-12 N" to "20000 1E-6 1E-20 Y")
POLY: @@ makes the following changes:
POLY: @@ 1) Changes "Maximum number of iterations" from the
POLY: @@ default 500 to 20000, which enforces 40 times more
POLY: @@ iterations for each of the calculations in order
POLY: @@ to obtain stable equilibria;
POLY: @@ 2) The "Required accuracy" remains the default value 1E-6.
POLY: @@ It can be changed to 1E-4, that allows less accurate
POLY: @@ calculations but makes it easier/faster to converge;
POLY: @@ 3) Changes "Smallest fraction" from the default site
POLY: @@ fraction of 1E-12 to 1E-20, which is more suitable
POLY: @@ for aqueous solution phases; and
POLY: @@ 4) The "Approximate driving force for metastable phases"
POLY: @@ is changed from the default of "N" to "Y" (meaning
POLY: @@ it should always approximately calculate driving
POLY: @@ forces for metastable phases).
POLY:
POLY: @@ These changes in the numerical limits are essential and
POLY: @@ useful for making sure of finding a converged solution of
POLY: @@ stable equilibria, especially when the heterogeneous
POLY: @@ interaction system becomes more complicated.
POLY: @@ -----
POLY:
POLY: s-n-l 20000 1e-6 1e-20 Y
... the command in full is SET_NUMERICAL_LIMITS
LIMITATIONS of the present version of Thermo-Calc
Max number of elements      : 80
Max number of species       :5000
Max number of sublattices in a phase      : 10
Max number of constituents in a phase:    : 200
Max number of constituents in an ideal phase :5000
POLY:
POLY:
POLY: @@ Calculate an equilibrium with only AQUEOUS:
POLY: c-st p *=sus
... the command in full is CHANGE_STATUS

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POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
AQUEOUS        ENTERED    0.000000E+00    6.138000E+03
SUSPENDED PHASES:
WUSTITE REF ELECTRODE NIO_S2 NIO_S1 NIOOH NIO2H2 NIFE2O4 NICR2O4 NAOH_S2
NAOH_S1 NAO2 NA2O S3 NA2O_S2 NA2O_S1 NA2O2_S2 NA2O2_S1 NA2FEO2 NA2CRO4_S2
NA2CRO4_S1 NA2CR2O4 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4
FE2O3_GAMMA FE2O2O2H2 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO_S COO2H2
COFE2O4 COCR2O4 CO3O4 BCC_A2 GAS
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL MINIMIZATION Y,,,,,,,,,
109 ITS, CPU TIME USED 1 SECONDS
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.11809565, MUR(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.57254E+01, Mass in grams 1.00599E+03
Total Gibbs energy -1.70641E+07, Enthalpy -1.59024E+07, Volume -4.21624E-08

Component      Moles      M-Fraction  Activity    Potential  Ref.stat
H2O             5.5508E+01  9.9611E-01  9.9606E-01  -9.7846E+00 AQUEOUS
H+1            -1.0027E-02 -1.7993E-04  1.0000E-07  -3.9956E+04 SER
ZE             3.7895E-02  6.8003E-04  1.0000E+00  0.0000E+00 REF_ELEC
NA             8.5554E-02  1.5353E-03  1.5211E-50  -2.8436E+05 SER
CL             8.5554E-02  1.5353E-03  1.1822E-30  -1.7083E+05 SER
FE             1.5041E-02  2.6991E-04  1.2285E-18  -1.0223E+05 SER
CR             1.9232E-03  3.4513E-05  1.6596E-45  -2.5561E+05 SER
NI             8.5193E-04  1.5288E-05  6.0058E-14  -7.5468E+04 SER
CO             1.6968E-04  3.0450E-06  3.2708E-16  -8.8391E+04 SER

AQUEOUS          Status ENTERED      Driving force 0.0000E+00
Moles 5.5725E+01, Mass 1.0060E+03, Volume fraction 1.0000E+00 Mole fractions:
H2O 9.96107E-01 ZE 6.80033E-04 NI 1.52881E-05
CL 1.53528E-03 FE 2.69915E-04 CO 3.04501E-06
NA 1.53528E-03 CR 3.45125E-05 H+1 -1.79930E-04
Constitution:      SiteFraction      Molality      Activity      log10Act
H2O                9.96604E-01      5.55084E+01    9.96157E-01    -0.0017
CL-1               1.53628E-03      8.55668E-02    6.59412E-02    -1.1808
NA+1               1.53628E-03      8.55668E-02    6.59591E-02    -1.1807
FE+2               1.56791E-04      8.73285E-03    3.08751E-03    -2.5104
FEOH+1             1.13299E-04      6.31049E-03    4.86919E-03    -2.3125
CRO+1              3.00740E-05      1.67505E-03    1.29247E-03    -2.8886
NI+2               1.52852E-05      8.51348E-04    3.02381E-04    -3.5194
CROH+2             3.38456E-06      1.88512E-04    6.68399E-05    -4.1750
CO+2               3.04698E-06      1.69710E-04    6.02711E-05    -4.2199
HCRO2              1.05903E-06      5.89856E-05    5.89799E-05    -4.2293
NIOH+1             1.28111E-08      7.13548E-07    5.50574E-07    -6.2592
CR+3               1.12056E-08      6.24122E-07    6.07385E-08    -7.2165
CRO2-1             6.16631E-09      3.43448E-07    2.65005E-07    -6.5767
OH-1               2.33522E-09      1.30066E-07    1.00231E-07    -6.9990
H+1               2.32641E-09      1.29576E-07    1.00000E-07    -7.0000
FEOH+2             1.10316E-12      6.14435E-11    2.17858E-11    -10.6618
CR+2               1.47493E-16      8.21498E-15    2.91275E-15    -14.5357
FE+3               6.69156E-17      3.72704E-15    3.61605E-16    -15.4418
FECCL+2            3.43228E-17      1.91170E-15    6.77823E-16    -15.1689
H2                 1.06276E-19      5.91933E-18    5.91876E-18    -17.2278
FE2O2H2+4          2.32944E-20      1.29744E-18    2.05117E-20    -19.6880
O3                 1.00000E-20      0.00000E+00    2.0444E-113    -112.6894
FEO3H3-1           1.00000E-20      0.00000E+00    4.15261E-44    -43.3817
H2O2               1.00000E-20      0.00000E+00    3.35251E-46    -45.4746
CRO4-2             1.00000E-20      0.00000E+00    1.67197E-26    -25.7768
HCL0               1.00000E-20      0.00000E+00    2.78756E-45    -44.5548
HCL02              1.00000E-20      0.00000E+00    1.00400E-87    -86.9983
CR2O7-2            1.00000E-20      0.00000E+00    9.28118E-52    -51.0324
HCRO4-1            1.00000E-20      0.00000E+00    5.05292E-27    -26.2965
HO2-1              1.00000E-20      0.00000E+00    7.09471E-51    -50.1491
CO1H2O2            1.00000E-20      0.00000E+00    5.9656E-101    -100.2243
CO+3               1.00000E-20      0.00000E+00    7.96270E-38    -37.0989
O2                 1.00000E-20      0.00000E+00    2.17014E-58    -57.6635
CLO4-1             1.00000E-20      0.00000E+00    5.4430E-133    -132.2642
CLO3-1             1.00000E-20      0.00000E+00    1.0463E-105    -104.9803
CLO2-1             1.00000E-20      0.00000E+00    1.05079E-82    -81.9785
CLO2               1.00000E-20      0.00000E+00    1.1394E-100    -99.9433
CLO-1              1.00000E-20      0.00000E+00    6.04311E-46    -45.2187
CL2                1.00000E-20      0.00000E+00    3.87204E-50    -49.4121
Solution Properties: pH = 7.0000 Eh = 0.0000 V I = 0.1094
pe = 0.0000 Ah = 0.0000 kJ m* = 0.1891
Aw = 0.9962 Os = 1.1300 pKw = 13.9973
At1= 1.0000E-20 At2= 1.3007E-07 (equiv_mol/kg_H2O)

POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
AQUEOUS        ENTERED    0.000000E+00    5.572540E+01
SUSPENDED PHASES:
WUSTITE REF ELECTRODE NIO_S2 NIO_S1 NIOOH NIO2H2 NIFE2O4 NICR2O4 NAOH_S2
NAOH_S1 NAO2 NA2O S3 NA2O_S2 NA2O_S1 NA2O2_S2 NA2O2_S1 NA2FEO2 NA2CRO4_S2
NA2CRO4_S1 NA2CR2O4 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4
FE2O3_GAMMA FE2O2O2H2 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO_S COO2H2
COFE2O4 COCR2O4 CO3O4 BCC_A2 GAS
POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.9899
N=55.725397
N(H2O)=55.508435, N(H+1)=-1.0026646E-2, N(ZE)=3.7895099E-2, N(NA)=8.5554E-2,
N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY:Hit RETURN to continuePOLY:
POLY: @@ Calculate an equilibrium with all phases (except for REF_ELE):
POLY:
POLY: c-st p *=ent 0
... the command in full is CHANGE_STATUS

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POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY: @@ Always set the REF_ELECTRODE phase as SUSPENDED:
POLY: c-st p REF_ELE=sus
... the command in full is CHANGE_STATUS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE	STATUS	DRIVING FORCE	MOLES
WUSTITE	ENTERED	0.000000E+00	0.000000E+00
NIO_S2	ENTERED	0.000000E+00	0.000000E+00
NIO_S1	ENTERED	0.000000E+00	0.000000E+00
NIOOH	ENTERED	0.000000E+00	0.000000E+00
NIO2H2	ENTERED	0.000000E+00	0.000000E+00
NIFE2O4	ENTERED	0.000000E+00	0.000000E+00
NICR2O4	ENTERED	0.000000E+00	0.000000E+00
NAOH_S2	ENTERED	0.000000E+00	0.000000E+00
NAOH_S1	ENTERED	0.000000E+00	0.000000E+00
NAO2	ENTERED	0.000000E+00	0.000000E+00
NA2O_S3	ENTERED	0.000000E+00	0.000000E+00
NA2O_S2	ENTERED	0.000000E+00	0.000000E+00
NA2O_S1	ENTERED	0.000000E+00	0.000000E+00
NA2O2_S2	ENTERED	0.000000E+00	0.000000E+00
NA2O2_S1	ENTERED	0.000000E+00	0.000000E+00
NA2FEO2	ENTERED	0.000000E+00	0.000000E+00
NA2CRO4_S2	ENTERED	0.000000E+00	0.000000E+00
NA2CRO4_S1	ENTERED	0.000000E+00	0.000000E+00
NA2CR2O4	ENTERED	0.000000E+00	0.000000E+00
MAGNETITE	ENTERED	0.000000E+00	0.000000E+00
HEMATITE	ENTERED	0.000000E+00	0.000000E+00
HALITE	ENTERED	0.000000E+00	0.000000E+00
FE0OH	ENTERED	0.000000E+00	0.000000E+00
FE03H3	ENTERED	0.000000E+00	0.000000E+00
FE02H2	ENTERED	0.000000E+00	0.000000E+00
FE02H2	ENTERED	0.000000E+00	0.000000E+00
FE2O3_GAMMA	ENTERED	0.000000E+00	0.000000E+00
FE2O2O2H2	ENTERED	0.000000E+00	0.000000E+00
FCC_A1	ENTERED	0.000000E+00	0.000000E+00
CRO3	ENTERED	0.000000E+00	0.000000E+00
CRO2	ENTERED	0.000000E+00	0.000000E+00
CR8O21	ENTERED	0.000000E+00	0.000000E+00
CR5O12	ENTERED	0.000000E+00	0.000000E+00
CR2O3	ENTERED	0.000000E+00	0.000000E+00
COO_S	ENTERED	0.000000E+00	0.000000E+00
COO2H2	ENTERED	0.000000E+00	0.000000E+00
COFE2O4	ENTERED	0.000000E+00	0.000000E+00
COCR2O4	ENTERED	0.000000E+00	0.000000E+00
CO3O4	ENTERED	0.000000E+00	0.000000E+00
BCC_A2	ENTERED	0.000000E+00	0.000000E+00
AQUEOUS	ENTERED	0.000000E+00	5.583623E+01
GAS	ENTERED	0.000000E+00	0.000000E+00

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SUSPENDED PHASES:
REF_ELECTRODE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
78 ITS, CPU TIME USED 0 SECONDS
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.11809565, MUR(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56976E+01, Mass in grams 1.00595E+03
Total Gibbs energy -1.70627E+07, Enthalpy -1.59010E+07, Volume -3.10120E-16

Component      Moles      M-Fraction  Activity    Potential  Ref.stat
H2O             5.5508E+01  9.9660E-01  9.9654E-01  -8.5924E+00 AQUEOUS
H+1            -5.2910E-02 -9.4995E-04  1.0000E-07  -3.9956E+04 SER
ZE             5.2936E-02  9.5042E-04  1.0000E+00  -4.4035E-12 REF_ELEC
NA             8.5554E-02  1.5360E-03  1.5537E-50  -2.8431E+05 SER
CL             8.5554E-02  1.5360E-03  1.2078E-30  -1.7077E+05 SER
FE             1.5041E-02  2.7005E-04  5.2232E-26  -1.4431E+05 SER
CR             1.9232E-03  3.4530E-05  1.2572E-53  -3.0196E+05 SER
NI             8.5193E-04  1.5296E-05  1.0073E-15  -8.5603E+04 SER
CO             1.6968E-04  3.0465E-06  1.5331E-20  -1.1310E+05 SER

AQUEOUS
Status ENTERED Driving force 0.0000E+00
Moles 5.5653E+01, Mass 1.0045E+03, Volume fraction 1.0000E+00 Mole fractions:
H2O 9.96925E-01 ZE 4.72606E-07 FE 1.08577E-11
CL 1.53727E-03 NI 2.36161E-07 CR 2.55062E-13
NA 1.53727E-03 CO 1.31447E-10 H+1 -2.25543E-10
Constitution:
SiteFraction      Molality      Activity      log10Act
H2O              9.96925E-01  5.55084E+01  9.96603E-01  -0.0015
CL-1            1.53727E-03  8.55948E-02  6.73703E-02  -1.1715
NA+1            1.53727E-03  8.55948E-02  6.73703E-02  -1.1715
NI+2            2.35950E-07  1.31376E-05  5.07139E-06  -5.2949
OH-1            2.28889E-09  1.27444E-07  1.00279E-07  -6.9988
H+1            2.27916E-09  1.26903E-07  1.00000E-07  -7.0000
NIOH+1          2.10599E-10  1.17261E-08  9.23842E-09  -8.0344
CO+2            1.31447E-10  7.31890E-09  2.82496E-09  -8.5490
FE+2            6.13590E-12  3.41645E-10  1.31278E-10  -9.8818
FEOH+1          4.72178E-12  2.62907E-10  2.07132E-10  -9.6838
CRO+1           2.23303E-13  1.24334E-11  9.79571E-12  -11.0090
CROH+2          2.36100E-14  1.31459E-12  5.06585E-13  -12.2953
HCRO2           8.03267E-15  4.47256E-13  4.47228E-13  -12.3495
CR+3            7.04094E-17  3.92037E-15  4.60120E-16  -15.3371
CRO2-1          4.58077E-17  2.55056E-15  2.00946E-15  -14.6969
H2              1.06307E-19  5.91913E-18  5.91876E-18  -17.2278
FEOH+2          4.31923E-20  2.40493E-18  9.26752E-19  -18.0330
O3              1.00000E-20  5.56796E-19  2.0474E-113  -112.6888
FEO3H3-1        1.00000E-20  5.56796E-19  1.76819E-51  -50.7525
FECL+2          1.00000E-20  5.56796E-19  2.94449E-23  -22.5310
FE2O2H2+4       1.00000E-20  5.56796E-19  3.71178E-35  -34.4304
FE+3            1.00000E-20  5.56796E-19  1.53750E-23  -22.8132
H2O2            1.00000E-20  5.56796E-19  3.35574E-46  -45.4742
HClO            1.00000E-20  5.56796E-19  2.84935E-45  -44.5453
CRO4-2          1.00000E-20  5.56796E-19  1.26903E-34  -33.8965
HClO2           1.00000E-20  5.56796E-19  1.02675E-87  -86.9885
HCRO4-1         1.00000E-20  5.56796E-19  3.83517E-35  -34.4162
CR2O7-2         1.00000E-20  5.56796E-19  5.34416E-68  -67.2721

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H02-1      1.00000E-20  5.56796E-19  7.10153E-51  -50.1486
CR+2       1.00000E-20  5.56796E-19  2.20654E-23  -22.6563
C01H2O2    1.00000E-20  5.56796E-19  2.7988E-105  -104.5530
CO+3       1.00000E-20  5.56796E-19  3.73219E-42  -41.4280
O2         1.00000E-20  5.56796E-19  2.17223E-58  -57.6631
CLO4-1     1.00000E-20  5.56796E-19  5.5717E-133  -132.2540
CLO3-1     1.00000E-20  5.56796E-19  1.0705E-105  -104.9704
CLO2-1     1.00000E-20  5.56796E-19  1.07460E-82  -81.9688
CLO2       1.00000E-20  5.56796E-19  1.1652E-100  -99.9336
CLO-1      1.00000E-20  5.56796E-19  6.17706E-46  -45.2092
CL2        1.00000E-20  5.56796E-19  4.04170E-50  -49.3934
Solution Properties:  pH = 7.0000  Eh = -0.0000 V  I = 0.0856
                    pe = -0.0000  Ah = -0.0000 kJ  m* = 0.1712
                    Aw = 0.9966  Os = 1.1033  pKw = 13.9973
                    At1= 1.0000E-20  At2= 1.2744E-07 (equiv_mol/kg_H2O)

HEMATITE           Status ENTERED      Driving force 0.0000E+00
Moles 3.3409E-02, Mass 1.0670E+00, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.20000E+00 NI 0.00000E+00 NA 0.00000E+00
H2O 6.00000E-01 CR 0.00000E+00 CO 0.00000E+00
FE 4.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00

NIFE2O4            Status ENTERED      Driving force 0.0000E+00
Moles 5.8715E-03, Mass 1.9660E-01, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.14286E+00 NI 1.42857E-01 NA 0.00000E+00
H2O 5.71429E-01 CR 0.00000E+00 CO 0.00000E+00
FE 2.85714E-01 CL 0.00000E+00 H+1 -1.14286E+00

CR2O3              Status ENTERED      Driving force 0.0000E+00
Moles 3.9597E-03, Mass 1.2037E-01, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.20000E+00 NI 0.00000E+00 NA 0.00000E+00
H2O 6.00000E-01 FE 0.00000E+00 CO 0.00000E+00
CR 4.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00

COCR2O4            Status ENTERED      Driving force 0.0000E+00
Moles 1.1877E-03, Mass 3.8504E-02, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.14286E+00 CO 1.42857E-01 NA 0.00000E+00
H2O 5.71429E-01 NI 0.00000E+00 FE 0.00000E+00
CR 2.85714E-01 CL 0.00000E+00 H+1 -1.14286E+00
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE              STATUS      DRIVING FORCE      MOLES
NIFE2O4            ENTERED      0.000000E+00      5.871536E-03
HEMATITE           ENTERED      0.000000E+00      3.340878E-02
CR2O3              ENTERED      0.000000E+00      3.959678E-03
COCR2O4            ENTERED      0.000000E+00      1.187738E-03
AQUEOUS            ENTERED      0.000000E+00      5.565313E+01
FE2O3              ENTERED      -1.007600E-01      0.000000E+00
FE2O2O2H2          ENTERED      -1.872978E-01      0.000000E+00
FEOOH              ENTERED      -2.260402E-01      0.000000E+00
COFE2O4            ENTERED      -8.149192E-01      0.000000E+00
FEO3H3             ENTERED      -1.157510E+00      0.000000E+00
NICR2O4            ENTERED      -1.415362E+00      0.000000E+00
FE2O3_GAMMA        ENTERED      -1.461433E+00      0.000000E+00
MAGNETITE          ENTERED      -1.556302E+00      0.000000E+00
NIO2H2             ENTERED      -3.146330E+00      0.000000E+00
NIO_S1             ENTERED      -4.159999E+00      0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.169527E+00
NIO_S2 HALITE COO2H2 FEO2H2 NA2CR2O4 NA2FEO2 CO3O4 WUSTITE COO_S2 CRO2
NA2CRO4_S1 NA2CRO4_S2 NIOOH CR5O12 NAOH_S1 NAOH_S2 CR8O21 CRO3 GAS NA2O2_S1
NA2O2_S2 NA2O_S1 NA2O_S2 NA2O_S3 NAO2 FCC_A1 BCC_A2
SUSPENDED PHASES:
REF ELECTRODE
POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.9467
N=55.697555
N(H2O)=55.508435, N(H+1)=-5.2909903E-2, N(ZE)=5.2936192E-2, N(NA)=8.5554E-2,
N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY:
POLY: @@ Save the workspace for the single-point equilibrium
POLY: @@ of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY:
POLY: save TCEX53_c.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continuePOLY:
POLY: @@ =====
POLY: @@ Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl
POLY: @@ =====
POLY:
POLY: @@ Define the mapping variables for Pourbaix diagram:
POLY: @@ pH from 0 to 14
POLY: @@ Eh from -1.2 to 1.5 (V)
POLY: s-a-v 1 lnacr(H+1) -32.22994 0 0.5
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 mur(Ze) -150000 200000 5000
... the command in full is SET_AXIS_VARIABLE
POLY: l-a-v
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: LNACR(H+1) Min: -32.22994 Max: 0 Inc: 0.5
Axis No 2: MUR(ZE) Min: -150000 Max: 200000 Inc: 5000
POLY:
POLY: @@ Add the starting points as initial equilibria:
POLY: @@ These may be enforced in 2 or 4 directions with
POLY: @@ the option >
POLY:
POLY: add 1>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -1>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add 2>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: @@ You can have more starting points at other pH-Eh
POLY: @@ conditions [corresponding to varied lnacr(H+1)
POLY: @@ and mur(Ze) values], and add them as initial equilibria.
POLY: @@ s-c lnacr(H+1)=-23.0
POLY: @@ s-c mur(ZE)=-2000
POLY: @@ l-c
POLY: @@ c-e

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POLY: @@ 1-e ,x
POLY:
POLY: li-in-eq
... the command in full is LIST INITIAL EQUILIBRIA
No 1 +1> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(Fe)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
No 2 -1> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(Fe)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
No 3 +2> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(Fe)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
No 4 -2> P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(Fe)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
POLY:
POLY: @@ Save the workspace for the Pourbaix diagram settings
POLY: @@ of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY: save TCEX53_d.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continuePOLY:
POLY: @@ Perform the mapping calculation:
POLY: @@ -----
POLY: @@ Due to the complexity of the aqueous solution model (SIT),
POLY: @@ a complete mapping calculation of the Pourbaix diagram
POLY: @@ may take a long time. Be patient...

POLY: @@ -----
POLY: MAP
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12

Phase region boundary 1 at: -1.541E+01 -4.404E-12
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
NIFE2O4
Calculated.. 35 equilibria
Terminating at axis limit.

Phase region boundary 2 at: -3.223E+01 -4.165E+04
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
NIFE2O4
Calculated. 38 equilibria

Phase region boundary 3 at: -1.404E+01 3.415E+03
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
** NIFE2O4

Phase region boundary 4 at: -1.404E+01 3.415E+03
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
Calculated. 7 equilibria

Phase region boundary 5 at: -1.110E+01 1.070E+04
AQUEOUS
** COCR2O4
CR2O3
** FECR2O4
HEMATITE

Phase region boundary 6 at: -1.110E+01 1.070E+04
AQUEOUS
CR2O3
** FECR2O4
HEMATITE
Calculated. 8 equilibria

Phase region boundary 7 at: -7.729E+00 1.905E+04
AQUEOUS
CR2O3
** FECR2O4
** HEMATITE

Phase region boundary 8 at: -7.729E+00 1.905E+04
AQUEOUS
CR2O3
** FECR2O4
Calculated. 9 equilibria

Phase region boundary 9 at: -7.729E+00 -1.955E+04
** GAS
AQUEOUS

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CR2O3
** FECR2O4

Phase region boundary 10 at: -7.729E+00 -1.955E+04
  GAS
  AQUEOUS
  CR2O3
  ** FECR2O4
Calculated.                4 equilibria

Phase region boundary 11 at: -7.169E+00 -1.817E+04
  GAS
  AQUEOUS
  ** CR2O3
  ** FECR2O4

Phase region boundary 12 at: -7.169E+00 -1.817E+04
  GAS
  AQUEOUS
  ** FECR2O4
Calculated                44 equilibria

Phase region boundary 13 at: -7.169E+00 -1.817E+04
  GAS
  AQUEOUS
  ** CR2O3
Calculated.                2 equilibria

Phase region boundary 14 at: -7.259E+00 -1.839E+04
  ** GAS
  AQUEOUS
  ** CR2O3

Phase region boundary 15 at: -7.259E+00 -1.839E+04
  AQUEOUS
  ** CR2O3
Calculated.                10 equilibria

Phase region boundary 16 at: -7.259E+00  2.259E+04
  AQUEOUS
  ** CR2O3
  ** HEMATITE

Phase region boundary 17 at: -7.259E+00  2.259E+04
  AQUEOUS
  ** CR2O3
  HEMATITE
Calculated.                32 equilibria

Phase region boundary 18 at: -1.110E+01  7.654E+04
  AQUEOUS
  ** COCR2O4
  ** CR2O3
  HEMATITE

Phase region boundary 19 at: -1.110E+01  7.654E+04
  AQUEOUS
  COCR2O4
  ** CR2O3
  HEMATITE
Calculated.                7 equilibria

Phase region boundary 20 at: -1.404E+01  6.628E+04
  AQUEOUS
  COCR2O4
  ** CR2O3
  HEMATITE
  ** NIFE2O4

Phase region boundary 21 at: -1.404E+01  6.628E+04
  AQUEOUS
  COCR2O4
  ** CR2O3
  HEMATITE
  NIFE2O4
Calculated..              38 equilibria
Terminating at axis limit.

Phase region boundary 22 at: -1.404E+01  6.628E+04
  AQUEOUS
  COCR2O4
  HEMATITE
  ** NIFE2O4
Calculated.                1 equilibria

Phase region boundary 23 at: -1.404E+01  6.733E+04
  AQUEOUS
  ** CO3O4
  COCR2O4
  HEMATITE
  ** NIFE2O4

Phase region boundary 24 at: -1.404E+01  6.733E+04
  AQUEOUS
  CO3O4
  COCR2O4
  HEMATITE
  ** NIFE2O4
Calculated.                2 equilibria

Phase region boundary 25 at: -1.404E+01  6.745E+04
  AQUEOUS
  CO3O4
  ** COCR2O4
  HEMATITE
  ** NIFE2O4

Phase region boundary 26 at: -1.404E+01  6.745E+04
  AQUEOUS
  CO3O4
  HEMATITE
  ** NIFE2O4
Calculated.                5 equilibria

Phase region boundary 27 at: -1.404E+01  8.332E+04
  ** GAS

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```

    AQUEOUS
    CO3O4
    HEMATITE
** NIFE2O4

Phase region boundary 28 at: -1.404E+01 8.332E+04
    GAS
    AQUEOUS
    CO3O4
    HEMATITE
** NIFE2O4
Calculated.                11 equilibria

Phase region boundary 29 at: -1.257E+01 8.794E+04
    GAS
    AQUEOUS
    CO3O4
** HALITE
    HEMATITE
** NIFE2O4

Phase region boundary 30 at: -1.257E+01 8.794E+04
    GAS
    AQUEOUS
    CO3O4
    HALITE
    HEMATITE
** NIFE2O4
Calculated                33 equilibria

Phase region boundary 31 at: -1.257E+01 8.794E+04
    GAS
    AQUEOUS
    CO3O4
** HALITE
    HEMATITE
Calculated.                9 equilibria

Phase region boundary 32 at: -8.749E+00 9.740E+04
    GAS
    AQUEOUS
** CO3O4
** HALITE
    HEMATITE

Phase region boundary 33 at: -8.749E+00 9.740E+04
    GAS
    AQUEOUS
** HALITE
    HEMATITE
Calculated.                18 equilibria

Phase region boundary 34 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
** HALITE
** HEMATITE

Phase region boundary 35 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
** HALITE
Calculated                44 equilibria

Phase region boundary 36 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
** HEMATITE
Calculated                5 equilibria

Phase region boundary 37 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
    HALITE
** HEMATITE
Calculated                27 equilibria

Phase region boundary 38 at: -8.749E+00 9.740E+04
    GAS
    AQUEOUS
** CO3O4
    HEMATITE
Calculated.                8 equilibria

Phase region boundary 39 at: -1.021E+01 9.281E+04
** GAS
    AQUEOUS
** CO3O4
    HEMATITE

Phase region boundary 40 at: -1.021E+01 9.281E+04
    AQUEOUS
** CO3O4
    HEMATITE
Calculated.                5 equilibria

Phase region boundary 41 at: -1.211E+01 7.398E+04
    AQUEOUS
** CO3O4
** COCR2O4
    HEMATITE

Phase region boundary 42 at: -1.211E+01 7.398E+04
    AQUEOUS
** CO3O4
    COCR2O4
    HEMATITE
Calculated.                5 equilibria
Terminating at known equilibrium

Phase region boundary 43 at: -1.211E+01 7.398E+04
    AQUEOUS
** COCR2O4
    HEMATITE
Calculated.                4 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 44 at: -1.211E+01 7.398E+04
  AQUEOUS
  CO3O4
  ** COCR2O4
  HEMATITE
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 45 at: -1.021E+01 9.281E+04
  ** GAS
  AQUEOUS
  HEMATITE
Calculated. 20 equilibria

Phase region boundary 46 at: -1.208E+00 1.151E+05
  ** GAS
  AQUEOUS
  ** HEMATITE
Calculated.. 4 equilibria
Terminating at axis limit.

Phase region boundary 47 at: -1.208E+00 1.151E+05
  ** GAS
  AQUEOUS
Calculated.. 4 equilibria
Terminating at axis limit.

Phase region boundary 48 at: -1.208E+00 1.151E+05
  AQUEOUS
  ** HEMATITE
Calculated. 28 equilibria
Terminating at known equilibrium

Phase region boundary 49 at: -1.208E+00 1.151E+05
  GAS
  AQUEOUS
  ** HEMATITE
Calculated 14 equilibria

Phase region boundary 50 at: -1.021E+01 9.281E+04
  ** GAS
  AQUEOUS
  CO3O4
  HEMATITE
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 51 at: -8.749E+00 9.740E+04
  GAS
  AQUEOUS
  ** CO3O4
  HALITE
  HEMATITE
Calculated 39 equilibria

Phase region boundary 52 at: -1.257E+01 8.794E+04
  GAS
  AQUEOUS
  CO3O4
  ** HALITE
  HEMATITE
  NIFE2O4
Calculated.. 41 equilibria
Terminating at axis limit.

Phase region boundary 53 at: -1.404E+01 8.332E+04
  ** GAS
  AQUEOUS
  CO3O4
  HEMATITE
  NIFE2O4
Calculated.. 38 equilibria
Terminating at axis limit.

Phase region boundary 54 at: -1.404E+01 6.745E+04
  AQUEOUS
  CO3O4
  ** COCR2O4
  HEMATITE
  NIFE2O4
Calculated. 27 equilibria

Phase region boundary 55 at: -2.249E+01 3.456E+04
  AQUEOUS
  CO3O4
  ** COCR2O4
  ** COFE2O4
  HEMATITE
  NIFE2O4

Phase region boundary 56 at: -2.249E+01 3.456E+04
  AQUEOUS
  CO3O4
  ** COCR2O4
  COFE2O4
  HEMATITE
  NIFE2O4
+++++

Phase region boundary 57 at: -2.249E+01 3.456E+04
  AQUEOUS
  CO3O4
  ** COFE2O4
  HEMATITE
  NIFE2O4
Calculated.. 21 equilibria
Terminating at axis limit.

Phase region boundary 58 at: -2.249E+01 3.456E+04
  AQUEOUS
  CO3O4
  COCR2O4
  ** COFE2O4
  HEMATITE
  NIFE2O4
Calculated. 2 equilibria

```

Phase region boundary 59 at: -2.239E+01 3.480E+04
 AQUEOUS
 ** CO3O4
 COCR2O4
 ** COFE2O4
 HEMATITE
 NIFE2O4

Phase region boundary 60 at: -2.239E+01 3.480E+04
 AQUEOUS
 COCR2O4
 ** COFE2O4
 HEMATITE
 NIFE2O4
 Calculated.. 21 equilibria
 Terminating at axis limit.

Phase region boundary 61 at: -2.239E+01 3.480E+04
 AQUEOUS
 ** CO3O4
 COCR2O4
 HEMATITE
 NIFE2O4
 Calculated. 18 equilibria
 Terminating at known equilibrium

Phase region boundary 62 at: -2.239E+01 3.480E+04
 AQUEOUS
 ** CO3O4
 COCR2O4
 COFE2O4
 HEMATITE
 NIFE2O4
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 63 at: -1.404E+01 6.628E+04
 AQUEOUS
 COCR2O4
 CR2O3
 HEMATITE
 ** NIFE2O4
 Calculated. 14 equilibria
 Terminating at known equilibrium

Phase region boundary 64 at: -1.110E+01 7.654E+04
 AQUEOUS
 ** COCR2O4
 CR2O3
 HEMATITE
 Calculated. 15 equilibria
 Terminating at known equilibrium

Phase region boundary 65 at: -7.259E+00 2.259E+04
 AQUEOUS
 CR2O3
 ** HEMATITE
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 66 at: -7.259E+00 -1.839E+04
 ** GAS
 AQUEOUS
 Calculated.. 16 equilibria
 Terminating at axis limit.

Phase region boundary 67 at: -7.259E+00 -1.839E+04
 ** GAS
 AQUEOUS
 CR2O3
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 68 at: -7.169E+00 -1.817E+04
 GAS
 AQUEOUS
 ** CR2O3
 FECCR2O4
 Calculated. 3 equilibria

Phase region boundary 69 at: -7.752E+00 -1.961E+04
 ** GAS
 AQUEOUS
 ** CR2O3
 FECCR2O4

Phase region boundary 70 at: -7.752E+00 -1.961E+04
 AQUEOUS
 ** CR2O3
 FECCR2O4
 Calculated. 9 equilibria

Phase region boundary 71 at: -7.752E+00 1.899E+04
 AQUEOUS
 ** CR2O3
 FECCR2O4
 ** HEMATITE

Phase region boundary 72 at: -7.752E+00 1.899E+04
 AQUEOUS
 ** CR2O3
 FECCR2O4
 HEMATITE
 Calculated. 8 equilibria
 Terminating at known equilibrium

Phase region boundary 73 at: -7.752E+00 1.899E+04
 AQUEOUS
 FECCR2O4
 ** HEMATITE
 Calculated. 16 equilibria

Phase region boundary 74 at: -1.286E+01 -1.893E+04
 AQUEOUS
 FECCR2O4
 ** HEMATITE

```

** MAGNETITE

Phase region boundary 75 at: -1.286E+01 -1.893E+04
  AQUEOUS
  FECR2O4
** HEMATITE
  MAGNETITE
Calculated.                4 equilibria

Phase region boundary 76 at: -1.395E+01 -2.164E+04
  AQUEOUS
** COFE2O4
  FECR2O4
** HEMATITE
  MAGNETITE

Phase region boundary 77 at: -1.395E+01 -2.164E+04
  AQUEOUS
  COFE2O4
  FECR2O4
** HEMATITE
  MAGNETITE
Calculated.                2 equilibria

Phase region boundary 78 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
** HEMATITE
  MAGNETITE
** NIFE2O4

Phase region boundary 79 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
** HEMATITE
  MAGNETITE
  NIFE2O4
Calculated..              38 equilibria
Terminating at axis limit.

Phase region boundary 80 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  MAGNETITE
** NIFE2O4
Calculated.                5 equilibria

Phase region boundary 81 at: -1.555E+01 -3.682E+04
  AQUEOUS
** BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
** NIFE2O4

Phase region boundary 82 at: -1.555E+01 -3.682E+04
  AQUEOUS
  BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
** NIFE2O4
Calculated..              35 equilibria
Terminating at axis limit.

Phase region boundary 83 at: -1.555E+01 -3.682E+04
  AQUEOUS
** BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
Calculated.                2 equilibria

Phase region boundary 84 at: -1.548E+01 -3.681E+04
  AQUEOUS
** BCC_A2
** COFE2O4
  FECR2O4
  MAGNETITE

Phase region boundary 85 at: -1.548E+01 -3.681E+04
  AQUEOUS
** BCC_A2
  FECR2O4
  MAGNETITE
Calculated.                4 equilibria

Phase region boundary 86 at: -1.473E+01 -3.690E+04
** GAS
  AQUEOUS
** BCC_A2
  FECR2O4
  MAGNETITE

Phase region boundary 87 at: -1.473E+01 -3.690E+04
  GAS
  AQUEOUS
** BCC_A2
  FECR2O4
  MAGNETITE
Calculated.                7 equilibria

Phase region boundary 88 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
** BCC_A2
  FECR2O4
** MAGNETITE

Phase region boundary 89 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
** BCC_A2

```

```

FECR2O4
Calculated.                8 equilibria

Phase region boundary 90 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  ** BCC_A2
  FECR2O4
  ** HALITE

Phase region boundary 91 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  ** BCC_A2
  FECR2O4
  HALITE
Calculated                201 equilibria

Phase region boundary 92 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  FECR2O4
  ** HALITE
Calculated.                14 equilibria

Phase region boundary 93 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
  ** FECR2O4
  ** HALITE

Phase region boundary 94 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
  ** HALITE
Calculated..                16 equilibria
Terminating at axis limit.

Phase region boundary 95 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
  ** FECR2O4
+
++

Phase region boundary 96 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
  ** FECR2O4
  HALITE
Calculated                72 equilibria

Phase region boundary 97 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  BCC_A2
  FECR2O4
  ** HALITE
Calculated.                6 equilibria

Phase region boundary 98 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECR2O4
  ** HALITE
  ** MAGNETITE

Phase region boundary 99 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECR2O4
  ** HALITE
  MAGNETITE
Calculated..                38 equilibria
Terminating at axis limit.

Phase region boundary 100 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECR2O4
  ** MAGNETITE
+
++

Phase region boundary 101 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECR2O4
  HALITE
  ** MAGNETITE
Calculated                61 equilibria

Phase region boundary 102 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
  FECR2O4
  ** MAGNETITE
Calculated.                3 equilibria

Phase region boundary 103 at: -1.472E+01 -3.688E+04
  ** GAS
  AQUEOUS
  FECR2O4
  ** MAGNETITE

Phase region boundary 104 at: -1.472E+01 -3.688E+04
  AQUEOUS
  FECR2O4
  ** MAGNETITE
Calculated.                5 equilibria
Terminating at known equilibrium

Phase region boundary 105 at: -1.472E+01 -3.688E+04
  ** GAS

```



```

    AQUEOUS
    FECR204
    Calculated.          15  equilibria
    Terminating at known equilibrium

Phase region boundary 106 at:  -1.472E+01 -3.688E+04
** GAS
    AQUEOUS
    FECR204
    MAGNETITE
    Calculated.          2  equilibria
    Terminating at known equilibrium

Phase region boundary 107 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR204
    ** MAGNETITE
    Calculated          46  equilibria

Phase region boundary 108 at:  -1.473E+01 -3.690E+04
** GAS
    AQUEOUS
    BCC_A2
    FECR204
    MAGNETITE
    Calculated..        38  equilibria
    Terminating at axis limit.

Phase region boundary 109 at:  -1.548E+01 -3.681E+04
    AQUEOUS
    ** COFE204
    FECR204
    MAGNETITE
    Calculated.          5  equilibria
    Terminating at known equilibrium

Phase region boundary 110 at:  -1.548E+01 -3.681E+04
    AQUEOUS
    BCC_A2
    ** COFE204
    FECR204
    MAGNETITE
    Calculated..        37  equilibria
    Terminating at axis limit.

Phase region boundary 111 at:  -1.555E+01 -3.682E+04
    AQUEOUS
    ** BCC_A2
    COFE204
    FECR204
    MAGNETITE
    NIFE204
    Calculated..        35  equilibria
    Terminating at known equilibrium
    Terminating at axis limit.

Phase region boundary 112 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE204
    FECR204
    HEMATITE
    MAGNETITE
    ** NIFE204
    Calculated.          1  equilibria

Phase region boundary 113 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE204
    FECR204
    HEMATITE
    ** MAGNETITE
    ** NIFE204

Phase region boundary 114 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE204
    FECR204
    HEMATITE
    ** NIFE204
    Calculated.          4  equilibria

Phase region boundary 115 at:  -1.404E+01 -1.073E+04
    AQUEOUS
    ** COCR204
    COFE204
    FECR204
    HEMATITE
    ** NIFE204

Phase region boundary 116 at:  -1.404E+01 -1.073E+04
    AQUEOUS
    COCR204
    COFE204
    FECR204
    HEMATITE
    ** NIFE204
    Calculated.          1  equilibria
    Terminating at known equilibrium

Phase region boundary 117 at:  -1.404E+01 -1.073E+04
    AQUEOUS
    ** COCR204
    COFE204
    FECR204
    HEMATITE
    Calculated.          2  equilibria

Phase region boundary 118 at:  -1.395E+01 -1.051E+04
    AQUEOUS
    ** COCR204
    ** COFE204
    FECR204
    HEMATITE

```

Phase region boundary 119 at: -1.395E+01 -1.051E+04
 AQUEOUS
 ** COCR2O4
 FECR2O4
 HEMATITE
 Calculated. 7 equilibria
 Terminating at known equilibrium

Phase region boundary 120 at: -1.395E+01 -1.051E+04
 AQUEOUS
 ** COFE2O4
 FECR2O4
 HEMATITE
 Calculated. 3 equilibria

Phase region boundary 121 at: -1.395E+01 -2.164E+04
 AQUEOUS
 ** COFE2O4
 FECR2O4
 HEMATITE
 ** MAGNETITE

Phase region boundary 122 at: -1.395E+01 -2.164E+04
 AQUEOUS
 ** COFE2O4
 FECR2O4
 HEMATITE
 MAGNETITE
 Calculated. 1 equilibria
 Terminating at known equilibrium

Phase region boundary 123 at: -1.395E+01 -2.164E+04
 AQUEOUS
 FECR2O4
 HEMATITE
 ** MAGNETITE
 Calculated. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 124 at: -1.395E+01 -2.164E+04
 AQUEOUS
 COFE2O4
 FECR2O4
 HEMATITE
 ** MAGNETITE
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 125 at: -1.395E+01 -1.051E+04
 AQUEOUS
 COCR2O4
 ** COFE2O4
 FECR2O4
 HEMATITE
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 126 at: -1.404E+01 -1.073E+04
 AQUEOUS
 ** COCR2O4
 COFE2O4
 FECR2O4
 HEMATITE
 NIFE2O4
 Calculated.. 38 equilibria
 Terminating at axis limit.

Phase region boundary 127 at: -1.404E+01 -2.186E+04
 AQUEOUS
 COFE2O4
 FECR2O4
 HEMATITE
 ** MAGNETITE
 NIFE2O4
 Calculated.. 38 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 128 at: -7.752E+00 1.899E+04
 AQUEOUS
 CR2O3
 FECR2O4
 ** HEMATITE
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 129 at: -7.752E+00 -1.961E+04
 ** GAS
 AQUEOUS
 CR2O3
 FECR2O4
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 130 at: -1.110E+01 1.070E+04
 AQUEOUS
 ** COCR2O4
 CR2O3
 FECR2O4
 HEMATITE
 Calculated. 1 equilibria
 Terminating at known equilibrium

Phase region boundary 131 at: -1.404E+01 3.415E+03
 AQUEOUS
 COCR2O4
 CR2O3
 FECR2O4
 HEMATITE
 ** NIFE2O4
 Calculated. 1 equilibria
 Terminating at known equilibrium

Phase region boundary 132 at: -1.541E+01 -4.404E-12
 AQUEOUS
 COCR2O4

```

    CR2O3
** FECR2O4
  HEMATITE
  NIFE2O4
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 133 at:  -3.020E+01 -4.404E-12
  AQUEOUS
  COCR2O4
** CR2O3
  HEMATITE
  NIFE2O4
Calculated..          9 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 134 at:  -3.020E+01 -4.404E-12
  AQUEOUS
  COCR2O4
** CR2O3
  HEMATITE
  NIFE2O4
Calculated.          54 equilibria
Terminating at known equilibrium

Phase region boundary 135 at:  -1.610E+01  5.964E+04
  AQUEOUS
** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.          21 equilibria
Terminating at known equilibrium

Phase region boundary 136 at:  -1.610E+01  5.964E+04
  AQUEOUS
** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.          7 equilibria
Terminating at known equilibrium

Phase region boundary 137 at:  -1.612E+01  5.959E+04
  AQUEOUS
** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 138 at:  -1.612E+01  5.959E+04
  AQUEOUS
** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 139 at:  -1.612E+01  5.825E+04
  AQUEOUS
  COCR2O4
** CR2O3
  HEMATITE
  NIFE2O4
Calculated..          34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 140 at:  -1.612E+01  5.825E+04
  AQUEOUS
  COCR2O4
** CR2O3
  HEMATITE
  NIFE2O4
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 141 at:  -1.612E+01 -1.748E+03
  AQUEOUS
  COCR2O4
  CR2O3
** FECR2O4
  HEMATITE
  NIFE2O4
Calculated..          34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 142 at:  -1.612E+01 -1.748E+03
  AQUEOUS
  COCR2O4
  CR2O3
** FECR2O4
  HEMATITE
  NIFE2O4
Calculated.          6 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex53\TCEx53_d.POLY3
CPU time for mapping          1069 seconds

POLY:
POLY: @@ Plot the calculated Pourbaix diagram (and others):
POLY: @@ -----
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: l-sym
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
  AH2O=55.508435, RNF=96485.309, ZERO=0
DEFINED FUNCTIONS AND VARIABLES%

```

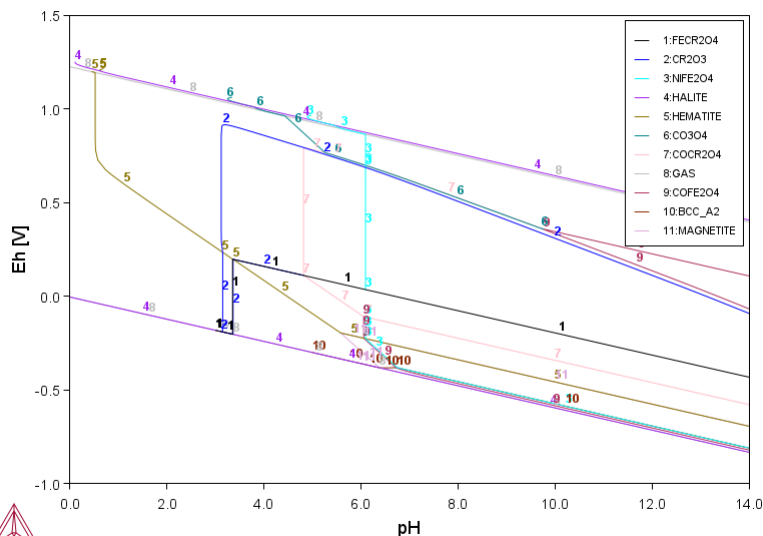
```

EH=MUR(ZE)/RNF
PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
TEMP_C=T-273.15
POST:Hit RETURN to continuePOST:

POST: s-d-a x pH
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n pH
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-d-a y Eh
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text y n Eh [V]
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-t-m-s y
... the command in full is SET_TRUE_MANUAL_SCALING
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-l-c e
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: s-s-s x n 0 14
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n -1.0 1.5
... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-a
... the command in full is SET_TITLE
POST: pl,,,
... the command in full is PLOT DIAGRAM

```

Thermo-Calc Example 53-a

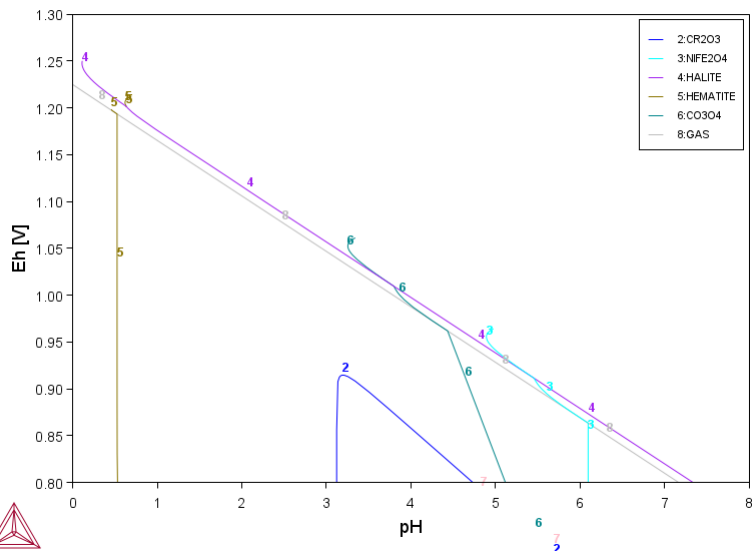


```

POST: make TCEX53.EXP y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST:
POST:
POST: sel-pl new
... the command in full is SELECT_PLOT
POST:
POST: s-s-s x n 0 8
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n .8 1.3
... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-b
... the command in full is SET_TITLE
POST:
POST: pl,,,
... the command in full is PLOT DIAGRAM

```

Thermo-Calc Example 53-b



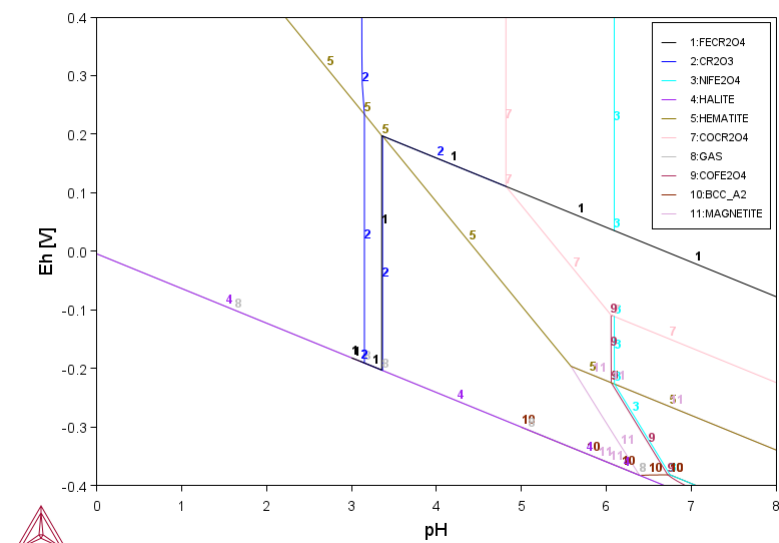
```

POST:Hit RETURN to continue
POST:

```

```
POST: sel-pl new
... the command in full is SELECT_PLOT
POST:
POST: s-s-s y n -.4 .4
... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-c
... the command in full is SET_TITLE
POST:
POST: pl,,,
... the command in full is PLOT_DIAGRAM
```

Thermo-Calc Example 53-c



```
POST:Hit RETURN to continue
POST:
POST:
POST: @@ -----
POST: @@ From the same mapping calculations, you can plot more
POST: @@ diagrams, using different X-Y axis variables (for such
POST: @@ purposes, it is convenient to use pre-defined symbols as
POST: @@ listed at the end of this macro file).
POST: @@ -----
POST:
POST: SET-INTERACTIVE
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex54

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex54\tcex54.TCM.test"

SYS: SET_ECHO

SYS:

SYS: @@ Simulating the solidification of a Al-2.1Cu-1Si alloy

SYS: @@ with a Scheil calculation including back diffusion

SYS:

SYS: @@ This is an example of a solidification simulation

SYS: @@ of a Al-2.1Cu-1Si alloy. The back diffusion option

SYS: @@ in the Scheil module is used, i.e. there is back

SYS: @@ diffusion in the primary phase, which is FCC_A1.

SYS:

SYS: GO SCHEIL

SCHEIL: USE-BACK-DIFFUSION YES

SCHEIL: START-WIZARD

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: ALDEMO

Current database: Aluminum Demo Database v5.0

VA /- DEFINED

Major element or alloy: AL

Composition input in mass (weight) percent? /Y/: N

Composition will be taken to be in mole percent

1st alloying element: CU

Mole percent /1/: 2.1

2nd alloying element: SI

Mole percent /1/: 1.0

Next alloying element:

Temperature (C) /2000/: 1000

VA /- DEFINED

REINITIATING GES

AL DEFINED

CU DEFINED

SI DEFINED

This database has following phases for the defined system

LIQUID:L	AL2CU_C16	ALCU_DEL
ALCU_EPS	ALCU_ETA	ALCU_ZETA
ALZR2_B82	BCC_A2	BCC_B2
C14_LAVES	C15_LAVES	C36_LAVES
CU15SI4_EPSILON	CU33SI7_DELTA	CU56SI11_GAMMA
CUSI_ETA	DIAMOND_A4	FCC_A1
GAMMA_D83	GAMMA_H	HCP_A3

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

LIQUID:L	AL2CU_C16	ALCU_DEL
ALCU_EPS	ALCU_ETA	ALCU_ZETA
ALZR2_B82	BCC_A2	BCC_B2
C14_LAVES	C15_LAVES	C36_LAVES
CU15SI4_EPSILON	CU33SI7_DELTA	CU56SI11_GAMMA
CUSI_ETA	DIAMOND_A4	FCC_A1
GAMMA_D83	GAMMA_H	HCP_A3

.....

OK? /Y/: Y

10:15:05,667 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

Mobility Database /MALDEMO/: MALDEMO

Current database: Al-Alloys Mobility demo database v3.0

VA /- DEFINED

AL DEFINED

CU DEFINED

SI DEFINED

This database has following phases for the defined system

LIQUID:L FCC_A1

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

```

LIQUID:L          FCC_A1
.....

OK? /Y/: Y
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

Use the command LIST_REFERENCES to see the list of references for assessed data

INFO: Forcing option USE_POLY3 for complex phase ALZR2_B82
INFO: Forcing option USE_POLY3 for complex phase BCC_A2
-OK-
Should any phase have a miscibility gap check? /N/: N
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/: NONE
Temperature time dependence /LINEAR/: LINEAR
Cooling rate (K/s) /1/: 0.1
Expression for secondary dendrite arm spacing /CONSTANT/: POWER_LAW
  Power law in the form c*(cooling rate)^-n
Exponent n /.33/: 0.33
Scaling factor c /5E-05/: 5.0E-5
Secondary dendrite arm spacing 0.1069E-03 m
Primary phase /AUTOMATIC/: AUTOMATIC
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=1273.15, X(CU)=2.1E-2, X(SI)=1E-2, P=100000, N=1   DEGREES OF FREEDOM 0
PHASE CHANGE AT 914.742752934
FCC_A1#1 forms
  Testing POLY result by global minimization procedure
Calculated      17676 grid points in      0.062 s
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

Phase Region from    914.833      for:
  LIQUID
Terminating at      914.933
Calculated      4 equilibria

Phase Region from    914.833      for:
  LIQUID
Global check of adding phase at 9.14743E+02
Calculated      3 equilibria

Phase Region from    914.743      for:
  LIQUID
  FCC_A1
Global test at 9.06833E+02 .... OK
Global test at 8.96833E+02 .... OK
Global test at 8.86833E+02 .... OK
Global test at 8.76833E+02 .... OK
Global test at 8.66833E+02 .... OK
Global test at 8.56833E+02 .... OK
Global test at 8.46833E+02 .... OK
Global test at 8.36833E+02 .... OK
Global test at 8.26833E+02 .... OK
Global test at 8.16833E+02 .... OK
Global test at 8.06833E+02 .... OK
Global test at 7.96833E+02 .... OK
Global check of removing phase at 7.94498E+02
Backtracking to find phase change for DIAMOND_A4#1
Global test at 7.95833E+02 .... OK
Global check of adding phase at 7.95274E+02
Calculated      123 equilibria

Phase Region from    795.274      for:
  LIQUID
  DIAMOND_A4
  FCC_A1
Global Check of removing phase at 7.94976E+02
Calculated      3 equilibria

Phase Region from    794.976      for:
  DIAMOND_A4
  FCC_A1
Calculated      4 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_3412.POLY3
  POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

  POSTPROCESSOR VERSION 3.2

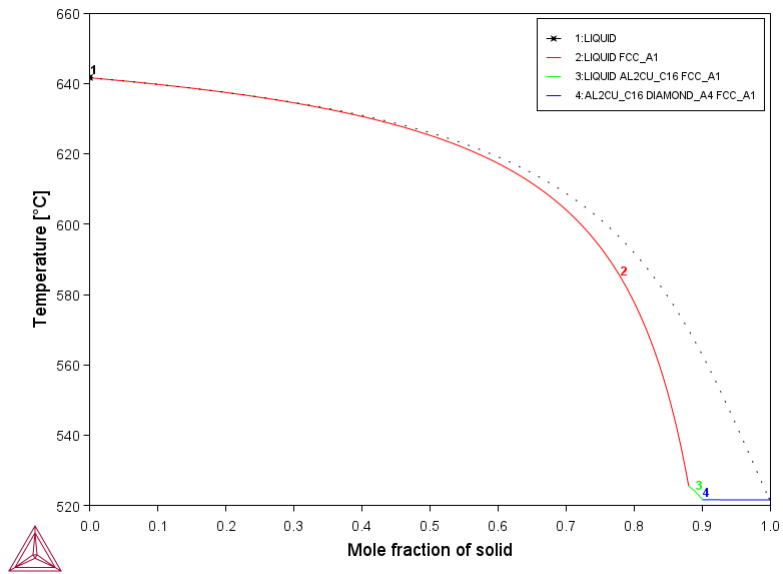
Setting automatic diagram axes

An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_3412.EXP
has been created to store the equilibrium solidification results.
  CALCULATING SCHEIL SOLIDIFICATION
FCC_A1#1 set as the primary phase
  T(C)      fraction solid
641.6828      0.000000
PHASE REGION:LIQUID + FCC_A1
  T(C)      fraction solid
641.5871      0.3328777E-03
640.5871      0.5644985E-01
639.5871      0.1068990
638.5871      0.1524203
637.5871      0.1936891
636.5871      0.2312634
635.5871      0.2656089
634.5871      0.2971165
633.5871      0.3261172
632.5871      0.3528931
631.5871      0.3776855
630.5871      0.4007028
629.5871      0.4221253
628.5871      0.4421098
627.5871      0.4607936
626.5871      0.4782973
625.5871      0.4947270

```

624.5871	0.5101768
623.5871	0.5247302
622.5871	0.5384614
621.5871	0.5514369
620.5871	0.5637164
619.5871	0.5753534
618.5871	0.5863962
617.5871	0.5968883
616.5871	0.6068692
615.5871	0.6163750
614.5871	0.6254381
613.5871	0.6340883
612.5871	0.6423528
611.5871	0.6502565
610.5871	0.6578222
609.5871	0.6650708
608.5871	0.6720217
607.5871	0.6786925
606.5871	0.6850998
605.5871	0.6912587
604.5871	0.6971832
603.5871	0.7028862
602.5871	0.7083800
601.5871	0.7136758
600.5871	0.7187839
599.5871	0.7237142
598.5871	0.7284756
597.5871	0.7330767
596.5871	0.7375255
595.5871	0.7418293
594.5871	0.7459950
593.5871	0.7500293
592.5871	0.7539382
591.5871	0.7577275
590.5871	0.7614025
589.5871	0.7649684
588.5871	0.7684300
587.5871	0.7717917
586.5871	0.7750579
585.5871	0.7782325
584.5871	0.7813194
583.5871	0.7843221
582.5871	0.7872441
581.5871	0.7900886
580.5871	0.7928587
579.5871	0.7955571
578.5871	0.7981867
577.5871	0.8007502
576.5871	0.8032499
575.5871	0.8056882
574.5871	0.8080674
573.5871	0.8103896
572.5871	0.8126569
571.5871	0.8148712
570.5871	0.8170342
569.5871	0.8191479
568.5871	0.8212138
567.5871	0.8232336
566.5871	0.8252089
565.5871	0.8271410
564.5871	0.8290314
563.5871	0.8308815
562.5871	0.8326925
561.5871	0.8344656
560.5871	0.8362021
559.5871	0.8379030
558.5871	0.8395695
557.5871	0.8412027
556.5871	0.8428034
555.5871	0.8443727
554.5871	0.8459114
553.5871	0.8474206
552.5871	0.8489010
551.5871	0.8503534
550.5871	0.8517787
549.5871	0.8531777
548.5871	0.8545509
547.5871	0.8558993
546.5871	0.8572233
545.5871	0.8585238
544.5871	0.8598013
543.5871	0.8610565
542.5871	0.8622899
541.5871	0.8635022
540.5871	0.8646938
539.5871	0.8658653
538.5871	0.8670172
537.5871	0.8681501
536.5871	0.8692644
535.5871	0.8703605
534.5871	0.8714391
533.5871	0.8725004
532.5871	0.8735449
531.5871	0.8745730
530.5871	0.8755852
529.5871	0.8765818
528.5871	0.8775632
527.5871	0.8785298
526.5871	0.8794819
525.7265	0.8802109
PHASE REGION:LIQUID + AL2CU_C16 + FCC_A1	
T(C)	fraction solid
525.6946	0.8803189
524.6946	0.8861368
523.6946	0.8914905
522.6946	0.8963827
521.6946	0.9008701
521.6628	0.9010006
PHASE REGION:AL2CU_C16 + DIAMOND_A4 + FCC_A1	
T(C)	fraction solid
521.6309	1.000000

Calculating properties ...
Liquidus temperature: 914.743 K
Solidus temperature: 794.781 K



.....

The following axis variables are available

T - Temperature in Celsius

NL/BL/VL - Mole/mass/volume fraction of liquid

NS/BS/VS - Mole/mass/volume fraction of all solid phases

NS(ph)/BS(ph) - Mole/mass fraction of a solid phase

VS(ph) - Volume fraction of a solid phase

W(ph,el) - Weight fraction of an element in a phase

X(ph,el) - Mole fraction of an element in a phase

Y(ph,el) - Site fraction of an element in a phase

NN(ph,el) - Distribution of an element in a phase

NH/BH - Heat release and Latent heat per mole/gram

CP/BCP - Apparent heat capacity per mole/gram

NV/NV(ph) - Molar volume of the system or a phase

DS/DS(ph) - Average density of the system or a phase

BT - Apparent volumetric TEC of the system

DVIS(ph) - Dynamic viscosity of a phase

KVIS(ph) - Kinematic viscosity of a phase

SURF(ph) - Surface tension of a liquid phase

ELRS/ELRS(ph) - Electrical resistivity of the system or a phase

ELCD/ELCD(ph) - Electrical conductivity of the system or a phase

THCD/THCD(ph) - Thermal conductivity of the system or a phase

THRS/THRS(ph) - Thermal resistivity of the system or a phase

THDF/THDF(ph) - Thermal diffusivity of the system or a phase

DGV - Driving force for evaporation

DHV - Evaporation enthalpy

MMG - Molar mass of gas

XAVG(el) - Mole fraction of an element in solid phases

WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively

"*" can be used as a wild character for "el" and "ph"

.....

POST:

POST: BACK

SCHEIL: SET-INTER

--OK---

SCHEIL:

tcex55

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex55\tcex55.TCM.test"

SYS:

SYS: @@ Plotting viscosity of Cr-Ni at 1873 K

SYS:

SYS: @@ Plotting viscosity of Cr-Ni at 1873 K

SYS: @@ The example includes an experimental

SYS: @@ data (*.exp) file called Cr-Ni_1873K.exp.

SYS:

SYS:

SYS: set-echo

SYS:

SYS: go da

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw FEDEMO

Current database: Iron Demo Database v6.0

VA /- DEFINED

TDB_FEDEMO: def-system ni cr

NI CR DEFINED

TDB_FEDEMO: reject-phase *

GAS:G	LIQUID:L	BCC_A2
C14 LAVES	CBCC_A12	CHI_A12
CUB_A13	FCC_A1	HCP_A3

SIGMA_D8B REJECTED

TDB_FEDEMO: restore-phase liquid

LIQUID:L RESTORED

TDB_FEDEMO: get

10:16:35,374 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_FEDEMO:

TDB_FEDEMO: go poly

POLY version 3.32

POLY: s-c t=1873 n=1 p=1e5 x(ni)=.2

POLY: c-e

Using global minimization procedure

Calculated 209 grid points in 0.164 s

Found the set of lowest grid points in 0.000 s

Calculated POLY solution 0.076 s, total time 0.240 s

POLY: s-a-v 1 x(ni) 0 1 ,,

POLY: step sep

Phase Region from 0.502463 for:
LIQUID

Phase Region from 0.502463 for:
LIQUID

*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST: ent-sym fun Dyn_visc_mPa_s=DVIS(liquid)*1000;

POST: s-d-a y Dyn_visc_mPa_s

POST: s-d-a x m-f ni

POST:

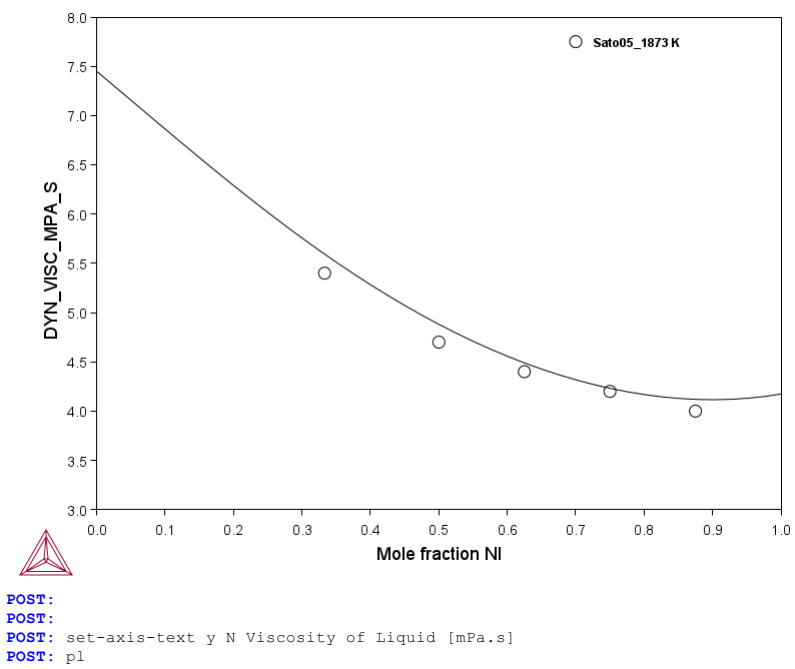
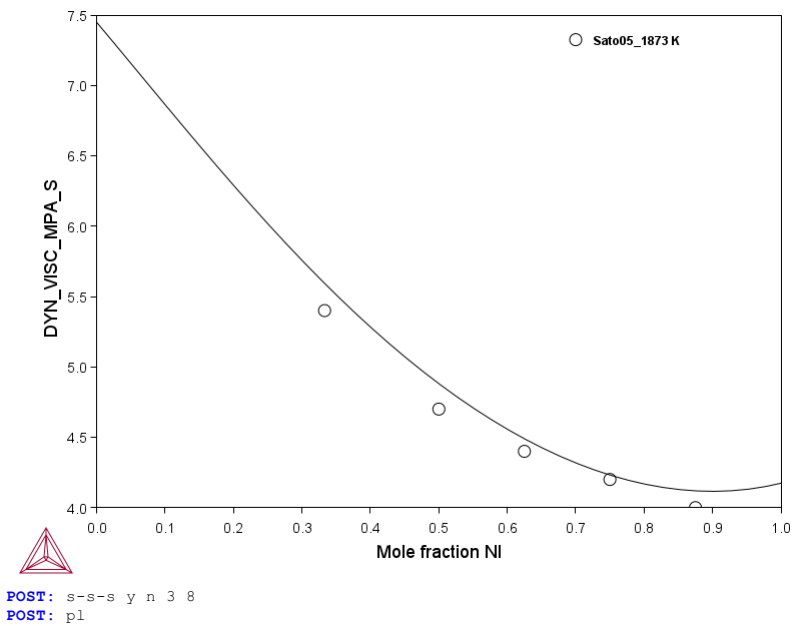
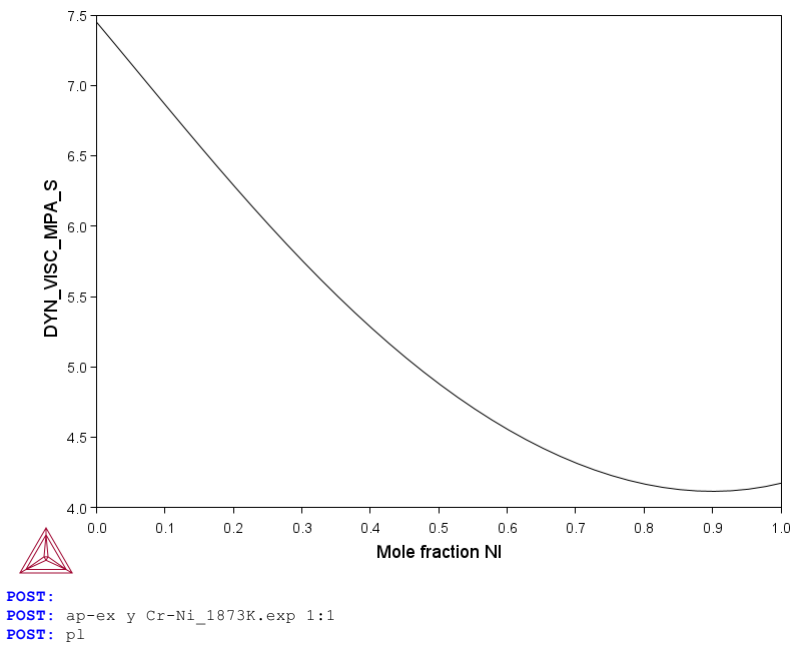
POST: SET_EXP_FILE_FORMAT 5

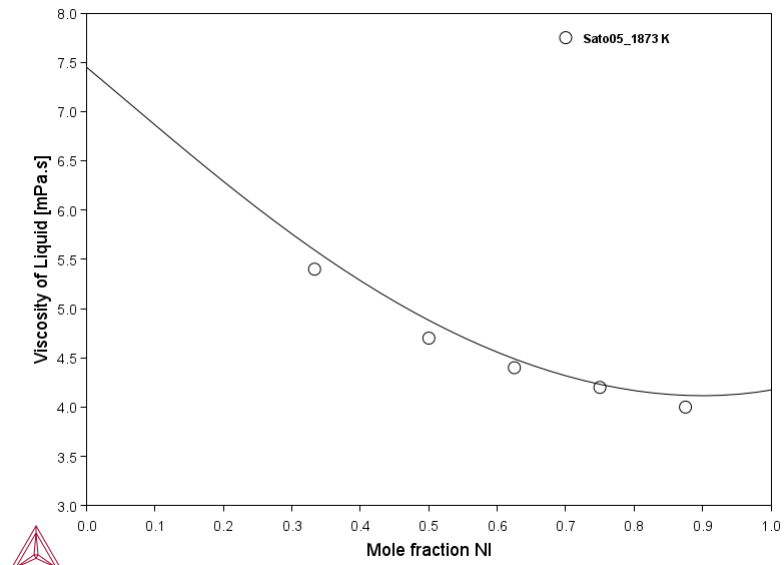
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot





POST:
POST: set-inter
POST:

tcex56

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex56\tcex56.TCM.test"

SYS: @@ Plotting Surface Tension of Cu-Zr at 1373 K

SYS:

SYS: @@ Plotting Surface Tension of Cu-Zr at 1373 K. The

SYS: @@ example includes an experimental data (*.exp) file

SYS: @@ called Cr-Zr_ALDEMO.exp.

SYS:

SYS: set-echo

SYS:

SYS: go data

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw aldemo

Current database: Aluminum Demo Database v5.0

VA /- DEFINED

TDB_ALDEMO:

TDB_ALDEMO: de-system cu zr

CU ZR DEFINED

TDB_ALDEMO: rej-phase *

LIQUID:L	AL2CU_C16	ALCU_EPS
ALCU_ETA	ALZR2_B82	BCC_A2
BCC_B2	C14_LAVES	C15_LAVES
C36_LAVES	FCC_A1	HCP_A3
REJECTED		

TDB_ALDEMO: res-phase liquid

LIQUID:L RESTORED

TDB_ALDEMO: get

10:18:44,784 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_ALDEMO:

TDB_ALDEMO: go poly

POLY version 3.32

POLY: s-c t=1373 n=1 p=1e5 x(zr)=.2

POLY: c-e

Using global minimization procedure

Calculated 209 grid points in 0.153 s

Found the set of lowest grid points in 0.001 s

Calculated POLY solution 0.074 s, total time 0.228 s

POLY:

POLY: set-axis-var 1 x(zr) 0 1 ,,

POLY: step sep

Phase Region from 0.502463 for:
LIQUID

Phase Region from 0.502463 for:
LIQUID

*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

POLY:

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST: set-diagram-axis y surf(liq)

POST: set-diagram-axis x m-f zr

POST:

POST: ap-exp y Cu-Zr_ALDEMO.exp 1:1

POST:

POST:

POST: set-axis

Ambiguous command use HELP

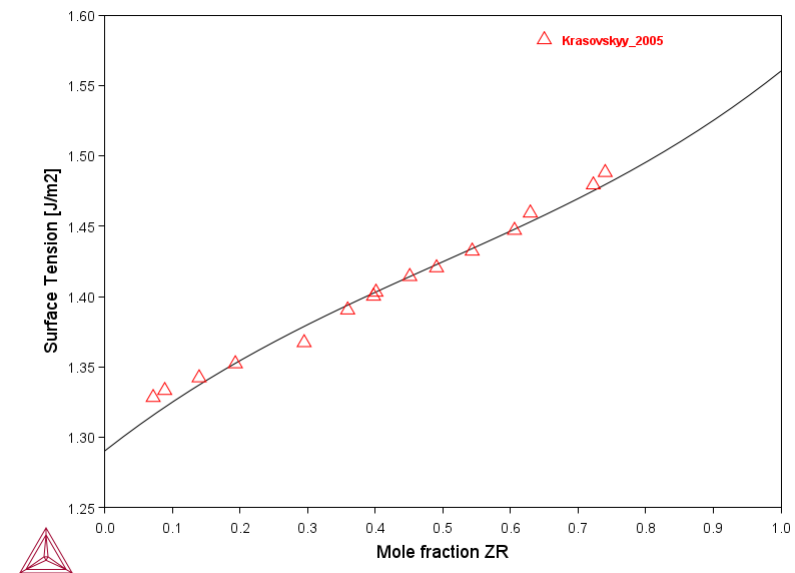
POST: set-axis-te

AXIS (X, Y OR Z) : y

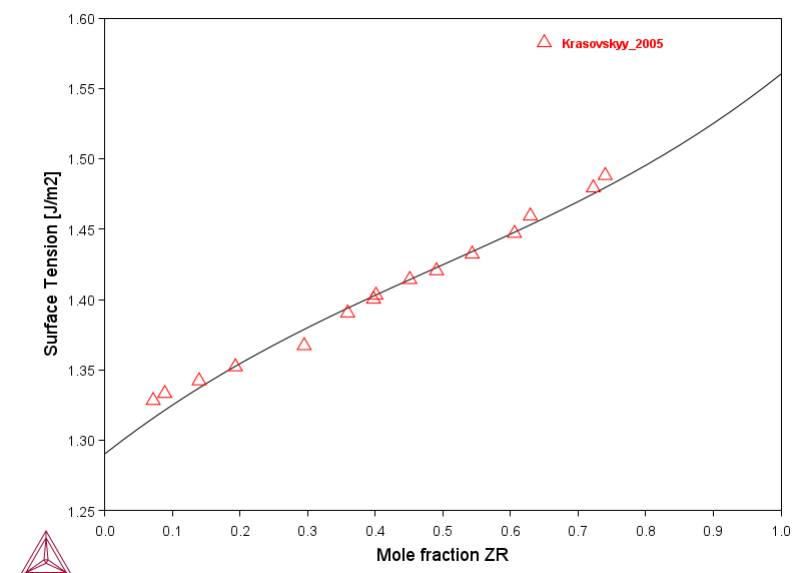
AUTOMATIC AXIS TEXT (Y OR N) /N/: N

AXIS TEXT : Surface Tension [J/m2]

POST: pl



```
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST: plot
```



```
POST:
POST: set-inter
POST:
```

tcex57

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex57\tcex57.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a Scheil with Solute Trapping Solidification in a Al-Si-Cu system

SYS:

SYS: set-log ex57,,,

SYS:

SYS: go scheil

... the command in full is GOTO_MODULE

SCHEIL:

SCHEIL: SOLUTE_TRAPPING Y

SCHEIL:

SCHEIL: start

... the command in full is START_WIZARD

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: ALDEMO

Current database: Aluminum Demo Database v5.0

VA /- DEFINED

Major element or alloy: al

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: si

Mass (weight) percent /1/: 7.5

2nd alloying element: cu

Mass (weight) percent /1/: 0.2

Next alloying element:

Temperature (C) /2000/: 2500

VA /- DEFINED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

AL DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

CU DEFINED

This database has following phases for the defined system

LIQUID:L	AL2CU_C16	ALCU_DEL
ALCU_EPS	ALCU_ETA	ALCU_ZETA
ALZR2_B82	BCC_A2	BCC_B2
C14_LAVES	C15_LAVES	C36_LAVES
CU15SI4_EPSILON	CU33SI7_DELTA	CU56SI11_GAMMA
CUSI_ETA	DIAMOND_A4	FCC_A1
GAMMA_D83	GAMMA_H	HCP_A3

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

LIQUID:L	AL2CU_C16	ALCU_DEL
ALCU_EPS	ALCU_ETA	ALCU_ZETA
ALZR2_B82	BCC_A2	BCC_B2
C14_LAVES	C15_LAVES	C36_LAVES
CU15SI4_EPSILON	CU33SI7_DELTA	CU56SI11_GAMMA
CUSI_ETA	DIAMOND_A4	FCC_A1
GAMMA_D83	GAMMA_H	HCP_A3

.....

OK? /Y/: Y

10:20:09,473 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

Should any phase have a miscibility gap check? /N/: N

LIQUID PHASE NAME: LIQUID

Expression for solidification speed /SCANNING_SPEED_AND_ANGLE/: SCANNING_SPEED_AND_ANGLE

Solidification speed (m/s) is calculated as $\dot{V} = (\text{scanning speed}) * \cos(\alpha)$

Scanning speed (m/s) /1/: 1

Alpha (degrees) /45/: 45

Solidification speed 0.7071 m/s

Primary phase /AUTOMATIC/: AUTOMATIC

... the command in full is COMPUTE_TRANSITION

This command is a combination of CHANGE_STATUS and SET_CONDITION

to calculate directly when a phase may form by releasing one condition.

You must release one of these conditions

T=2773.15, W(SI)=7.5E-2, W(CU)=2E-3, P=100000, N=1 DEGREES OF FREEDOM 0

PHASE CHANGE AT 885.72250905

FCC_A1#1 forms

Testing POLY result by global minimization procedure

Calculated 17676 grid points in 0.062 s

```

CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
... the command in full is ADD_INITIAL_EQUILIBRIUM
... the command in full is ENTER_SYMBOL
... the command in full is ADVANCED_OPTIONS
... the command in full is STEP_WITH_OPTIONS
...OK

Phase Region from      885.813      for:
LIQUID
Terminating at      885.913
Calculated      4 equilibria

Phase Region from      885.813      for:
LIQUID
Global check of adding phase at      8.85723E+02
Calculated      3 equilibria

Phase Region from      885.723      for:
LIQUID
FCC_A1
Global test at      8.77813E+02 .... OK
Global test at      8.67813E+02 .... OK
Global test at      8.57813E+02 .... OK
Global check of adding phase at      8.49559E+02
Calculated      39 equilibria

Phase Region from      849.559      for:
LIQUID
DIAMOND_A4
FCC_A1
Global check of removing phase at      8.46181E+02
Calculated      6 equilibria

Phase Region from      846.181      for:
DIAMOND_A4
FCC_A1
Calculated      4 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_1072.POLY3
POSTPROCESSOR VERSION 3.2

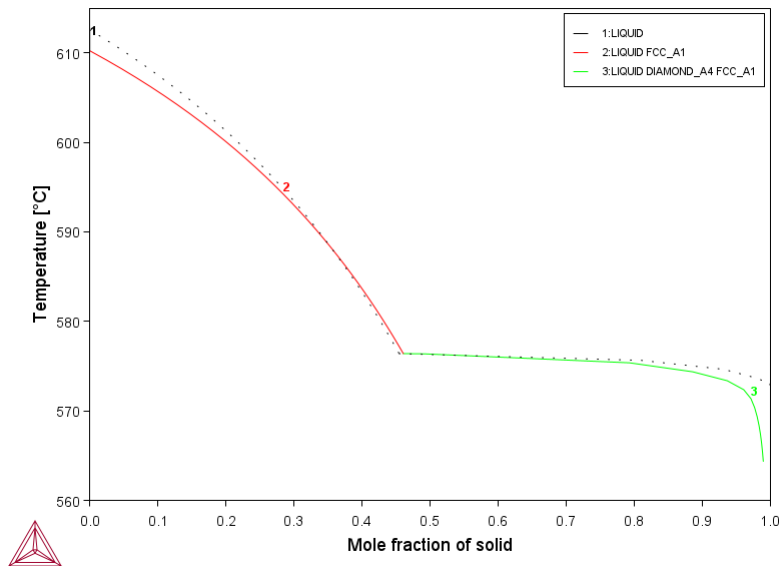
Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is ENTER_SYMBOL
... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_1072.EXP
has been created to store the equilibrium solidification results.
... the command in full is READ_WORKSPACES
CALCULATING SCHEIL SOLIDIFICATION
FCC_A1#1 set as the primary phase
T(C)      fraction solid
612.6625      0.000000
611.6625      0.000000
610.6625      0.000000
610.2481      0.000000
PHASE REGION:LIQUID + FCC_A1
T(C)      fraction solid
610.2163      0.3148144E-03
609.2163      0.2406990E-01
608.2163      0.4679047E-01
607.2163      0.6854047E-01
606.2163      0.8937880E-01
605.2163      0.1093598
604.2163      0.1285336
603.2163      0.1469466
602.2163      0.1646419
601.2163      0.1816592
600.2163      0.1980355
599.2163      0.2138054
598.2163      0.2290009
597.2163      0.2436518
596.2163      0.2577860
595.2163      0.2714295
594.2163      0.2846067
593.2163      0.2973404
592.2163      0.3096520
591.2163      0.3215615
590.2163      0.3330877
589.2163      0.3442483
588.2163      0.3550599
587.2163      0.3655382
586.2163      0.3756979
585.2163      0.3855530
584.2163      0.3951166
583.2163      0.4044010
582.2163      0.4134180
581.2163      0.4221787
580.2163      0.4306935
579.2163      0.4389724
578.2163      0.4470249
577.2163      0.4548598
576.4194      0.4609507
Can't find a solute trapping partitioning at first attempt, iterating...
Iteration from previous temperature successful
PHASE REGION:LIQUID + DIAMOND_A4 + FCC_A1
T(C)      fraction solid
576.3875      0.4921089
575.3875      0.7935046
574.3875      0.8862770
573.3875      0.9372088
572.3875      0.9613926
571.3875      0.9719953
570.3875      0.9774242
569.3875      0.9811188
568.3875      0.9839099
567.3875      0.9860544
566.3875      0.9877322
565.3875      0.9890754
564.3875      0.9901738
Calculating properties ...
Liquidus temperature:      883.398 K
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is APPEND_EXPERIMENTAL_DATA

```

The following axis variables are available

T - Temperature in Celsius
 NL/BL/VL - Mole/mass/volume fraction of liquid
 NS/BS/VS - Mole/mass/volume fraction of all solid phases
 NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
 VS(ph) - Volume fraction of a solid phase
 W(ph,el) - Weight fraction of an element in a phase
 X(ph,el) - Mole fraction of an element in a phase
 Y(ph,el) - Site fraction of an element in a phase
 NN(ph,el) - Distribution of an element in a phase
 NH/BH - Heat release and Latent heat per mole/gram
 CP/BCP - Apparent heat capacity per mole/gram
 NV/NV(ph) - Molar volume of the system or a phase
 DS/DS(ph) - Average density of the system or a phase
 BT - Apparent volumetric TEC of the system
 DVIS(ph) - Dynamic viscosity of a phase
 KVIS(ph) - Kinematic viscosity of a phase
 SURF(ph) - Surface tension of a liquid phase
 ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
 ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
 THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
 "*" can be used as a wild character for "el" and "ph"

POST:
 POST:
 POST: set-inter
 ... the command in full is SET_INTERACTIVE_MODE
 POST:

tcex58

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex58\tcex58.TCM.test"

SYS: @@ Calculate volumetric thermal expansion coefficients

SYS: @@ of the L12-type Al3Sc.

SYS:

SYS: GO DA

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: SW Aldemo

Current database: Aluminum Demo Database v5.0

VA /- DEFINED

TDB_ALDEMO: DEF-ELE AL SC

AL SC DEFINED

TDB_ALDEMO: GET

10:21:41,639 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_ALDEMO:

TDB_ALDEMO: go p-3

POLY version 3.32

POLY:

POLY: c-s ph *=sus

POLY: c-s ph al3sc,liquid,fcc_al=ent 1

POLY:

POLY: s-c n=1 p=1e5

POLY:

POLY: s-c x(sc)=0.25 t=273

POLY:

POLY: ent func avAl3Sc=vm(al3sc).t/vm(al3sc);

POLY:

POLY: c-e

Using global minimization procedure

Calculated 419 grid points in 0.241 s

Found the set of lowest grid points in 0.001 s

Calculated POLY solution 0.106 s, total time 0.348 s

POLY:

POLY: s-a-v 1 t 100 2000,,

POLY:

POLY: step

Option? /NORMAL/:

No initial equilibrium, using default

Step will start from axis value 273.000

...OK

Phase Region from 273.000 for:

AL3SC

FCC_A1

Global test at 3.53000E+02 OK

Global test at 4.53000E+02 OK

Global check of adding phase at 5.52137E+02

Calculated 30 equilibria

Phase Region from 552.137 for:

LIQUID

AL3SC

FCC_A1

Calculated 2 equilibria

Phase Region from 552.137 for:

LIQUID

AL3SC

Global test at 6.23000E+02 OK

Global test at 7.23000E+02 OK

Global test at 8.23000E+02 OK

Global test at 9.23000E+02 OK

Global test at 1.02300E+03 OK

Global test at 1.12300E+03 OK

Global test at 1.22300E+03 OK

Global test at 1.32300E+03 OK

Global test at 1.42300E+03 OK

Global test at 1.52300E+03 OK

QBSMER trying to find equilibrium at 1.5970000E+03

QBSMER trying to find equilibrium at 1.5970000E+03

QBSMER forced phase set change at 1597.000000000000

Calculated 109 equilibria

Phase Region from 1597.00 for:

LIQUID

Global test at 1.66900E+03 OK

Global test at 1.76900E+03 OK

Global test at 1.86900E+03 OK

Global test at 1.96900E+03 OK

Terminating at 2000.00

```

Calculated      45 equilibria

Phase Region from    273.000      for:
  AL3SC
  FCC Al
Global Test at  1.93000E+02 .... OK
Global test at  1.00000E+02 .... OK
Terminating at    100.000
Calculated      21 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

```

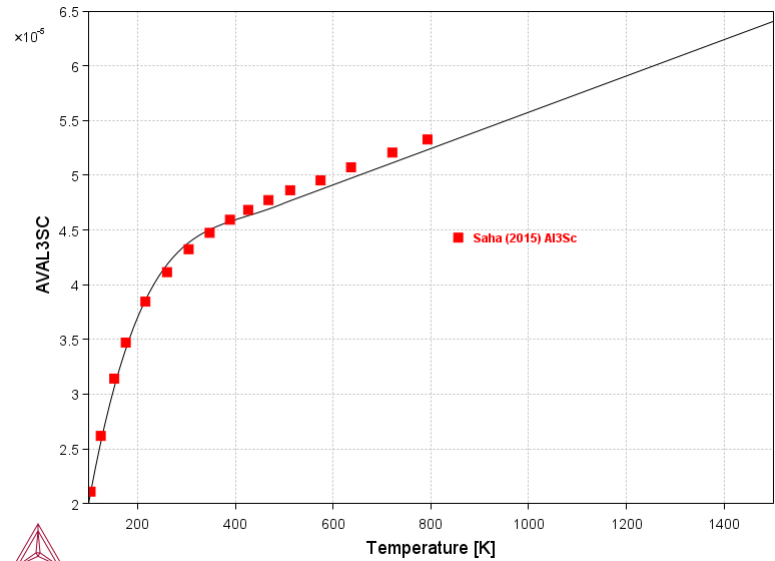
Setting automatic diagram axes

```

```

POST:
POST:@?plot_expansion_coefficient
POST: a-e y Al3X.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST:
POST: set-ras y,,
POST: s-d-a x t-k
POST: s-s-s x n 100 1500
POST: s-d-a y avAl3Sc
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

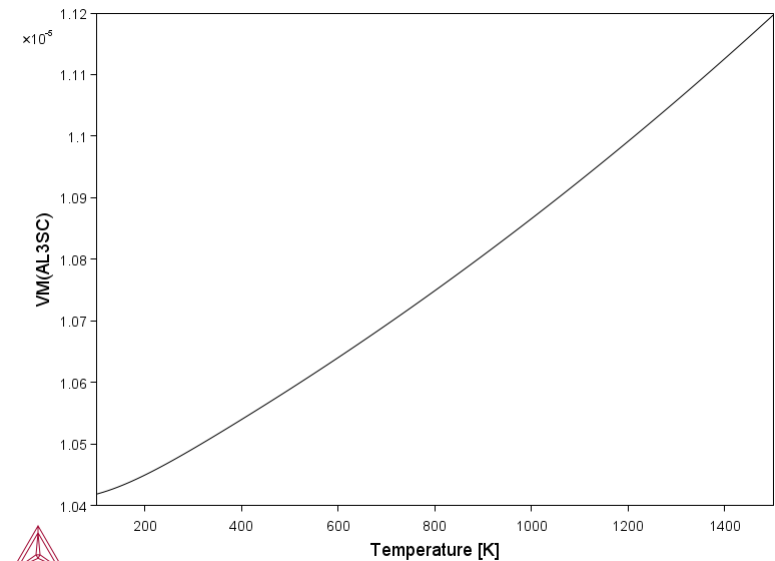
```



```

POST:
POST:@?plot_molar_volume
POST: select,,,
POST: s-d-a y vm(al3sc)
POST: a_e n,,,
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

```



```

POST:
POST: set-inter
POST:

```

tcex59

SYS>About

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Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex59\tcex59.TCM.test"

SYS: @@ Calculate volumetric thermal expansion coefficients

SYS: @@ of the L12-type Al3Zr.

SYS:

SYS: GO DA

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: SW Aldemo

Current database: Aluminum Demo Database v5.0

VA /- DEFINED

TDB_ALDEMO: DEF-ELE AL Zr

AL ZR DEFINED

TDB_ALDEMO: GET

10:22:44,317 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_ALDEMO:

TDB_ALDEMO: go p-3

POLY version 3.32

POLY:

POLY: c-s ph *=sus

POLY: c-s ph al3sc,liquid,fcc_al=ent 1

POLY:

POLY: s-c n=1 p=1e5

POLY:

POLY: s-c x(Zr)=0.25 t=273

POLY:

POLY: ent func avAl3Zr=vm(al3sc).t/vm(al3sc);

POLY:

POLY: c-e

Using global minimization procedure

Calculated 419 grid points in 0.198 s

Found the set of lowest grid points in 0.001 s

Calculated POLY solution 0.088 s, total time 0.287 s

POLY:

POLY: s-a-v 1 t 100 2000,,

POLY:

POLY: step

Option? /NORMAL/:

No initial equilibrium, using default

Step will start from axis value 273.000

...OK

Phase Region from 273.000 for:

AL3SC

FCC_A1

Global test at 3.53000E+02 OK

Global test at 4.53000E+02 OK

Global test at 5.53000E+02 OK

Global test at 6.53000E+02 OK

Global test at 7.53000E+02 OK

Global test at 8.53000E+02 OK

Global test at 9.53000E+02 OK

Global test at 1.05300E+03 OK

Global check of adding phase at 1.09736E+03

Calculated 85 equilibria

Phase Region from 1097.36 for:

LIQUID

AL3SC

FCC_A1

Calculated 2 equilibria

Phase Region from 1097.36 for:

LIQUID

AL3SC

Global test at 1.17300E+03 OK

Global test at 1.27300E+03 OK

Global test at 1.37300E+03 OK

Global test at 1.47300E+03 OK

Global test at 1.57300E+03 OK

Global test at 1.67300E+03 OK

Global test at 1.77300E+03 OK

QBSMER trying to find equilibrium at 1.7990000E+03

QBSMER trying to find equilibrium at 1.7990000E+03

QBSMER forced phase set change at 1799.000000000000

Calculated 75 equilibria

Phase Region from 1799.00 for:

LIQUID

Global test at 1.87100E+03 OK

Global test at 1.97100E+03 OK

```

Terminating at      2000.00
Calculated      24 equilibria

Phase Region from    273.000      for:
AL3SC
FCC_Al
Global test at 1.93000E+02 .... OK
Global test at 1.00000E+02 .... OK
Terminating at      100.000
Calculated      21 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

```

```

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

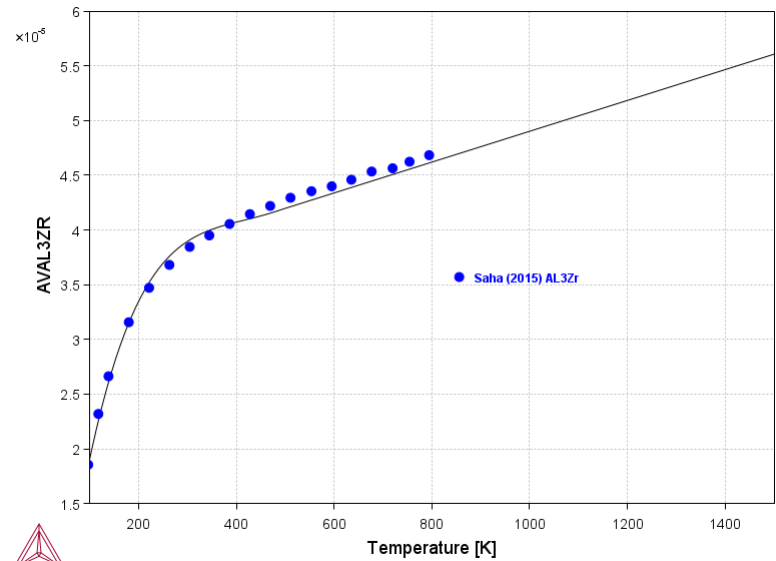
Setting automatic diagram axes

```

```

POST:
POST:@?plot_expansion_coefficient
POST: a-e y Al3X.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 2
POST:
POST: set-ras y,,
POST: s-d-a x t-k
POST: s-s-s x n 100 1500
POST: s-d-a y avAl3Zr
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

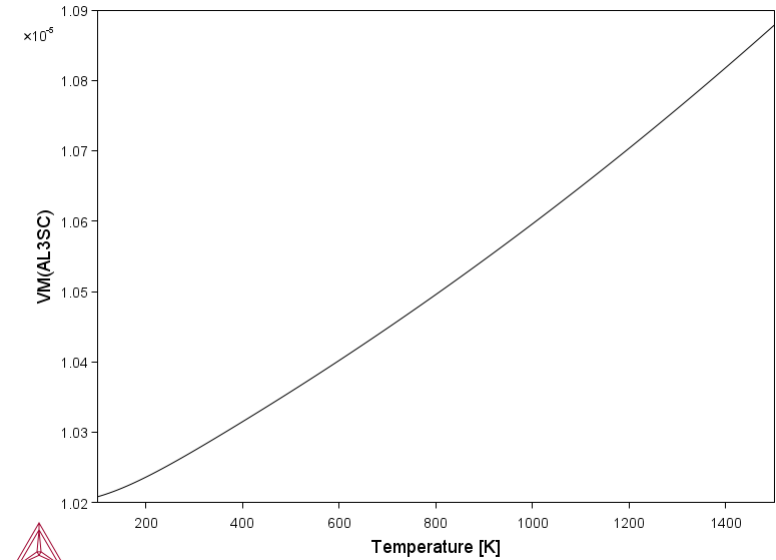
```



```

POST:
POST:@?plot_molar_volume
POST: select,,,,
POST: s-d-a y vm(al3sc)
POST: a_e n,,,
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

```



```

POST:
POST:
POST: set-inter
POST:

```


tcex60

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software running on Windows 64-bit wordlength
Compiler: unknown compiler
License library version: 9.7.0.0036
Linked: Sun May 11 17:31:44 2025

SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_console_examples\examples\tcex60\tcex60.TCM.test"

SYS: @@ Calculate the electrical resistivity (ELRS) and
SYS: @@ thermal conductivity (THCD) from FCC_A1 to liquid.

SYS:

SYS:

SYS: @@ This example makes a step calculation of pure Cu

SYS: @@ over a wide temperature range, covering both the

SYS: @@ FCC_A1 state and the liquid state. It plots thermal @@ conductivity of the system (pure Cu, for both

SYS: @@ FCC_A1 and liquid) and that of a single phase

SYS: @@ (taking FCC_A1 as an example), respectively.

SYS: @@ Also plots electrical resistivity of the system

SYS: @@ and that of FCC_A1.

SYS:

SYS: go da

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\dev_pipeline\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA FCC_A1 REJECTED

TDB_TCFE11: sw aldemo

Current database: Aluminum Demo Database v5.0

VA /- DEFINED

TDB_ALDEMO: def-ele Cu

CU DEFINED

TDB_ALDEMO: get

10:23:47,269 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

TDB_ALDEMO:

TDB_ALDEMO: go p-3

POLY version 3.32

POLY: s-c n=1 p=1e5 t=300

POLY:

POLY: c-s ph *

Status: /ENTERED/: sus

POLY: c-s ph fcc_al liquid

Status: /ENTERED/: ENTERED

Start value, number of mole formula units /0/: 1

POLY:

POLY: c-e

Using global minimization procedure

Calculated 2 grid points in 0.163 s

POLY:

POLY: s-a-v 1 t 200 6000

Increment /145/: 67.5

POLY:

POLY: step

Option? /NORMAL/: NORMAL

No initial equilibrium, using default

Step will start from axis value 300.000

...OK

Phase Region from 300.000 for:

FCC_A1

Global test at 3.80000E+02 OK

Global test at 4.80000E+02 OK

Global test at 5.80000E+02 OK

Global test at 6.80000E+02 OK

Global test at 7.80000E+02 OK

Global test at 8.80000E+02 OK

Global test at 9.80000E+02 OK

Global test at 1.08000E+03 OK

Global test at 1.18000E+03 OK

Global test at 1.28000E+03 OK

Global check of adding phase at 1.35777E+03

Calculated 108 equilibria

Phase Region from 1357.77 for:

LIQUID

FCC_A1

Calculated 2 equilibria

Phase Region from 1357.77 for:

LIQUID

Global test at 1.43000E+03 OK

Global test at 1.53000E+03 OK

Global test at 1.63000E+03 OK

Global test at 1.73000E+03 OK

Global test at 1.83000E+03 OK

Global test at 1.93000E+03 OK

Global test at 2.03000E+03 OK

Global test at 2.13000E+03 OK

Global test at 2.23000E+03 OK

Global test at 2.33000E+03 OK

Global test at 2.43000E+03 OK

```

Global test at 2.53000E+03 .... OK
Global test at 2.63000E+03 .... OK
Global test at 2.73000E+03 .... OK
Global test at 2.83000E+03 .... OK
Global test at 2.93000E+03 .... OK
Global test at 3.03000E+03 .... OK
Global test at 3.13000E+03 .... OK
Global test at 3.23000E+03 .... OK
Global test at 3.33000E+03 .... OK
Global test at 3.43000E+03 .... OK
Global test at 3.53000E+03 .... OK
Global test at 3.63000E+03 .... OK
Global test at 3.73000E+03 .... OK
Global test at 3.83000E+03 .... OK
Global test at 3.93000E+03 .... OK
Global test at 4.03000E+03 .... OK
Global test at 4.13000E+03 .... OK
Global test at 4.23000E+03 .... OK
Global test at 4.33000E+03 .... OK
Global test at 4.43000E+03 .... OK
Global test at 4.53000E+03 .... OK
Global test at 4.63000E+03 .... OK
Global test at 4.73000E+03 .... OK
Global test at 4.83000E+03 .... OK
Global test at 4.93000E+03 .... OK
Global test at 5.03000E+03 .... OK
Global test at 5.13000E+03 .... OK
Global test at 5.23000E+03 .... OK
Global test at 5.33000E+03 .... OK
Global test at 5.43000E+03 .... OK
Global test at 5.53000E+03 .... OK
Global test at 5.63000E+03 .... OK
Global test at 5.73000E+03 .... OK
Global test at 5.83000E+03 .... OK
Global test at 5.93000E+03 .... OK
Terminating at 6000.00
Calculated 468 equilibria

```

```

Phase Region from 300.000 for:
FCC_A1

```

```

Global test at 2.20000E+02 .... OK
Terminating at 200.000
Calculated 13 equilibria

```

```

*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

```

POLY:

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:

POST:@?plot_thcd_of_system

POST: s-d-a x t-k

POST: s-d-a y thcd

POST: s-s-s x n 200 6000

POST: a-e y 1972Ho_cu_thcd

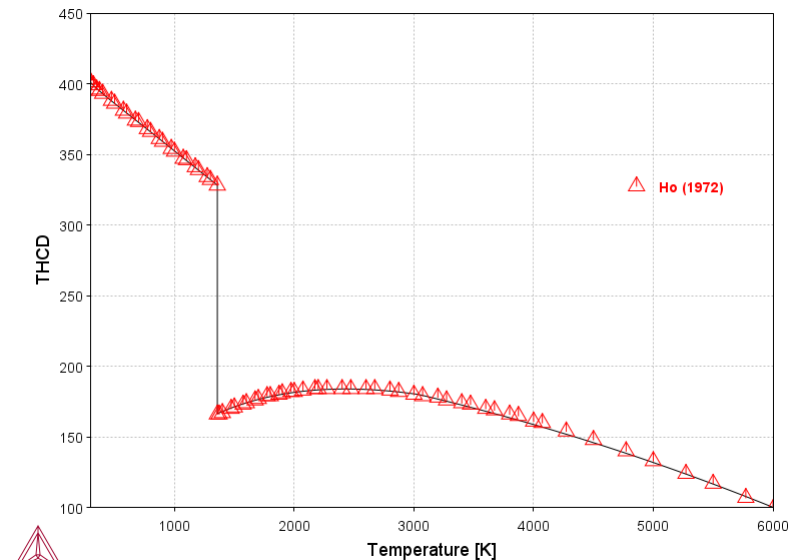
PROLOGUE NUMBER: /0/: 1

DATASET NUMBER(s): /-1/: 1 2 3

POST: set-ras y

POST: set-tic 4

POST: pl,,



POST:

POST:@?plot_thcd_of_fcc_a1_only

POST: select,,

POST: s-d-a y thcd(fcc_a1)

POST: s-s-s x n 200 6000

POST: a-e y 1972Ho_cu_thcd

PROLOGUE NUMBER: /1/: 1

DATASET NUMBER(s): /-1/: 1 2

POST:

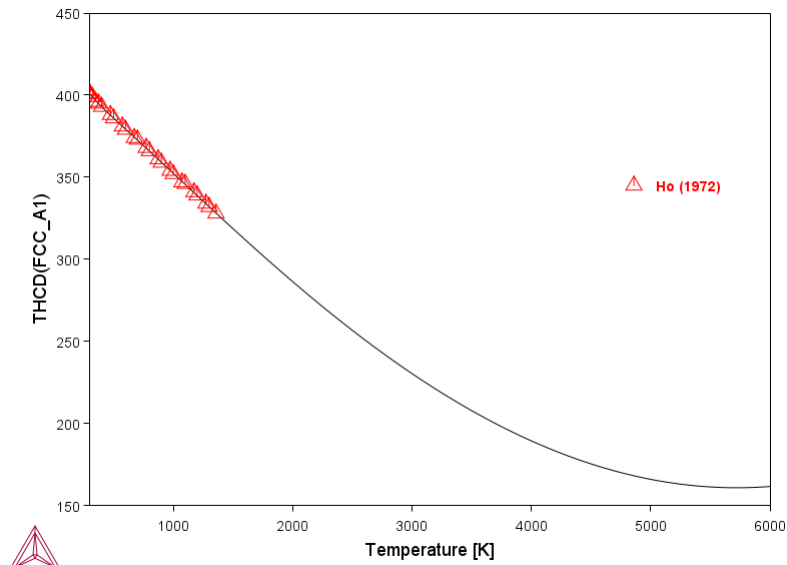
POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y

POST: SET_EXP_FILE_FORMAT 10

POST:

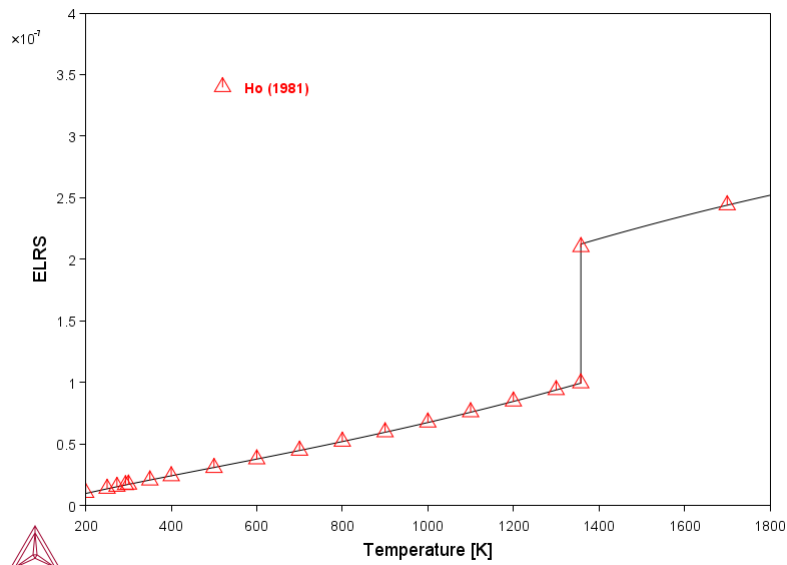
POST: plot,,



```

POST:
POST:@?plot_elrs_of_system
POST: select,,,
POST: s-d-a y elrs
POST: s-s-s y n 0 4e-7
POST: a-e y 1981Ho_cu_elrs
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 1 2 3
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

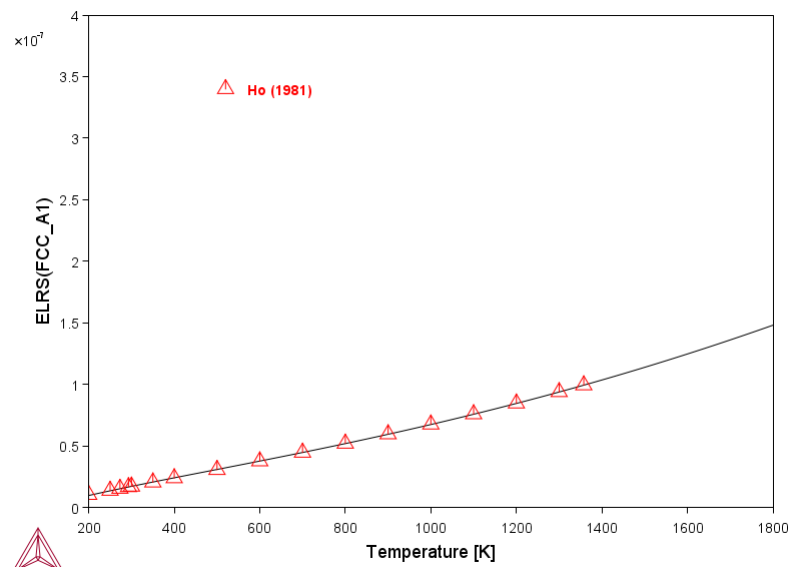
```



```

POST:
POST:@?plot_elrs_of_fcc_a1_only
POST: select,,,
POST: s-d-a y elrs(fcc_a1)
POST: s-s-s y n 0 4e-7
POST: a-e y 1981Ho_cu_elrs
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 1 2
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

```



POST:
POST: set-inter
POST:

