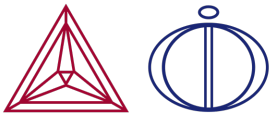
TQ-Interface

SDK Programmer's Guide

Thermo-Calc 2020a



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The TQ-Interface

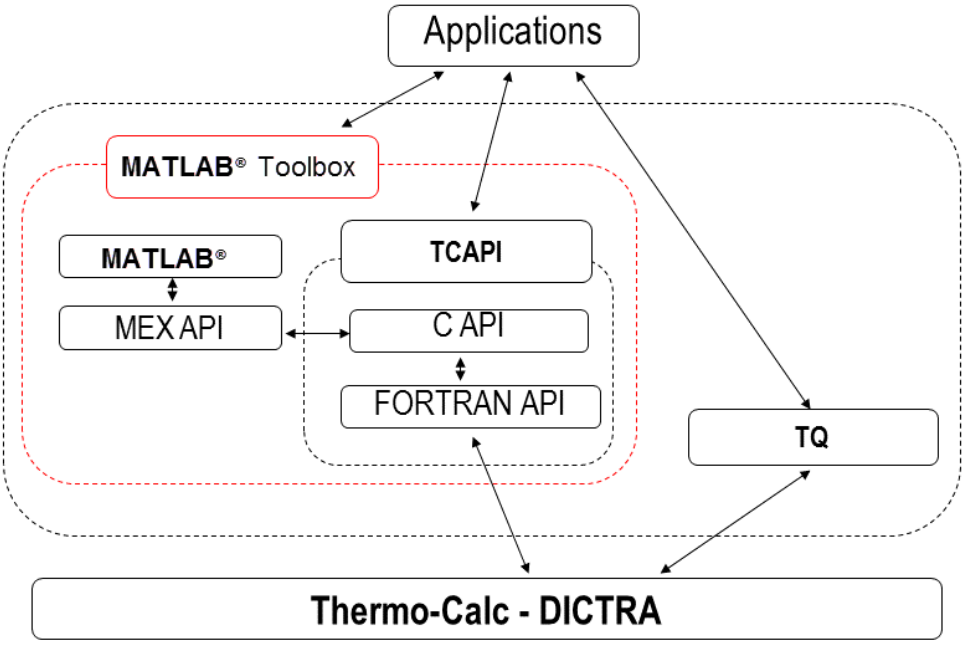
In this section:

Introduction to the TQ-Interface

TQ-Interface is an application programming interface for Thermo-Calc, a general software package for multicomponent phase equilibrium calculations. TQ-Interface is for application programmers to write programs using the Thermo-Calc kernel. With this programming interface, it is easy to make Thermo-Calc an integral part of application programs such as those for process simulation, microstructure evolution modeling and materials property prediction.

THERMO-CALC APIS

Interfacing with the Thermo-Calc Engine



The thermodynamic properties and phase equilibrium data that can be obtained by using the TQ-Interface include Gibbs energy, enthalpy, entropy, heat capacity, first and second derivatives of Gibbs energy with respect to composition, chemical potential, phase amount, phase composition, partition coefficients, liquidus or solidus points, invariant temperature, heat of reaction, adiabatic combustion temperature, and volume, etc.

Through appending the mobility databases into the workspace, you can also obtain assessed mobility or diffusivity data via the TQ-Interface. The TQ-Interface can also be used to predict metastable or non-equilibrium states by changing the status of the phases under consideration.

The TQ-Interface is available for both Windows and Linux platforms. It is supplied in the form of DLLs (*Dynamically Linked Libraries*) meaning there is no need to recompile existing application programs when a new version of TQ-Interface is released.

TQ-Interface is written in FORTRAN as many software packages for scientific calculations are developed in this language. The Subroutines and Functions topic outlines categories of what is available in the TQ-Interface.

The computer language to implement application programs is not restricted to FORTRAN, for example a GUI application written in C++ can realize its various functionalities by using TQ-Interface subroutines with the appropriate calling conventions.

Programming Languages

The Subroutines and Functions

The FORTRAN subroutines and functions available in the TQ-Interface can be classified into categories based on purpose:

1. Initialization Subroutines. For example, initializing the workspace, reading the thermodynamic data files, setting default units for thermodynamic quantities, selecting the input and output options, changing the program input and output units
2. System Data Manipulation Subroutines. For example, identifying system components, phases, and constituents, redefining the system components, changing the status of components and phases or the system reference state.
3. Condition, Stream and Segment Subroutines. For example, defining conditions for an equilibrium calculation, setting conditions for a thermodynamic equilibrium calculation, and setting a new equilibrium segment.
4. Calculations and Results Subroutines. For example, calculate equilibriums, get molar Gibbs energy values, and calculate interfacial energy between a matrix phase and a precipitate phase.
5. Miscellaneous Subroutines. For example, reinitiate the calculation workspace, set error codes and messages, or set equilibrium calculation options.

Essentially, only subroutines 1, 3, and 4 are required to use the TQ- Interface. In the simplest case, only one or two subroutines are needed from each category.

Additional subroutines are grouped as follows:

- Extra Subroutines–Phase Properties. For example, get Gibbs energy of a phase, mobility of a species in a phase, or check if mobility data for a phase is available.

- Database Subroutines For example, get lists of database names, reject a selected element and get data from the selected database.
- Adaptive Interpolation Schemes. For example, define a function or state variable to be interpolated and get statistics on the usage of the interpolation scheme.
- Composition Set Reordering Routines . For example, initialize IWSR workspace and set ideal composition in a phase.

Installing and Using the TQ-Interface

If you have not used Thermo-Calc before, start with the Basic Concepts. Several simple application examples are given in the installed SDK folder.

If you are an experienced Thermo-Calc user you can start by copying a suitable example. You make it work for problems by changing, adding or deleting some callings to TQ-Interface subroutines and functions.

It is strongly recommended that at least one or two examples should be compiled and linked (and tested) to make sure the linked executables can be run successfully.

In this section:

Installing the TQ-Interface and Examples

The TQ-Interface requires an additional license key, which is purchased along with the Thermo-Calc software/database package. For both Windows and Linux platforms, the TQ-Interface is supplied as a dynamically linked library.

All the examples in this document are included in the SDK installation directory. For example, for a network installation on Windows, the directory is here:

`C:\Users\<username>\Documents\Thermo-Calc\<version>\SDK\TQ\<Windows>`

On Windows, once Thermo-Calc and the SDKs are installed go to **Start → All Programs** or **All Apps → Thermo-Calc** and click **SDK** to open the folders.

For installation and directory locations, see the *Thermo-Calc Installation Guide*.

TQ-Interface Examples

Example Name	Description
TQEX01	This sample program shows how to retrieve data from a Thermo-Calc data file, then defines a set of conditions for a single equilibrium calculation, gets the equilibrium phases and their amounts and compositions. The method of calculating the liquidus and solidus temperature is also demonstrated.
TQEX02	This sample program calculates the To line for the fcc and bcc phase in the Fe-C system.
TQEX03	This sample program simulates the non-equilibrium solidification under the Scheil-Guilliver condition.
TQEX04	This sample program simulates the non-equilibrium solidification under the Scheil-Guilliver condition.
TQEX05	This example demonstrates how to use stream calculation to get the enthalpy of a reaction, i.e., the enthalpy difference between the reaction products at one temperature and the reactants at another temperature. By setting the enthalpy of reaction to zero, the adiabatic temperature can be easily calculated.

Example Name	Description
TQEX06	This example demonstrates how to use stream calculation to obtain the chill factors in the steelmaking industry.[1]O.Kubaschewski and C.B. Alock, Metellurgical Thermochemistry, 1979, Page 211.
TQEX07	This sample program calculates the A3 temperature of a steel and determines the influence of each alloying element on this temperature. It demonstrates that some very special quantities, such as the composition derivative of temperature, can be obtained easily via the TQ interface.
TQEX08	This sample program displays the diffusion matrix in a multicomponent system.
TQEX09	This sample program show how to retrieve Gibbs energy, Gibbs energy derivatives and mobilities.
TQEX10	This sample program is the same as Example 9 except that it demonstrates how to convert mole fractions to site fractions and first derivatives of Gm w.r.t. site fractions to that w.r.t. mole fractions.
TQEX11	This sample program shows how to get information about the paraequilibrium transformation from Fcc to Bcc in a steel.
TQEX12	This sample program demonstrates how to use subroutines getting system data from a database and how to restart new calculation on a different system in the same application program.
TQEX13	This sample program demonstrates that the number of phases can increase due to the use of global mininization for equilibrium calculation during which additional composition set(s) can be added automatically if a miscibility gap is detected.
TQEX14	This sample program show how to use the functionality for setting how different composition sets should correspond to different compositions. For example, that in the Ni-Al system the composition set fcc_l12#1 should correspond to gamma and fcc_l12#2 to gamma-prime.
TQEX15	TQ library example to illustrate the use the adaptive interpolation scheme. This example calculates the liquidus temperature in a part of the C-CR-FE system and displays a selection of the results.

Example Name	Description
	The MPI examples only show how the TQ-Interface can be used in applications together with MPI. Thermo-Calc Software AB or Thermo-Calc Software, Inc. is not available to answer support questions related to MPI.
MPExample1	This is an MPI (Message Passing Interface) example that calculates the Gibbs energy for a composition grid C with a density of "npoints" at 1273K in the Mn-Ni-Fe system.
MPExample2	This is an MPI (Message Passing Interface) example where a set of equilibrium calculations are distributed over all processes. Then the Gibbs energy of the system is retrieved and collected in a single vector in the master process.

Using this Guide

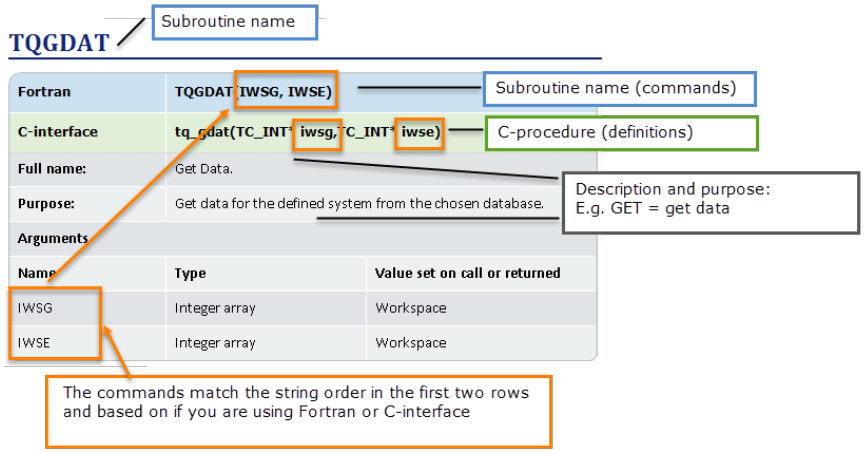
The topic names in this guide are the same as the FORTRAN routine names. Also included in each topic are details for both the FORTRAN and C programming languages.

Programming Languages

Note the following conventions to distinguish between the programming languages.

- Routines starting with **TQ**XXX, for example, *TQGDAT*, are in the Fortran interface
- Routines starting with **tq_**xxxx, for example *tq_gdat*, are in the C-interface.
- In Fortran, all routines are subroutines and do not return any values except where explicitly declared as functions.
- All the C procedures are declared as void and do not return any values except where explicitly otherwise declared.

An example of how to read the subroutine definitions.



Programming Languages

You can program your TQ-library with the FORTRAN or C programming languages.

FORTRAN

No special consideration is needed when interfacing the TQ-library with a program written in FORTRAN; the main core of the TQ-library is written in FORTRAN. By default all parameters are passed to routines by reference, except for strings, which are passed by descriptor.

C-Interface

The C-interface acts as a translation layer in between the calling C-program and the underlying FORTRAN TQ-library.

For a C-interface, the default parameter passing mechanism is by *value* and not by reference. Some decisions must be made as to how parameters, which are updated in the TQ-Interface, are then passed into the library. For example:

- The *C procedures* are defined in the file **tqroot.h** which should be included in the procedures using the library calls in C.
- The **tqroot.h** file also includes the file **tc_data_defs.h** where the datatypes are defined.

The definition of some of these data types vary depending on what platform and compiler is used. It is important to define these and for the definitions to be correctly set (see Compiler Settings).

COMMON C-PROCEDURE DEFINITIONS

The commonly used definitions in the C-interface are listed in the table. Note that:

- TC_INT and TC_FLOAT are used when only the value of the variables is necessary to pass.
- TC_INT* and TC_FLOAT* are used when the variables are updated and values are returned within these.
- When a TC_STRING is updated, the allocated size of the string must be passed into the interface in a variable declared as TC_STRING_LENGTH.

Routine	Definitions
TC_INT	An integer of platform dependent length passed by value.
TC_INT*	Address of an integer of platform dependent length.
TC_FLOAT	A 64-bit real passed by value.
TC_FLOAT*	Address of a 64-bit real.
TC_STRING	Address of a character string.
TC_STRING_LENGTH	An integer of platform dependent length passed by value defining the length of the string.

Basic Concepts

A thermodynamic system is made up of *components* and *phases*. A number of *state variables* define the properties and the relationships.

A **component** is a system-wide entity; sometimes it is specifically called a *system component*. A component has a unique name and some thermodynamic properties are associated with it, for example, its amount and activity or chemical potential. At equilibrium the activity or chemical potential of the components are the same in the whole system.

A **phase** is a system-wide entity, which has a composition expressed in the amounts of components, enthalpy content, a volume, and many other properties. The phase has *constituents* that may be different from the components. The **constituents** have a stoichiometry that can be expressed in terms of the components and possibly a charge. *Condensed phases* may have an internal structure like sub-lattices or clusters, and these clusters may be modeled as constituents.

Naming Components, Phases and Constituents

Naming Conventions

The name of a component, phase or constituent can be maximum of 24 characters and must start with a letter (A-Z or a-z) and contain only letters, digits and these special characters:

- underscore (_)
- full stop (.)
- parentheses (and)
- plus (+)
- minus (-)
- slash (/)

COMPONENTS

The TQ Interface maintains a list of *components*. These are numbered sequentially from `1` up to the number of components.

A component has a name which can be identical to a chemical formula or any string of letters such as `h2o`, `c2h2cl_cis`, or `au3cu_cvm1`.

Several subroutines are available to get information about the components and to manipulate them, for example:

- TQGCOM returns the total number of components and all component names
- TQGSCI returns the index of one component name
- TQSCOM enables you to re-define the components.

The *component index* is used in most subroutines for defining conditions, etc.

Components can be suspended by TQCSSC, thus leaving gaps in the component list because suspending one component does not change the sequential numbering. The logical function TQGSSC can be used to check if a specific component is suspended or not.

PHASES

The TQ-Interface maintains a list of *phases*. These are numbered sequentially from `1` up to the

number of phases in the system.

A phase has many properties and most importantly a list of constituents (see Phase Constituents). Subroutines are available to get information about the phases, for example:

- TQGNP for the total number of phases
- TQGPN for the name of a phase
- TQGPI for the name of its index
- TQGNPC for the number of phase constituents

Phases can be suspended or set dormant by TQCSP, thus leaving gaps in the list because suspending one phase does not change the sequential numbering. The logical function TQGSP can be used to check if a specific phase is suspended or not.

Phase Constituents

The TQ Interface maintains a list of the constituents of each phase (the *phase constituents*). These are numbered sequentially from `1` up to the number of constituents in the phase. The number of constituents can be different in each phase. If a phase has sub-lattices, the numbering goes from the first constituent in the first sub-lattice over all sub-lattices to the last constituent in the last sub-lattice.

Subroutines are available to get information about the constituents, for example:

- TQGNPC for the number of constituents of a phase
- TQGPCN (or its index TQGPCI) for the name of a phase constituent
- TQGPCS for the stoichiometry of a constituent expressed in terms of the components

About Adaptive Interpolation Schemes

A general dynamic interpolation scheme is implemented in the TQ-library. At a slight cost of accuracy, this scheme allows you to rapidly obtain equilibrium values for state variables and functions for many different values of a predefined set of conditions.

Multiple sets of conditions and requested variable values can be defined in order to obtain different values for different situations. These are stored internally as different branches.

The accuracy of the scheme can be adjusted by setting the number of steps in the composition/temperature/pressure space where the interpolation is performed.

For a given set of conditions (a *branch*), the scheme builds up an interpolation matrix within the bounds of the conditions that have been previously defined. As long as the subsequent condition values are kept within these limits, the returned values are calculated from the interpolation matrix. If the condition values are outside these limits then the scheme automatically extends the interpolation matrix. With this procedure the scheme extends the interpolation matrix so that it can return values from a growing range of conditions in composition, temperature and pressure.

For each set of condition values within a branch a unique identifying number is calculated. This number is used to find the correct position in the interpolation matrix using a *hash table*.

If the memory requirements to extend the interpolation exceeds the available memory, the nodes in the matrix that are less frequently used are removed to free up some memory.

For a general reference about the interpolation scheme, see Larsson and Höglund (2015): "A Scheme for More Efficient Usage of CALPHAD Data in Simulations', *Calphad*, 50, 1–5.

Initialization Subroutines

Purpose	Subroutine
Initialize TQ-Interface with user-specified database and temporary directories	TQINI3
Initialize TQ-Interface	TQINI
Set input/output option	TQSIO
Get input/output option	TQGIO
Read thermodynamic data file	TQRFIL
Set unit for a system quantity	TQSSU
Get unit for a system quantity	TQGSU
Check if the system is the same	TQSAME
Retrieve information about the TQ-library	TQGVER

Units for TQSSU and TQGSU

Quantity	Unit	Comment
Temperature	K, C, F	K=Kelvin (default); C=Celsius, calculated as K-273.15; F=Fahrenheit
Volume	M3	Cubic meter (default)
	L	Liter. Calculated as 0.001 M^3
	IN3	Cubic inch.
	FT3	Cubic feet
	USG	US gallon
Energy	J	Joule (default)
	Cal	Calories. Calculated as J/4.184
	BTU	British thermal units.
Pressure	Pa	Pascal (default)
	Psi	Pounds/sq. inch
	Bar	Bar. Calculated as 0.00001*Pa
	Atm	Atmosphere. Calculated as Pa/101325
	Torr	Torricelli. Calculated as 758*Pa/101325

Quantity	Unit	Comment
Mass	kg, g, lb	kg=Kilograms (default); g=Grams; lb=Pounds

Legal Input/Output Options for TQSIO and TQGIO

Option	Meaning	Default value
INPUT	Input unit	0
OUTPUT	Output unit	0
ERROR	Error output	0
LIST	List output	0

TQINI3

Fortran	**TQINI3(DATABASE_PATH, TEMP_PATH, NWSG, NWSE, IWSG, IWSE)**	
C-interface	**tq_ini3(TC_STRING database_path, TC_STRING temp_path, TC_INT nwsg, TC_INT nwse, TC_INT* iwsg, TC_INT* iwse);**	
Full name:	Initialize TQ-Interface with user-specified database and temporary directories. If a GES file is used (i.e. no databases are opened) the directories can be empty strings.	
Purpose:	The application program initializes the Thermo-Calc package for thermodynamic calculations. This or TQINI must be called before using any other subroutines in the TQ-Interface.	
Arguments		
Name	**Type**	**Value set on call or returned**
database_path	Character*256	Path to the directory holding the data directory, which in turn contains the databases.  See the examples collection for a default value for this parameter.
temp_path	Character*256	Path to the directory for temporary and log file output. This directory has to be writable by the user who runs the application.

Fortran	TQINI3(DATABASE_PATH, TEMP_PATH, NWSG, NWSE, IWSG, IWSE)	
C-interface	**tq_ini3(TC_STRING database_path, TC_STRING temp_path, TC_INT nwsg, TC_INT nwse, TC_INT* iwsg, TC_INT* iwse);**	
		 See the examples collection for a default value for this parameter.
NWSG	Integer	Set to size of the workspace IWSG.
NWSE	Integer	Set to size of the workspace IWSE.
IWSG	Integer array	Memory area for storage of data inside the package.
IWSE	Integer array	Memory area for storage of data inside the package.

TQINI

Fortran	TQINI(NWSG, NWSE, IWSG, IWSE)	
C-interface	**tq_ini(TC_INT nwsg, TC_INT nwse,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Initialize TQ Interface.	
Purpose:	With this subroutine the application program initializes the Thermo-Calc package for thermodynamic calculations. This or TQINI3 must be called before using any other subroutines in the TQ-Interface.	
Arguments		
Name	**Type**	**Value set on call or returned**
NWSG	Integer	Set to size of the workspace IWSG.
NWSE	Integer	Set to size of the workspace IWSE.
IWSG	Integer array	Memory area for storage of data inside the package.
IWSE	Integer array	Memory area for storage of data inside the package.

TQSIO

Fortran	TQSIO(OPTION, IVAL)	
C-interface	tq_sio(TC_STRING option,TC_INT ival);	
Full name:	Set Input/Output Option.	
Purpose:	With this subroutine the application program can re-direct input and output from the Thermo-Calc package.	
Comments:	OPTION is a character identifying the Input/Output option. The current internal value is set to the value in IVAL. If the value is illegal the error condition is set.	
Arguments		
Name	Type	Value set on call or returned
OPTION	Character*8	Set to a value given in Legal Input/Output Options for TQSIO and TQGIO
IVAL	Integer	Set to an internal value.

TQGIO

Fortran	TQGIO(OPTION, IVAL)	
C-interface	tq_gio(TC_STRING option,TC_INT* ival);	
Full name:	Get Input/output Unit.	
Purpose:	Obtain a value of Input/Output option.	
Comments:	OPTION is a character identifying the Input/Output option. IVAL is an integer where its current internal value is returned.	
Arguments		
Name	Type	Value set on call or returned
OPTION	Character*8	Set to a value given in Legal Input/Output Options for TQSIO and TQGIO.
IVAL	Integer	Return the current internal value.

TQRFIL

Fortran	**TQRFIL(FILE, IWSG, IWSE)**	
C-interface	**tq_rfil(TC_STRING file,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Read File.	
Purpose:	Read a thermodynamic data file in the Thermo-Calc format.	
Comments:	The default set of components is supplied by the thermodynamic input file. The thermodynamic data file should contain at least the following information. • System: name of the elements, molecular mass for elements, list of phases • Phase: list of constituents, type of solution model (if not fixed composition), thermodynamic model parameters • Constituents: name, chemical formula (stoichiometric matrix), molecular mass, thermodynamic properties All this data are not necessarily stored separately, for example the molecular weight for a constituent can be calculated from the masses of the elements.  The TQ-Interface is not intended to read from a database or a database file and thus selections of data from a database must be made in Thermo-Calc and then stored in a GES file by using the save command in the Gibbs-Energy-System module inside Thermo-Calc. When the GES file is read into the workspace by this subroutine it is possible to manipulate data by changing components and status for components or phases.	
Arguments		
Name	**Type**	**Value set on call or returned**
FILE	Character*60	Legal file name
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSSU

Fortran	TQSSU(QUANT, UNIT, IWSG, IWSE)	
C-interface	tq_ssu(TC_STRING quant,TC_STRING unit,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Set System Unit.	
Purpose:	Set the unit for a quantity (like mass, volume, etc.).	
Comments:	Default units are SI unless changes are made by this subroutine. The legal quantities and units are listed in Units for TQSSU and TQGSU.	
Arguments		
Name	Type	Value set on call or returned
QUANT	Character*60	Set to a legal quantity
UNIT	Character*60	Set to a legal unit
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGSU

Fortran	TQGSU(QUANT, UNIT, IWSG, IWSE)	
C-interface	tq_gsu(TC_STRING quant,TC_STRING unit,TC_STRING_LENGTH strlen_unit,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get System Unit.	
Purpose:	To find what units the TQ-Interface is currently using for a system quantity.	
Comments:	The legal quantities and units are listed in Units for TQSSU and TQGSU.	
Arguments		
Name	Type	Value set on call or returned
QUANT	Character*60	Set to a legal quantit.
UNIT	Character*60	Return the current unit.

Fortran	**TQGSU(QUANT, UNIT, IWSG, IWSE)**	
C-interface	**tq_gsu(TC_STRING quant,TC_STRING unit,TC_STRING_LENGTH strlen_unit,TC_INT* iwsg,TC_INT* iwse);**	
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSAME

Fortran	**TQSAME(ICODE, IWSG, IWSE)**	
C-interface	**tq_same(TC_INT* icode,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Same System.	
Purpose:	The application program can check if the thermochemical system has been changed, i.e., not just the conditions but the components or the phases. This is useful if several independent systems operate on the same equilibrium description.	
Comments:	ICODE is an integer with positive value identifying current system. If ICODE is not the same next time TQSAME is called, the system has been changed.This routine may have to be used if the set of components or the set of phases has been changed. The value of ICODE is changed if there are changes of the components, phases, etc., but not with changes in the conditions, or values of thermodynamic model parameters etc.	
Arguments		
Name	**Type**	**Value set on call or returned**
ICODE	Integer	Returns an internal code
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGVER

Fortran	**TQGVER(VERS, LNKDAT, OSNAME, BUILD, CMPLER)**	
C-interface	**void tq_gver(TC_STRING version,TC_STRING_LENGTH strlen_ version,TC_STRING lnkdat,TC_STRING_LENGTH strlen_lnkdat,TC_ STRING osname,TC_STRING_LENGTH strlen_osname,TC_STRING build,TC_STRING_LENGTH strlen_build,TC_STRING cmpler,TC_ STRING_LENGTH strlen_cmpler);**	
Full name:	Get version.	
Purpose:	The application program gets information about the TQ-library.	
Arguments		
Name	**Type**	**Value set on call or returned**
VERS	Character*32	Returns the version of TQ-library.
LNKDAT	Character*32	Returns the date and time the TQ-library was built.
OSNAME	Character*32	Returns the name of operating system the TQ-library was built for.
BUILD	Character*32	Returns the software revision version of the TQ-library.
CMPLER	Character*72	Returns the name and version of the compiler with which the TQ-library was built.

System Data Manipulation Subroutines

Purpose	Subroutine
Identify components, phases and constituents	
Get number of system components	TQGNC
Set system components	TQSCOM
Get system components	TQGCOM
Get system component index	TQGSCI
Get number of phases	TQGNP
Get phase name	TQGPN
Get phase index	TQGPI
Get phase constituent name	TQGPCN
Get phase constituent index	TQGPCI
Get component chemical formula	TQGCCF
Get phase constituent stoichiometry	TQGPCS
Get number of phase constituents	TQGNPC
Change the status of components, phases, and component reference states	
Change status of system component	TQCSSC
Get status of system component	TQGSSC*
Change status of phase	TQCSP
Get status of phase	TQGSP*
Set reference state	TQSETR
Add a composition set to a phase	TQPACS
	* Logical function
Contributions to the Gibbs energy of a phase	
Set Gibbs energy addition	TQSGA
Get Gibbs energy addition	TQGGA

Legal Component Status

Status	Meaning
ENTERED	The component is included in the system for an equilibrium calculation.
SUSPENDED	The component is excluded from the system and, as a result, some phases may become suspended if their constituents contain this component.
SPECIAL	The specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).

Legal Phase Status

Status	Meaning
ENTERED	The phase is included in an equilibrium calculation. It may be stable or unstable.
DORMANT	The phase is included in an equilibrium calculation but not allowed to become stable. The phase should be stable if the calculation shows that its driving force is positive (or activity is larger than unity)
FIXED	The phase is included in an equilibrium calculation and it must be stable.
SUSPENDED	The phase is ignored in an equilibrium calculation.

TQGNC

Fortran	**TQGNC (NCOM, IWSG, IWSE)**	
C-interface	**tq_gnc(TC_INT* ncom, TC_INT* iwsg, TC_INT* iwse);**	
Full name:	Get Number of components.	
Purpose:	With this subroutine the application program can get numbers of components.	
Arguments		
Name	**Type**	**Value set on call or returned**
NCOM	Integer	Return the number of components.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSCOM

Fortran	**TQSCOM(NCOM, NAMES, STOI, IWSG, IWSE)**	
C-interface	**tq_scom(TC_INT num,tc_components_strings* components,TC_FLOAT* stoi,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Set System Component.	
Purpose:	A new set of system components can be defined. The new number of components must be the same as previously. The number of system components can be changed by suspending a component by TQCSSC.	

Comments:	• The set of components must be linearly independent.
	• The names of the new system components are given in NAMES.
	• STOI is a matrix with dimension STOI (1:NCOM,1:NCOM) which gives the stoichiometry of the new components expressed in the old ones.
	• The default set for components is taken from in the input thermodynamic data file.
	• Legal values for the array elements in NAMES are constituent names.
	• The components are numbered as 1 NCOM in the order they are supplied in this call. The conversion from component name to index is also done by TQGSCI.
	
	EXAMPLE
	
	For example, to transform from the components A, B, C to `A2B`, `B4CC2` use the following values of STOI:
	
	`A2B2.0 1.0 0.0`
	
	`B4C 0.0 4.0 1.0`
	
	`C2 0.0 0.0 2.0`	

Arguments		
Name	**Type**	**Value set on call or returned**
NCOM	Integer	Set to the number of components.
NAMES	Character*24 array	Set to component names.
STOI	Double precision matrix	Stoichiometry matrix in old components.

Fortran	**TQSCOM(NCOM, NAMES, STOI, IWSG, IWSE)**	
C-interface	**tq_scom(TC_INT num,tc_components_strings* components,TC_FLOAT* stoi,TC_INT* iwsg,TC_INT* iwse);**	
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGCOM

Fortran	**TQGCOM(NCOM, NAMES, IWSG, IWSE)**	
C-interface	**tq_gcom(TC_INT* num,tc_components_strings* components,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get System Component.	
Purpose:	Get components of a system	
Comments:	The number of components are returned in NCOM and their names are returned in NAMES. They are returned in an internal sequential order of the TQ-Interface. In other subroutines one must in some cases use the index of a component rather than the name.  Also see TQGSCI.	
Arguments		
Name	**Type**	**Value set on call or returned**
NCOM	Integer	Return the current number of components.
NAMES	Character*24 array	Return the current names of components.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGSCI

Fortran	TQGSCI(INDEXC, NAME, IWSG, IWSE)	
C-interface	tq_gsci(TC_INT* index,TC_STRING component,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get System Component Index.	
Purpose:	Get index of a system component.	
Comments:	This is a way to translate from a name to an index. In order to translate from a component index to a name, use TQGCOM. The application program may call TQGCOM only once and maintain itself a list of component names stored by indices.	
Arguments		
Name	Type	Value set on call or returned
INDEXC	Integer	Return the index of the component.
NAMES	Character*24	Set to a component name.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGNP

Fortran	TQGNP (NPH, IWSG, IWSE)	
C-interface	tq_gnp(TC_INT* nph,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get Number of Phases.	
Purpose:	The application gets the numbers of phases.	
Comments:	The phases may have any status. They are numbered sequentially from 1 to NPH. Phases with miscibility gap and thus having more than one composition set are counted separately.	
Arguments		
Name	Type	Value set on call or returned

Fortran	TQGNP (NPH, IWSG, IWSE)	
C-interface	**tq_gnp(TC_INT* nph,TC_INT* iwsg,TC_INT* iwse);**	
NPH	Integer	Return the number of phases.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGPN

Fortran	TQGPN (INDEXP, NAME, IWSG, IWSE)	
C-interface	**tq_gpn(TC_INT index,TC_STRING phase,TC_STRING_LENGTH strlen_phase,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Phase Name.	
Purpose:	With this subroutine theapplication program can convert a phase index to the name of the phase.	
Comments:	The conversion from phase name to phase index is done by TQGPI. Note that phases with miscibility gaps must appear with each possible composition set as a separate phase. These are named as BCC#1, BCC#2 etc.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to the index of a phase.
NAME	Character*24	Return the name of the phase.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGPI

Fortran	TQGPI (INDEXP, NAME, IWSG, IWSE)	
C-interface	tq_gpi(TC_INT* index,TC_STRING phase,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get Phase Index.	
Purpose:	With this subroutine the application program can get the index of a named phase.	
Comments:	The conversion from phase index to phase name is done by TQGPN.	
Arguments		
Name	Type	Value set on call or returned
INDEXP	Integer	Return the index of a phase.
NAME	Character*24	Set to a phase name.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGPCN

Fortran	TQGPCN(INDEXP, INDEXC, NAME, IWSG, IWSE)	
C-interface	tq_gpcn(TC_INT indexp,TC_INT indexc,TC_STRING name,TC_STRING_LENGTH strlen_name,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get Phase Constituent Name.	
Purpose:	With this subroutine the application program can get the name of an indexed constituent.	
Comments:	If the same species appear in more than one sublattice site of a phase, they are named as A#2, A#3, etc., which means A on the second sublattice and A on the third sublattice, etc. The opposite conversion is done by TQGPCI.	
Arguments		
Name	Type	Value set on call or returned

Fortran	TQGPCN(INDEXP, INDEXC, NAME, IWSG, IWSE)	
C-interface	**tq_gpcn(TC_INT indexp,TC_INT indexc,TC_STRING name,TC_STRING_LENGTH strlen_name,TC_INT* iwsg,TC_INT* iwse);**	
INDEXP	Integer	Set to a phase index.
INDEXC	Integer	Set to the constituent index.
NAME	Character*24	Return the constituent name.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGPCI

Fortran	TQGPCI(INDEXP, INDEXC, NAME, IWSG, IWSE)	
C-interface	**tq_gpci(TC_INT indexp,TC_INT* indexc,TC_STRING name,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Phase Constituent Index.	
Purpose:	With this subroutine the application program can get the index of a constituent if its name is known.	
Comments:	The opposite conversion is done by TQGPCN.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index.
INDEXC	Integer	Return the constituent index.
NAME	Character*24	Set to the constituent name.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGCCF

Fortran	TQGCCF(INDEXC, NEL, ELNAM, STOI, MMASS, IWSG, IWSE)	
C-interface	tq_gccf(TC_INT indexc,TC_INT* nel,tc_elements_strings* elname,TC_FLOAT* stoi,TC_FLOAT* mmass,TC_INT* iwsg, TC_INT* iwse);	
Full name:	Get Component Chemical Formula.	
Purpose:	Get the stoichiometry array for a system component in terms of element.	
Comments:	Obtain the real elements in a component. All other subroutines just deal with a name that does not have to be related to the actual chemical formula. This is also the only subroutine that can provide the symbols of the actual elements in the system.  The dimension of ELNAM and STOI is NEL (number of elements in the component).	
Arguments		
Name	Type	Value set on call or returned
INDEXC	Integer	Set to system a component index.
NEL	Integer	Number of elements in chemical formula.
ELNAM	Character*2 array	Element symbols.
STOI	Double precision array	Stoichiometry array.
MMASS	Double precision	Total mass.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGPCS

Fortran	TQGPCS (INDEXP, INDEXC, STOI, MMASS, IWSG, IWSE)	
C-interface	tq_gpcs(TC_INT indexp,TC_INT indexc,TC_FLOAT* stoi,TC_FLOAT* mmass,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get Phase Constituent Stoichiometry.	
Purpose:	With this subroutine the application program can obtain the stoichiometry of a constituent expressed in the system components and also the molecular mass.	
Comments:	This does not give the chemical formula in terms of elements for the constituent. The dimension of STOI is NCOM (number of components) get by calling TQGCOM.	
Arguments		
Name	Type	Value set on call or returned
INDEXP	Integer	Set to a phase index.
INDEXC	Integer	Set to the constituent index.
STOI	Double precision array	Return the stoichiometry array.
MMASS	Double precision	Return the mass.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGNPC

Fortran	TQGNPC(INDEXP, NPCON, IWSG, IWSE)
C-interface	tq_gnpc(TC_INT indexp,TC_INT* npcon,TC_INT* iwsg,TC_INT* iwse);
Full name:	Get Number of Phase Constituent.
Purpose:	With this subroutine the number of constituents in a phase can be obtained.
Comments:	To have also the names, fractions etc. of the constituents, use TQGPD.

Fortran	TQGNPC(INDEXP, NPCON, IWSG, IWSE)	
C-interface	tq_gnpc(TC_INT indexp,TC_INT* npcon,TC_INT* iwsg,TC_INT* iwse);	
Arguments		
Name	Type	Value set on call or returned
INDEXP	Integer	Set to a phase index.
NPCON	Integer	Return the number of the phase constituents.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQCSSC

Fortran	TQCSSC (INDEXC, STATUS, IWSG, IWSE)	
C-interface	tq_cssc(TC_INT index,TC_STRING status,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Change Status of System Component	
Purpose:	With this subroutine the application program can change status for a system component.	
Comments:	The legal values for STATUS are ENTERED, SUSPENDED and SPECIAL  Also see Legal Component Status. By suspending a system component some phases may also become suspended if they contain this component. For example, in the system Fe-O-S if O is suspended all phases that must dissolve oxygen is automatically suspended. The fraction of oxygen is set to zero in phases that can dissolve oxygen but can also exist without oxygen.	
Arguments		
Name	Type	Value set on call or returned
INDEXC	Integer	Set to a component index.
STATUS	Character*12	Set to the new status

Fortran	TQCSSC (INDEXC, STATUS, IWSG, IWSE)	
C-interface	**tq_cssc(TC_INT index,TC_STRING status,TC_INT* iwsg,TC_INT* iwse);**	
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGSSC

This is a logical function.

Fortran	STATUS=TQGSSC (INDEXC, IWSG, IWSE)	
C-interface	**status=tq_gssc(TC_INT index,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Status of System Component.	
Purpose:	This function returns TRUE if the system component is ENTERED or FALSE if it is SUSPENDED.	
Comments:	The legal values for STATUS are given in Legal Component Status.If the C-interface is used the value returned is of type: TC_BOOL.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXC	Integer	Set to a component index.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQCSP

Fortran	TQCSP (INDEXP, STATUS, VAL, IWSG, IWSE)	
C-interface	tq_csp(TC_INT index,TC_STRING status,TC_FLOAT amount,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Change Status of Phase.	
Purpose:	Change status for a phase.	
Comments:	The legal values for STATUS are given in Legal Phase Status. For ENTERED phase, VAL is provided as a start value. It is normally set to zero if the phase is not likely to be stable and one if expected to be stable. Setting a phase SUSPENDED or DORMANT is a way to calculate a metastable equilibrium if the phase would be stable. With the DORMANT status one can know if it would be stable or not. For these two statuses, VAL is irrelevant and may be simply put to zero. For FIXED phase the exact amount of the phase must be given. Note that the amount is in number of mole formula units. Setting a phase FIXED decreases the degrees of freedom in the system by 1. To restore the lost degree of freedom the phase should be reset ENTERED. Set a FIXED phase to zero amount is the best way to get the phase stability limits like liquidus or solidus.	
Arguments		
Name	Type	Value set on call or returned
INDEXP	Integer	Set to a phase index.
STATUS	Character*12	Set to the status code
VAL	Double precision	Set to phase amount in number of mole formula units.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGSP

This is a logical function.

Fortran	STATUS=TQGSP (INDEXP, STATUS, VAL, IWSG, IWSE)	
C-interface	**status=tq_gsp(TC_INT index,TC_STRING status,TC_STRING_LENGTH strlen_status,TC_FLOAT* amount,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Status of Phase.	
Purpose:	This function is TRUE if the phase is ENTERED or FIXED. If the phase is SUSPENDED or DORMANT it is FALSE. The status is also returned in STATUS. The application program can test the status of a phase by calling this function.	
Comments:	The legal values for STATUS are listed in Legal Phase Status. If the C-interface is used the value returned is of type: TC_BOOL.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index.
STATUS	Character*12	Return the current status code.
VAL	Double precision	Return the phase amount as mole formula units.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSETR

Fortran	TQSETR (INDEXC, INDEXP, TEMP, PRES, IWSG, IWSE)
C-interface	**tq_setr(TC_INT indexc,TC_INT indexp,TC_FLOAT temp,TC_FLOAT press,TC_INT* iwsg, TC_INT* iwse);**
Full name:	Set Reference State.
Purpose:	Reset the reference state of a system component.
Comments:	By default the reference state for a component is determined by the thermodynamic data file. With this subroutine an application may select a different reference state if the one in the data file does not suit a calculation purpose. If the current temperature or pressure should be used for the calculation, the value given should not be larger than zero.

Fortran	**TQSETR (INDEXC, INDEXP, TEMP, PRES, IWSG, IWSE)**	
C-interface	**tq_setr(TC_INT indexc,TC_INT indexp,TC_FLOAT temp,TC_FLOAT press,TC_INT* iwsg, TC_INT* iwse);**	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXC	Integer	Set to a component index.
INDEXP	Integer	Set to a phase index.
TEMP	Double precision	Set to a temperature value.
PRES	Double precision	Set to a pressure value.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQPACS

Fortran	**TQPACS (INDEXP, IWSG, IWSE)**	
C-interface	**tq_pacs(TC_INT indexp,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Add composition set to phase.	
Purpose:	Add another composition set to a phase.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSGA

Fortran	TQSGA (INDEXP, VALUE, IWSG, IWSE)	
C-interface	**tq_gga(TC_INT indexp,TC_FLOAT value,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Set Gibbs energy addition.	
Purpose:	Add an amount of extra contribution to the Gibbs energy of a phase	
Comments:	The extra contribution may be due to elastic strain energy, surface energy, etc.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index.
VALUE	Double precision	Set to the value of extra contribution (J/(mol formula unit)
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGGA

Fortran	TQGGA (INDEXP, VALUE, IWSG, IWSE)	
C-interface	**tq_gga(TC_INT indexp,TC_FLOAT* value,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Gibbs energy addition.	
Purpose:	The contribution added to the Gibbs energy of a phase can be retrieved.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index.
VALUE	Double precision	Return the value of extra contribution (J/(mol formula unit).
IWSG	Integer array	Workspace

Fortran	**TQGGA (INDEXP, VALUE, IWSG, IWSE)**	
C-interface	**tq_gga(TC_INT indexp,TC_FLOAT* value,TC_INT* iwsg,TC_INT* iwse);**	
IWSE	Integer array	Workspace

Condition, Stream and Segment Subroutines

A *stream* is considered as a non-reactive medium for transferring matter to a reaction zone. It has constant temperature and pressure, and contains one or more phases of a certain composition, i.e., for each stream, temperature, pressure, and input amounts of phase constituents must be defined. Different sets of equilibrium *conditions* can be defined for the same system in different *segments*.

Purpose	Subroutine
Set condition	TQSETC
Remove condition	TQREMC
Save current conditions	TQSCURC
Remove all conditions	TQREMAC
Restore saved conditions	TQRESTC
Create stream	TQCSTM
Set stream constituent amount	TQSSC
Set stream invariant state variable	TQSSIC
Delete stream	TQDSTM
Create new equilibrium segment	TQNSEG
Select equilibrium segment	TQSSEG

Possible State Variables to Set Conditions in TQSETC

STAVAR	INDEXP	INDEXC	Meaning	Comments
T			Temperature	of the whole system
P			Pressure	of the whole system
MU	note [1.]	Yes	Chemical potential	of a system component
MUC	Yes	Yes	Chemical potential	of a phase constituent
AC	note[1]	Yes	Activity	of a system component

[1.] Giving a phase index means to define the reference state. If no phase index is given the previous reference state is used. The default reference state is SER (Standard Element Reference) if the thermodynamic data file is created from a SGTE (Scientific Group Thermodata Europe) database. It is necessary that the phase can exist with the constituent as its single constituent. It is an error to set FCC as reference state for carbon if carbon dissolves interstitially in FCC.

STAVAR	INDEXP	INDEXC	Meaning	Comments
ACC	Yes	Yes	Activity	of a system constituent
V			Volume	of the whole system
G			Gibbs energy	of the whole system
H			Enthalpy	of the whole system
S			Entropy	of the whole system
N			Moles	of all system components
N		Yes	Moles	of a system component
NP	note [1.]		Moles	of a phase
M			Total mass	of all system components
M		Yes	Mass	of a system component
BP	note[2]		Mass	of a phase
IN	Yes	Yes	Input amount	in moles of phase constituents
IM	Yes	Yes	Input amount	in mass units of phase constituents
X		Yes	Mole fraction	of a system component
W		Yes	Mass (Weight) fraction	of a system component
X%		Yes	Mole percent	of a system component
W%		Yes	Mass (Weight) fraction	of a system component

TQSETC

Fortran	**TQSETC(STAVAR, INDEXP, INDEXC, VAL, NUMCON, IWSG, IWSE)**
C-interface	**tq_setc(TC_STRING condition,TC_INT indexp,TC_INT indexc,TC_ FLOAT val,TC_INT* numcon,TC_INT* iwsg,TC_INT* iwse);**
Full name:	Set Condition.
Purpose:	To set conditions for an equilibrium calculation.
Comments:	In STAVAR the mnemonic of the state variable must be given, see Possible State

[1.] Not recommended to be used for setting conditions. To calculate stability limit one should use TQCSP with FIXED status and amount of the phase set to zero.

Fortran	**TQSETC(STAVAR, INDEXP, INDEXC, VAL, NUMCON, IWSG, IWSE)**	
C-interface	**tq_setc(TC_STRING condition,TC_INT indexp,TC_INT indexc,TC_FLOAT val,TC_INT* numcon,TC_INT* iwsg,TC_INT* iwse);**	
	Variables to Set Conditions in TQSETC. In some cases just the mnemonic is needed, like for temperature or pressure, but in many cases a phase index or a component index must be used to specify the condition. If both a phase index and a constituent index is supplied the condition is set for the specified constituent in the specified phase. The application program must set exactly the same number of conditions as degrees of freedom in the defined system. The degrees of freedom are equal to the number of system components plus two (usually temperature and pressure). Setting a phase FIXED using TQCSP decrease the degrees of freedom in the system by 1. Resetting the phase ENTERED using TQCSP restores one degree of freedom. Possible combinations of STAVAR and indices are listed in Possible State Variables to Set Conditions in TQSETC. Here it is shown that the same value of STAVAR may be used with or without an index. In the case there should not be an index, the value of INDEXP or INDEXC must be negative. Some combination of conditions may be thermodynamically impossible. The TQ-Interface provides relevant help for such cases.	
Arguments		
Name	**Type**	**Value set on call or returned**
STAVAR	Character*8	Set as a state variable
INDEXP	Integer	Set as a phase index (if needed).
INDEXC	Integer	Set as a component or constituent index (if needed).
VAL	Double precision	Set to the value.
NUMCON	Integer	Returned as an identification of the condition.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

EXAMPLES

Set the temperature to 800 Celsius

```
CALL TQSSU('Temperature','C',IWSG,IWSE)
CALL TQSETC('T',-1,-1,800.0D0,NCOND,IWSG,IWSE)
Set the incoming amount of a liquid phase constituent named Al2O3 to 1.5 moles
CALL TQGPI(INDEXP,'LIQUID',IWSG,IWSE)
CALL TQGPCI(INDEXP,INDEXC,'AL2O3',IWSG,IWSE)
CALL TQSETC('IN',INDEXP,INDEXC,1.5D0,NCOND,IWSG,IWSE)
```

Set the mass percent of the system component Cr to 13%.

```
CALL TQGSCI(INDEX,'cr',IWSG,IWSE)
CALL TQSETC('W%',-1,INDEX,13.0D0,NCOND,IWSG,IWSE)
```

Set the total amount of system to 1.0 mole components

```
CALL TQSETC('N',-1,-1,1.0D0,NCOND,IWSG,IWSE)
```

Set the mole fraction of H2O in GAS to 5 mol percent

```
CALL TQGPI(INDEXP,'GAS',IWSG,IWSE)
CALL TQGPCI(INDEXP,INDEXC,'H2O1',IWSG,IWSE)
CALL TQSETC('X',INDEXP,INDEXC,0.05D0,NCOND,IWSG,IWSE)
```

TQREMC

Fortran	**TQREMC(NUMCON, IWSG, IWSE)**	
C-interface	**tq_remc(TC_INT numcon,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Remove Condition.	
Purpose:	Remove the condition numbered NUMCON.	
Comments:	TQSETC and TQCSTM return an index for each condition set. This value must be supplied in this call. In order to change a condition to something else, not just a new value, one must first remove the condition. If one just wants to change the value of a condition one may call TQSETC again instead.	
Arguments		
Name	**Type**	**Value set on call or returned**
NUMCON	Integer	Set to a condition number.

Fortran	TQREMC(NUMCON, IWSG, IWSE)	
C-interface	tq_remc(TC_INT numcon,TC_INT* iwsg,TC_INT* iwse);	
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSCURC

Fortran	TQSCURC(IWSG, IWSE)	
C-interface	tq_scurc(TC_INT* iwsg,TC_INT* iwse);	
Full name:	Save Current Conditions.	
Purpose:	Save all conditions in case they need to be restored.	
Comments:	The saved conditions can be restored if necessary by using TQRESTC.	
Arguments		
Name	Type	Value set on call or returned
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQREMAC

Fortran	TQREMAC(IWSG, IWSE)	
C-interface	tq_remac(TC_INT* iwsg,TC_INT* iwse);	
Full name:	Remove All Conditions.	
Purpose:	TQREMAC provides the easiest way to remove all conditions. After calling TQREMAC, one can set completely new or restore previously saved conditions.	
Arguments		
Name	Type	Value set on call or returned
IWSG	Integer array	Workspace

Fortran	TQREMAC(IWSG, IWSE)	
C-interface	tq_remac(TC_INT* iwsg,TC_INT* iwse);	
IWSE	Integer array	Workspace

TQRESTC

Fortran	TQRESTC(IWSG, IWSE)	
C-interface	tq_restc(TC_INT* iwsg,TC_INT* iwse);	
Full name:	Restore Condition.	
Purpose:	Restore saved conditions.	
Comments:	Before calling TQRESTC, remove all present conditions.	
Arguments		
Name	Type	Value set on call or returned
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQCSTM

Fortran	TQCSTM(IDENT, TEMP, PRESS, IWSG, IWSE)
C-interface	tq_cstm(TC_STRING stream,TC_FLOAT temp,TC_FLOAT press,TC_INT* iwsg,TC_INT* iwse);
Full name:	Create Stream
Purpose:	To set the system conditions by stream input. Stream calculations are useful when calculating differences between an initial state and a final state. The streams define the initial state of the system components by specifying reactants of different phases at given temperatures and pressures.
Comments:	A stream is a non-reacting media for transferring matter to a reaction zone. A stream may contain several phases at the same given temperature and pressure. Phases with different temperatures and pressures should be grouped into different streams. Several streams can be transferred to a reaction zone.

Fortran	TQCSTM(IDENT, TEMP, PRESS, IWSG, IWSE)	
C-interface	tq_cstm(TC_STRING stream,TC_FLOAT temp,TC_FLOAT press,TC_INT* iwsg,TC_INT* iwse);	
	The input constituents of each phase do not react in a stream.	
Arguments		
Name	Type	Value set on call or returned
IDENT	Character*24	Set as identifier of the stream.
TEMP	Double precision	Input temperature of stream.
PRESS	Double precision	Input pressure of stream.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSSC

Fortran	TQSSC(IDENT, INDEXP, INDEXC, VALUE, NUMIN, IWSG, IWSE)	
C-interface	tq_ssc(TC_STRING stream,TC_INT iph,TC_INT icmp,TC_FLOAT value,TC_INT icond,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Set Stream Constituent Amount.	
Purpose:	Set the amount of phase constituent in a stream.	
Comments:	The last one takes effect if the amount of the same phase constituent have been set several times, i.e., the amount cannot be set additively.	
Arguments		
Name	Type	Value set on call or returned
IDENT	Character*24	Set as identifier of the stream.
INDEXP	Integer	Set as a phase index
INDEXC	Integer	Set as a constituent index.
VALUE	Double precision	Set to an amount of the constituent INDEXC in

Fortran	TQSSC(IDENT, INDEXP, INDEXC, VALUE, NUMIN, IWSG, IWSE)	
C-interface	**tq_ssc(TC_STRING stream,TC_INT iph,TC_INT icmp,TC_FLOAT value,TC_INT icond,TC_INT* iwsg,TC_INT* iwse);**	
		the stream.
NUMIN	Integer	Returned as identification of the input constituent in the stream.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSSIC

Fortran	TQSSIC(STAVAR, VALUE, IWSG, IWSE)	
C-interface	**tq_ssic(TC_STRING stavar,TC_FLOAT value,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Set Stream Invariant State Variable.	
Purpose:	To specify the invariant state variable for calculating the reaction of all streams.	
Comments:	The state variables that could be used are G, H, S, and V with a suffix D, which means difference between initial and final states of the reaction.	
Arguments		
Name	**Type**	**Value set on call or returned**
STAVAR	Character*8	Set as the mnemonic of a state variable.
VALUE	Double precision	Set to change in value of STAVAR.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

EXAMPLES

Calculation of adiabatic temperature for knallgas.

```
DIMENSION TPA(2)
C...set input temperature and pressure
TEMP=298.15D0
PRES=1.0D5
C...create the stream
CALL TQCSTM('knallgas',TEMP,PRES,IWSG,IWSE)
C...set amount of H2 and O2 in the stream
CALL TQGPCI(1,INDEXC,'H2',IWSG,IWSE)
CALL TQSSC('knallgas',1,INDEXC,2.0D0,NUMIN,IWSG,IWSE)
CALL TQGPCI(1,INDEXC,'O2',IWSG,IWSE)
CALL TQSSC('knallgas',1,INDEXC,1.0D0,NUMIN,IWSG,IWSE)
C...set the global temperature and pressure for the reaction
CALL TQSETC('T',-1,-1,500.0D+0,NUMC,IWSG,IWSE)
CALL TQSETC('P',-1,-1,PRES,NUMC,IWSG,IWSE)
C...get  the enthalpy of reaction
CALL TQCE(' ',-1,-1,0.0D+0,IWSG,IWSE)
CALL TQGETV1('HD',-1,-1,ENT,IWSG,IWSE)
WRITE(*,*)'Calculated enthalpy of reaction are '
&, ENT, ' at 500 K. '
C...set that the enthalpy shall be constant in the calculation
CALL TQSSIC('HD',0.0D0,IWSG,IWSE)
C...calculate
CALL TQCE('T',-1,-1,1.0D+0,IWSG,IWSE)
C...get temperature
CALL TQGETV1('T',-1,-1,TEMP,IWSG,IWSE)
WRITE(*,*)'Calculated temperature ',TEMP
```

TQDSTM

Fortran	**TQDSTM(IDENT, IWSG, IWSE)**
C-interface	**tq_dstm(TC_STRING stream, TC_INT* iwsg,TC_INT* iwse);**
Full name:	Delete Stream.
Purpose:	Delete all or one stream.
Comments:	Use an empty string as IDENT removes all the streams entered.

Fortran	TQDSTM(IDENT, IWSG, IWSE)	
C-interface	tq_dstm(TC_STRING stream, TC_INT* iwsg,TC_INT* iwse);	
Arguments		
Name	Type	Value set on call or returned
IDENT	Character*24	Set as identifier of the stream.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQNSEG

Fortran	TQNSEG(ID, IWSG, IWSE)	
C-interface	tq_nseg(TC_STRING id, TC_INT* iwsg,TC_INT* iwse);	
Full name:	New Equilibrium Segment.	
Purpose:	With this subroutine the application program can create a new equilibrium description with the same thermodynamic data. This subroutine is useful when simulating several equilibria representing local conditions, for example, in the reactor simulator.	
Comments:	TQNSEG does not read any thermodynamic file. This must have already been done with TQRFIL. Note that when several segments are used, an equilibrium should be computed when a segment is selected before any data is retrieved.	
Arguments		
Name	Type	Value set on call or returned
ID	Character*24	Set as identifier of the equilibrium segment.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSSEG

Fortran	**TQSSEG(ID, IWSG, IWSE)**	
C-interface	**tq_sseg(TC_STRING id, TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Select Equilibrium.	
Purpose:	When the application program has created several equilibrium segments using TQNSEG, this subroutine makes it possible to select a current equilibria which the subroutine calls refer to.	
Comments:	When several segments are used, and before any data is retrieved, an equilibrium should be computed when a segment is selected.	
Arguments		
Name	**Type**	**Value set on call or returned**
ID	Character*24	Set to an equilibrium identification.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

Calculations and Results Subroutines

Purpose	Subroutine
Calculate equilibrium	TQCE
Calculate global equilibrium	TQCEG
Get equilibrium property values (TQGET) and Get one value (TQGET1)	TQGETV and TQGET1
Get chemical potential value. It is a double precision function.	TQGMU
Get molar Gibbs energy value. It is a double precision function.	TQGGM
Get phase data	TQGPD
Get driving force and local equilibrium compositions for ortho- or para-equilibrium phase transformation	TQGDF2
Get interfacial energy between a matrix phase and a precipitate phase	TQGSE

State Variables Available for TQGETV and TQGET1

STAVAR	INDEXP	INDEXC	Meaning	Comments
T			Temperature	of the whole system
P			Pressure	of the whole system
MU	(yes)	Yes	Chemical potential	of a system component
MUC	Yes	yes	Chemical potential	of a constituent in a gas phase
AC	(yes)	Yes	Activity	of a system component
ACC	Yes	Yes	Activity	of a constituent in a gas phase
QF	Yes		Phase stability function	Negative when phase composition is inside a spinodal, otherwise positive. Can be used to find out if an equilibrium is within the miscibility gap for a solution phase. Cannot be used as a condition.
V			Volume	of the whole system
V	Yes		Volume	of a phase
G*			Gibbs energy	of the whole system

STAVAR	INDEXP	INDEXC	Meaning	Comments
G*	Yes		Gibbs energy	of a phase
H*			Enthalpy	of the whole system
H*	Yes		Enthalpy	of a phase
S*			Entropy	of the whole system
S*	Yes		Entropy	of a phase
CP			Heat capacity	of the system
CP	Yes		Heat capacity	of a phase
DG	Yes		Driving force	of a phase
N			Moles	of all system components
N		Yes	Moles	of a system component
NP	Yes		Moles	of a system phase
M			Total mass	of all system components
M		Yes	Mass	of a system component
BP	Yes		Mass	of a system phase
IN	Yes	Yes	Input amount	in moles of phase constituents
IM	Yes	Yes	Input amount	in mass units of phase constituents
X		Yes	Mole fraction	of a component in the whole system
X	Yes	Yes	Mole fraction	of a component in a phase
W		Yes	Mass (Weight) fraction	of a component in the whole system
W	Yes	Yes	Mass (Weight) fraction	of a component in a phase
X%		Yes	Mole percent	of a component in the whole system
X%	Yes	Yes	Mole	of a component in a phase

STAVAR	INDEXP	INDEXC	Meaning	Comments
			percent	
W%		Yes	Mass (Weight) fraction	of a component in the whole system
W%	Yes	Yes	Mass (Weight) fraction	of a component in a phase
Y	Yes	Yes	Constituent fraction	of a phase constituent

* You can add a normalizing suffix like M (per mole), W (per mass) or V (per volume) on G, H, S, etc. R can also be added as a suffix on G, H, S to get a value that is calculated with respect to the reference state specified by calling TQSETR.

Additional Variables Available for TQGETV and TQGET1

STAVAR	Meaning	Unit
M(phase,J)	Mobility coefficient where J=diffusing species	m^2/s
LOGM(phase,J)	10log of the mobility coefficient	m^2/s
DT(phase,J)	Tracer diffusion coefficient where J=diffusing species	m^2/s
LOGDT(phase,J)	10log of the tracer diffusion coefficient	m^2/s
DC(phase,J,K,N)	Chemical diffusion coefficient where K=gradient specie, and N=reference specie	m^2/s
LOGDC(phase,J,K,N)	10log of the chemical diffusion coefficient	m^2/s
DI(phase,J,K,N)	Intrinsic diffusion coefficient	m^2/s
LOGDI(phase,J,K,N)	10log of the intrinsic diffusion coefficient	m^2/s
QC(phase,J,K,N)	Q=R(*ln*(DC{T1})-*ln*(DC{T1+ε}))/(1/(T1+ε)-1/T1)	J/mol
QT(phase,J)	Q=R(*ln*(DT{T1})-*ln*(DT{T1+ε}))/(1/(T1+ε)-1/T1)	J/mol
QI(phase,J,K,N)	Q=R(*ln*(DI{T1})-*ln*(DI{T1+ε}))/(1/(T1+ε)-1/T1)	J/mol
FC(phase,J,K,N)	D0=exp(ln(DC{T1})+Q/R/T1)	m^2/s
FI(phase,J,K,N)	D0=exp(ln(DI{T1})+Q/R/T1)	m^2/s

STAVAR	Meaning	Unit
FT(phase,J)	D0=exp(ln(DT{T1})+Q/R/T1)	m^2/s

TQCE

Fortran	TQCE(TARGET, INDEXP, INDEXC, VALUE, IWSG, IWSE)	
C-interface	tq_ce(TC_STRING var,TC_INT indexp,TC_INT indexc,TC_FLOAT value,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Calculate Equilibrium.	
Purpose:	Calculate the equilibrium with current settings of conditions or streams.	
Comments:	Some software needs a TARGET specified for certain types of calculations. A TARGET is a state variable as specified in TQSETC. When working with Thermo-Calc, it is only useful in stream reaction calculations, where an initial guess of the target variable may be of some help. Otherwise, TARGET is normally set as an empty string and the values of INDEXP, INDEXC, and VALUE are irrelevant.	
Arguments		
Name	Type	Value set on call or returned
TARGET	Character*8	Set to a state variable, if necessary.
INDEXP	Integer	Set to a phase index, if necessary.
INDEXC	Integer	Set to a component index, if necessary.
VALUE	Double precision	Set to an estimate of the target variable.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

EXAMPLE

Calculate enthalpy for an equilibrium gas mixture SO3, SO2 and O2. Input SO3 2%, O2 10% and 88% SO2.

```
CALL TQGPI('GAS',INDEXP,IWSG,IWSE)
```

```
C...set temperature, pressure and total amount of moles
CALL TQSETC('T',-1,-1,800.0D0,NCOND,IWSG,IWSE)
CALL TQSETC('P',-1,-1,1.0D5,NCOND,IWSG,IWSE)
CALL TQSETC('N',-1,-1,1.0D0,NCOND,IWSG,IWSE)
C...set mole fraction of SO3 and O2
CALL TQGPI(INDEXP,'GAS',IWSG,IWSE)
CALL TQGPCI(INDEXP,INDEXC,'SO2',IWSG,IWSE)
CALL TQSETC('IN',INDEXP,INDEXC,8.8D-1,NCOND,IWSG,IWSE)
CALL TQGPCI(INDEXP,INDEXC,'O2',IWSG,IWSE)
CALL TQSETC('IN',INDEXP,INDEXC,1.0D-1,NCOND,IWSG,IWSE)
CALL TQGPCI(INDEXP,INDEXC,'SO3',IWSG,IWSE)
CALL TQSETC('IN',INDEXP,INDEXC,2.0D-2,NCOND,IWSG,IWSE)
CALL TQCE(' ',0,0,0.0D+0,IWSG,IWSE)
CALL TQGETV1('H',-1,-1,ENT,IWSG,IWSE)
```

In this way an application program can calculate the incoming enthalpy into the system. If there is more than one incoming flow it can calculate the enthalpies for each flow and sum them up.

TQCEG

Fortran	**TQCEG(IWSG, IWSE)**
C-interface	**tq_ceg(TC_INT* iwsg,TC_INT* iwse);**
Full name:	Calculate Equilibrium Global.
Purpose:	Calculate Equilibrium using Global Minimization Algorithm.
Comments:	The use of global minimization algorithm is meant to avoid metastable or unstable equilibrium and to obtain truly stable equilibrium. This is mainly due to its ability to find automatically miscibility gap and create accordingly new composition sets. As a consequence, the number of phases may increase after calling TQCEG. The newly added phases (new composition sets of old phases) are always put in the end of the phase list. In this way, the indexes of old phases remain the same as before See Example 13. The global minimization technique starts with discretizing the composition

Fortran	TQCEG(IWSG, IWSE)	
C-interface	tq_ceg(TC_INT* iwsg,TC_INT* iwse);	
	space and calculating Gibbs energy values at each grid point for each phase at a given temperature. This usually leads to a significant increase of computation time. Therefore, it is not recommended to use TQCEG in time-critical application programs. In the cases where phases involved are well known, for example, identifying the local equilibrium at a phase interface, it is absolutely not necessary to use TQCEG. If TQCEG is needed, irrelevant phases should better be rejected in the beginning when fetching thermodynamic data from a database.	
Arguments		
Name	Type	Value set on call or returned
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGETV and TQGET1

Fortran	TQGETV(STAVAR, INDEXP, INDEXC, NUMBER, VALAR, IWSG, IWSE) TQGET1(STAVAR, INDEXP, INDEXC, VAL, IWSG, IWSE)
C-interface	tq_getv(TC_STRING stavar,TC_INT indexp,TC_INT indexc,TC_INT number,TC_FLOAT* valar,TC_INT* iwsg,TC_INT* iwse); tq_get1(TC_STRING stavar,TC_INT indexp,TC_INT indexc,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);
Full name:	Get Values. With TQGETV an array of values can be returned; with TQGET1 a single value only.
Purpose:	These subroutines return the value of any variable in the system after an equilibrium calculation, for example, thermodynamic properties for phases and constituents, temperature, pressure and volume of the system, and amount of the system, a phase or a constituent.
Comments:	If an equilibrium is not established, the error code is set on return. Go to State Variables Available for TQGETV and TQGET1 for obtaining values.

Fortran	**TQGETV(STAVAR, INDEXP, INDEXC, NUMBER, VALAR, IWSG, IWSE)** **TQGET1(STAVAR, INDEXP, INDEXC, VAL, IWSG, IWSE)**
C-interface	**tq_getv(TC_STRING stavar,TC_INT indexp,TC_INT indexc,TC_INT number,TC_FLOAT* valar,TC_INT* iwsg,TC_INT* iwse);** **tq_get1(TC_STRING stavar,TC_INT indexp,TC_INT indexc,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);**
	Valid INDEXC or INDEXP has a positive value. Setting INDEXC or INDEXP to -1 means it is not relevant. Using 0 for INDEXC or INDEXP in TQGETV means all components or all phases, respectively.

Arguments

Name	Type	Value set on call or returned
STAVAR	Character*32	Set to mnemonic of state variable
INDEXP	Integer	Set to a phase index
INDEXC	Integer	Set to a component or constituent index
NUMBER	Integer	Set to the number of values in VALAR.
VALAR	Double precision array	Return the values
VAL	Double precision	Return the value
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

EXAMPLES

Get temperature of the system

```
CALL TQGET1('T',-1,-1,VAL,IWSG,IWSE)
```

Get overall mole fraction of system component Cr

```
CALL TQGSCI(INDEXC,'CR',IWSG,IWSE)
CALL TQGET1('X',-1,INDEXC,VAL,IWSG,IWSE)
```

Get overall mole fractions of all components

```
CALL TQGETV('x',-1,0,NCOM,VALAR,IWSG,IWSE)
```

Get activity of system component SiC

```
CALL TQGSCI(INDEXC,'sic',IWSG,IWSE)
CALL TQGET1('AC',-1,INDEXC,VAL,IWSG,IWSE)
```

Get activity of gas phase constituent SiC (gas is phase 1)

```
CALL TQGPCI(1,INDEXC,'sic',IWSG,IWSE)
CALL TQGET1('AC',1,INDEXC,VAL,IWSG,IWSE)
```

Get total mass of system

```
CALL TQGET1('M',-1,-1,VAL,IWSG,IWSE)
CALL TQGET1('M',0,0,VAL,IWSG,IWSE)
```

Get total mass of liquid phase

```
CALL TQGPI(INDEXP,'LIQUID',IWSG,IWSE)
```

or

```
CALL TQGET1('BP',INDEXP,-1,VAL,IWSG,IWSE)
```

Get mass of all constituents of liquid phase

```
CALL TQGPI(INDEXP,'LIQUID',IWSG,IWSE)
CALL TQGETV('IM',INDEXP,0,NVAL,VALAR,IWSG,IWSE)
```

Get mass of SIC in liquid phase

```
CALL TQGPI(INDEXP,'LIQUID',IWSG,IWSE)
CALL TQGPCI(INDEXP,INDEXC,'sic',IWSG,IWSE)
CALL TQGET1('IM',INDEXP,INDEXC,VAL,IWSG,IWSE)
```

Get volume of GAS phase

```
CALL TQGET1('V',1,-1,VAL,IWSG,IWSE)
```

Get constituent mole fraction of H2O in GAS

```
CALL TQGPCI(1,INDEXC,'h2o',IWSG,IWSE)
CALL TQGET1('y',1,INDEXC,VAL,IWSG,IWSE)
```

Get partial pressure of H2O in GAS (equal to the total pressure times the constituent mole fraction)

```
CALL TQGPCI(1,INDEXC,'h2o',IWSG,IWSE)
CALL TQGET1('y',1,INDEXC,VAL,IWSG,IWSE)
```

```
CALL TQGET1('p',-1,-1,PVAL,IWSG,IWSE)
PH2O = PVAL*VAL
```

Get chemical potentials of all constituents in slag

```
CALL TQGPI(INDEXP,'slag',IWSG,IWSE)
CALL TQGETV('MUC',INDEXP,0,NCON,VALAR,IWSG,IWSE)
```

TQGMU

This is a double precision function.

Fortran	**TQGMU (INDEXC, IWSG, IWSE)**	
C-interface	**tq_gmu(TC_INT indexc, TC_INT* iwsg, TC_INT* iwse);**	
Full name:	Get Chemical Potential.	
Purpose:	This function returns the chemical potential of a component in a faster way.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXC	Integer	Set to a component index
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGGM

This is a double precision function.

Fortran	**TQGGM (INDEXP, IWSG, IWSE)**	
C-interface	**tq_ggm(TC_INT indexp, TC_INT* iwsg, TC_INT* iwse);**	
Full name:	Get Molar Gibbs Energy.	
Purpose:	This function returns the molar Gibbs energy of a phase more quickly.	
Arguments		
Name	**Type**	**Value set on call or returned**

Fortran	TQGGM (INDEXP, IWSG, IWSE)	
C-interface	**tq_ggm(TC_INT indexp, TC_INT* iwsg, TC_INT* iwse);**	
INDEXP	Integer	Set to a phase index
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGPD

Fortran	TQGPD (INDEXP, NSUB, NSCON, SITES, YFRAC, EXTRA, IWSG, IWSE)	
C-interface	**tq_gpd(TC_INT indexp,TC_INT* nsub,TC_INT* nscon,TC_FLOAT* sites,TC_FLOAT* yfrac,TC_FLOAT* extra,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Phase Data.	
Purpose:	The application program can get data for the constituents of a phase.	
Comments:	With this subroutine the application program can determine the structure of the phase and the fraction of the constituents and other things. Note that YFRAC is constituent fraction, not mole fractions.A substitutional phase has NSUB equal to 1, which is identical to no sublattice. That is true for the gas phase too. The maximum number of sublattices are 10. The constituents of a phase are numbered sequentially from 1 for the first constituent on the first sublattice, to NPCON (See TQGNPC) for the last constituent on the last sublattice. NSCON (L) is the number of constituents on sublattice L. The sum of NSCON over all sublattices is equal to NPCON. Note that constituents that are DORMANT and SUSPENDED still are counted in NPCON and NSCON. They also have a fraction in YFRAC (which must be zero of course). EXTRA may contain extra information about the phase, total mass for example. These are yet to be defined.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index
NSUB	Integer	Return the number of sublattices.

Fortran	TQGPD (INDEXP, NSUB, NSCON, SITES, YFRAC, EXTRA, IWSG, IWSE)	
C-interface	tq_gpd(TC_INT indexp,TC_INT* nsub,TC_INT* nscon,TC_FLOAT* sites,TC_FLOAT* yfrac,TC_FLOAT* extra,TC_INT* iwsg,TC_INT* iwse);	
NSCON	Integer array	Return the number of constituents on each sublattice.
SITES	Double precision array	Return the number of sites on each sublattice.
YFRAC	Double precision array	Return the fractions of the constituents.
EXTRA	Double precision array	Return some special values (see Comments)
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

EXAMPLES

To list the constituent names and fractions by sublattices. It is assumed that there are max 10 sublattices and max 500 constituents on all sublattices altogether.

```
DIMENSION NSCON(10),SITES(10),YFRAC(500),EXTRA(5)
CHARACTER NAME*24
LOGICAL TQGSPC
...
CALL TQGPN(INDEXP,NAME,IWSG,IWSE)
CALL TQGPD(INDEXP,NSUB,NSCON, SITES,YFRAC,EXTRA, &IWSG,IWSE)
KK=0
WRITE(*,190)NAME,NSUB
190 FORMAT(' The phase ',A,' has ',I2,' sublattices')
DO 300 LS=1,NSUB
WRITE(*,191)LS,SITES(LS),NSCON(LS)
191 FORMAT('On sublattice ',I2,' there are ',F8.4,&' sites and',I3,' constituents')
DO 200 LC=1,NSCON(LS)
KK=KK+1
CALL TQGPCN(INDEXP,KK,NAME,IWSG,IWSE)
```

```
WRITE(*,192)NAME,YFRAC(KK)
192 FORMAT('Constituent ',A,' has fraction',&1P1E15.8)
200 CONTINUE
300 CONTINUE
```

TQGDF2

Fortran	**TQGDF2 (MODE, IMATR, IPREC, NIE, IIE, XMATR, TEMP, DF, XPREC, XEM, XEP, MUI, IWSG, IWSE)**	
C-interface	**tq_gdf2(TC_INT mode,TC_INT imatr,TC_INT iprec,TC_INT nie,TC_INT *iie,TC_FLOAT* xmatr,TC_FLOAT temp,TC_FLOAT* df,TC_FLOAT* xprec,TC_FLOAT* xem,TC_FLOAT* xep,TC_FLOAT* mui,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get the driving force of nucleation and local equilibrium concentration for a phase transformation under para- or ortho-equilibrium condition.	
Purpose:	Obtain data on both the chemical driving force for the nucleation of a precipitate and the local equilibrium concentration at the matrix/precipitate interface under para- or ortho-equilibrium conditions.  See Example 11.	
Comments:	For ortho-equilibrium calculations, XPREC can be inputs or outputs, depending on whether its values are known before the calculation or not. If unknown, the values of XPREC should be set to zero or negative when calling this subroutine and on return one obtains the composition of the precipitate at which the maximum driving force is available. The use of this subroutine for the ortho-equilibrium calculation supersedes that of the obsolete subroutine TQGDF.	
Arguments		
Name	**Type**	**Value set on call or returned**
MODE	Integer	Set type of output and type of composition to use (±1, ±2, and ±3 correspond to mole fraction, weight fraction and U-fraction respectively. However, ±3 can be used only with para-equilibrium calculations. If negative, calculate and output only driving force data. This saves the time for equilibrium calculation when you are not interested in local equilibrium concentrations)
IMATR	Integer	Set index of matrix phase

Fortran	**TQGDF2 (MODE, IMATR, IPREC, NIE, IIE, XMATR, TEMP, DF, XPREC, XEM, XEP, MUI, IWSG, IWSE)**	
C-interface	**tq_gdf2(TC_INT mode,TC_INT imatr,TC_INT iprec,TC_INT nie,TC_INT *iie,TC_FLOAT* xmatr,TC_FLOAT temp,TC_FLOAT* df,TC_FLOAT* xprec,TC_FLOAT* xem,TC_FLOAT* xep,TC_FLOAT* mui,TC_INT* iwsg,TC_INT* iwse);**	
IPREC	Integer	Set index of precipitate phase
NIE	Integer	Set number of interstitial element(s). Zero implies no para-equilibrium calculation
IIE	Integer array	Set index of interstitial element(s), only relevant for para-equilibrium condition
XMATR	Double precision array	Set composition of matrix phase. Composition type depends on MODE
TEMP	Double precision	Set temperature in Kelvin
DF	Double precision	Return driving force in J/mol of atoms if MODE = ±1, ±2 and J/mole of substitional atoms if MODE = ±3
XPREC	Double precision array	Return composition of the precipitate phase at the maximum driving force under para/ ortho-equilibrium condition or set to a known composition of the precipitate in order to get the driving force of phase transformation. Composition type depends on MODE
XEM	Double precision array	Return, if both MODE and DF are positive, local equilibrium composition of matrix phase. Composition type depends on MODE
XEP	Double precision array	Return, if both MODE and DF positive, local equilibrium composition of precipitate phase. Composition type depends on MODE
MUI	Double precision array	Return, if both MODE and DF are positive, chemical potential of interstitial elements. Relevant for only para-equilibrium calculation.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGSE

Fortran	TQGSE (IMATR, IPREC, IMC,TEMP, U, VOLM,VOLP, IWSG, IWSE)	
C-interface	tq_gse (TC_INT imatr,TC_INT iprec,TC_INT imc,TC_FLOAT temp,TC_FLOAT* u,TC_FLOAT volm,TC_FLOAT volp,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get interfacial energy between a matrix phase and a precipitate phase.	
Purpose:	With this subroutine the application program can estimate the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. The approximation model is based on Becker's bond energy approach is available as the *Interfacial Energy* model included with the Property Model Calculator and Precipitation Module (TC-PRISMA). For systems with interstitial elements note the following: • The composition array must contain so-called u-fractions. ▶ The u-Fraction Variable in the *Thermo-Calc Console Mode User Guide*. • The molar volumes of the matrix and precipitate should be with respect to substitutional elements. This can be achieved by first setting the component status to 'SPECIAL' for the interstitial elements with TQCSSC, and then retrieve the correct molar volume with TQGET1 ('VM',...). An equilibrium calculation is not required prior to using this function.	
Arguments		
Name	**Type**	**Value set on call or returned**
IMATR	Integer	Set index of matrix phase
IPREC	Integer	Set index of precipitate phase
IMC	Integer	Set index of major component
TEMP	Double precision	Set temperature in Kelvin
U	Double precision array	Set overall alloy composition in u-fraction

Fortran	**TQGSE (IMATR, IPREC, IMC,TEMP, U, VOLM,VOLP, IWSG, IWSE)**	
C-interface	**tq_gse (TC_INT imatr,TC_INT iprec,TC_INT imc,TC_FLOAT temp,TC_FLOAT* u,TC_FLOAT volm,TC_FLOAT volp,TC_INT* iwsg,TC_INT* iwse);**	
VOLM	Double precision	Set molar volume of matrix phase with respect to substitutional elements
VOLP	Double precision	Set molar volume of precipitate phase with respect to substitutional elements
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace
Return Value		
TQGSE	Double precision	The interfacial energy in J/m^2

Miscellaneous Subroutines

Purpose	Subroutine
List status	TQLS
List conditions	TQLC
List equilibrium	TQLE
Force automatic start values	TQFASV
Keep composition set numbers	TQKEEP_CS_NUMBERS
Set default major constituent	TQSDMC
Set start phase constitution	TQSSPC
Set start value of a state variable	TQSSV
Reinitiate the calculation workspace	TQPINI
Set numerical limits	TQSNL
Set maximum number of grid points	TQSMNG
Set equilibrium calculation options	TQSECO
Set error code and give message	ST1ERR
Set error code	ST2ERR
Get error code and give message	SG1ERR or TQG1ERR *
Get error code	SG2ERR or TQG2ERR *
Get error code and message	SG3ERR or TQG3ERR *
Reset error code and message	RESERR or TQRSERR
Save a POLY-3 file	TQSP3F
	* Logical function

TQLS

Fortran	TQLS(IWSG, IWSE)	
C-interface	tq_ls(TC_INT* iwsg,TC_INT* iwse);	
Full name:	List Status.	
Purpose:	Listing status of all components, phases, and species in a system.	
Comments:	If necessary, use this subroutine to check if the status of all components, phases, and species has been correctly set in an application program. It should only be used for debugging purpose.	
Arguments		
Name	Type	Value set on call or returned
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQLC

Fortran	TQLC(IWSG, IWSE)	
C-interface	tq_lc(TC_INT* iwsg,TC_INT* iwse);	
Full name:	List Conditions.	
Purpose:	Listing conditions set for the current equilibrium calculation.	
Comments:	If necessary, use this subroutine to check if the conditions for an equilibrium calculation in the application program has been correctly set. It should only be used for debugging purpose.	
Arguments		
Name	Type	Value set on call or returned
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQLE

Fortran	**TQLE(IWSG, IWSE)**	
C-interface	**tq_le(TC_INT* iwsg,TC_INT* iwse);**	
Full name:	List Equilibrium.	
Purpose:	Listing results from the most recent equilibrium calculation. The output depends on the package used and the listing displays on the current output unit.	
Comments:	If necessary, use this subroutine to check if an equilibrium calculation is successful. It should only be used for debugging purpose.	
Arguments		
Name	**Type**	**Value set on call or returned**
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQFASV

Fortran	**TQFASV(IWSG, IWSE)**	
C-interface	**tq_fasv(TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Force Automatic Start Value.	
Purpose:	To force automatic start-values for all phases in a single equilibrium calculation.	
Comments:	This is not required unless the calculation fails.	
Arguments		
Name	**Type**	**Value set on call or returned**
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQKEEP_CS_NUMBERS

Fortran	TQKEEP_CS_NUMBERS(IWSE, KEEP)	
C-interface	tq_keep_cs_numbers(TC_INT* iwse, TC_BOOL* keep);	
Full name:	Keep composition set numbers.	
Purpose:	To prevent composition set ID-numbers from switching between consecutive equilibrium calculations.	
Comments:	This subroutine turns on/off the functionality to keep the composition set numbers from the previous equilibrium calculations. By default the setting is off. Once turned on, it affects all subsequent equilibrium calculations until explicitly turned off again.	
Arguments		
Name	Type	Value set on call or returned
IWSE	Integer array	Workspace
KEEP	Logical	TRUE will turn the functionality on, FALSE off

TQSDMC

Fortran	TQSDMC(INDEXP, IWSG, IWSE)	
C-interface	tq_sdmc(TC_INT indexp,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Set Default Major Constituents.	
Purpose:	To set the major phase constituents to the default ones defined in the thermodynamic data file.	
Comments:	Major constituents in a phase can be set in the Gibbs (GES) module of Thermo-Calc and then saved into a thermodynamic data file for the use of this interface.	
Arguments		
Name	Type	Value set on call or returned

Fortran	**TQSDMC(INDEXP, IWSG, IWSE)**	
C-interface	**tq_sdmc(TC_INT indexp,TC_INT* iwsg,TC_INT* iwse);**	
INDEXP	Integer	Set as a phase index
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSSPC

Fortran	**TQSSPC(INDEXP, YF, IWSG, IWSE)**	
C-interface	**tq_sspc(TC_INT indexp,TC_FLOAT* yf,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Set Start Phase Constitution.	
Purpose:	To set start-values for the constitution of an individual phase.	
Comments:	It is not necessary unless the calculation fails, especially when involving a miscibility gap or an ordering phase.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set as a phase index
YF	Double precision array	Set to the site fraction of each constituent.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSSV

Fortran	TQSSV(STAVAR, IP, IC, VALUE, IWSG, IWSE)	
C-interface	tq_ssv(TC_STRING stavar,TC_INT ip,TC_INT ic,TC_FLOAT value,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Set Start Variable.	
Purpose:	To set start-value for a state variable.	
Comments:	It is not necessary unless the calculation fails.	
Arguments		
Name	Type	Value set on call or returned
STAVAR	Character*8	Set as a state variable listed in Possible State Variables to Set Conditions in TQSETC
IP	Integer	Set as a phase index (if needed).
IC	Integer	Set as a component or constituent index (if needed).
VALUE	Double precision	Set to the value.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQPINI

Fortran	TQPINI(IWSG, IWSE)
C-interface	tq_pini(TC_INT* iwsg,TC_INT* iwse);
Full name:	Poly-3 reINItiation.
Purpose:	Reinitiate the POLY-3 workspace in Thermo-Calc kernel.
Comments:	Preparing for a fresh calculation.
Arguments	

Fortran	TQPINI(IWSG, IWSE)	
C-interface	tq_pini(TC_INT* iwsg,TC_INT* iwse);	
Name	Type	Value set on call or returned
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSNL

Fortran	TQSNL(MAXIT, ACC, YMIN, ADG, IWSG, IWSE)	
C-interface	tq_snl(TC_INT maxit,TC_FLOAT acc,TC_FLOAT ymin,TC_STRING adg,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Set Numerical Limits	
Purpose:	To set the Numerical Limits to be used inside POLY-3.	
Comments:	It is not necessary unless the calculation fails.	
Arguments		
Name	Type	Value set on call or returned
MAXIT	Double precision	Set maximum number of iterations when calculating equilibrium. Default value is 500.
ACC	Double precision	Set required relative accuracy when calculating equilibrium. Default value is 1E-6.
YMIN	Double precision	Set smallest fraction to assign to unstable constituents. Default value is 1E-30.
ADG	Character*1	Specify if the calculation should be forced to converge also for the meta stable phases. Legal options are Y or N, where Y means yes and N means no. N is default.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSMNG

Fortran	TQSMNG(NGP, IWSG, IWSE)	
C-interface	tq_smng(TC_INT ngp,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Set Maximum Number of Grid points for each phase.	
Purpose:	To change the maximum number of grid points that can be used for each phase.	
Comments:	The global minimization technique starts with discretizing the composition space and calculating Gibbs energy values at each grid point for each phase. To balance its efficiency and robustness, an appropriate density of grid points should be chosen. The default value of NGP is 2000. In practice, the number of grid points generated during a normal calculation is much less than this value. However, under certain circumstances, one does need to increase the density of grid point for some phases in order to find a true stable equilibrium.	
Arguments		
Name	Type	Value set on call or returned
NGP	Integer	Number of grid points
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSECO

Fortran	TQSECO(IPDH, ICSS, IWSG, IWSE)	
C-interface	tq_seco(TC_INT ipdh,TC_INT icss,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Set Equilibrium Calculation Option.	
Purpose:	To choose equilibrium calculation options.	
Comments:	TQ starts with IPDH=1 and ICSS=1 by default.	
Arguments		
Name	Type	Value set on call or returned

Fortran	TQSECO(IPDH, ICSS, IWSG, IWSE)	
C-interface	**tq_seco(TC_INT ipdh,TC_INT icss,TC_INT* iwsg,TC_INT* iwse);**	
IPDH	Integer	1 = Force positive definite Hessian0 = Do not force positive definite Hessian
ICSS	Integer	1 = Control stepsize during minimization 0 = Do not control stepsize during minimization
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

ST1ERR

Fortran	ST1ERR(IERR, SUBR, MESS)
C-interface	**tq_st1err(TC_INT ierr,TC_STRING subr,TC_STRING mess);**
Full name:	Set Error Code and Give Message.
Purpose:	This is called when an error that cannot be handled by the current program unit occurs. The error message is printed on the error unit but also saved internally in the error handling package. The program unit should return to the calling program.
Comments:	The error-handling routines are those defined by SGTE for use in the thermodynamic model package. Note that the error-handling is constructed in such a way that when a subroutine detects an error it cannot handle, it should first call an ST* subroutine to set an appropriate error code and then return to the calling subroutine. In that subroutine the error code should be tested, and possibly that subroutine can correct the error and proceed, otherwise it should return to its calling subroutine and so on, until either the error is corrected or the top level of the program is reached.In this way it is possible to design a program where minor problems at a low level do not cause program to terminate. Instead, the error is passed up to a higher level where it can be corrected or ignored. The normal subroutines to use are ST2ERR to set the error code and SG2ERR to check it. The other subroutines are less used.

Fortran	ST1ERR(IERR, SUBR, MESS)	
C-interface	tq_st1err(TC_INT ierr,TC_STRING subr,TC_STRING mess);	
	The TQ subroutines normally do not clear the error code when called. An error set in an earlier subroutine but not tested and detected after that call may cause strange error messages later on. This should be used only for fatal or almost fatal errors.	
Arguments		
Name	Type	Value set on call or returned
IERR	Integer	Set to an error code.
SUBR	Character*6	Set to the current subroutine name.
MESS	Character*72	Set to the error message to be printed

ST2ERR

Fortran	ST2ERR(IERR, SUBR, MESS)	
C-interface	tq_st2err(TC_INT ierr,TC_STRING subr,TC_STRING mess);	
Full name:	Set Error Code.	
Purpose:	Called when an error occurs that cannot be handled by the current program unit. The program unit should return to the calling program.	
Comments:	Identical to ST1ERR except that it is silent, i.e., no error message is printed. This should be the normal subroutine to call when detecting errors that should be handled by a higher level of the program.	
Arguments		
Name	Type	Value set on call or returned
IERR	Integer	Set to an error code.
SUBR	Character*6	Set to the current subroutine name.
MESS	Character*72	Set to the error message to be printed

SG1ERR or TQG1ERR

This is a logical function.

Fortran	ERROR=SG1ERR(IERR) or ERROR=TQG1ERR(IERR)	
C-interface	error=tq_sg1err(TC_INT* ierr);	
Full name:	Get Error Code and Give Message.	
Purpose:	This is a logical function which could be called after calling a TQ subroutine that can detect an error when the error message should be displayed. If there is an error the function value is .TRUE and the appropriate error code is in IERR. This subroutine also prints the error message on the error unit.	
Comments:	Use when the error is almost fatal. Note that it is possible that the error message is already printed by ST1ERR. Use SG2ERR in most cases. If no error the function value is .FALSE and IERR is zero. If the C-interface is used the value returned is of type: TC_BOOL.	
Arguments		
Name	Type	Value set on call or returned
IERR	Integer	Set to the error code

SG2ERR or TQG2ERR

This is a logical function.

Fortran	ERROR=SG2ERR(IERR) or ERROR=TQG2ERR(IERR)
C-interface	error=tq_sg2err(TC_INT* ierr);
Full name:	Get Error Code.
Purpose:	This is a logical function which should be called after calling any TQ subroutine that can detect an error. If there is an error the function value is .TRUE and the appropriate error code is in IERR. This subroutine does not print the error message.
Comments:	Use for the normal error checking. Note that it is possible that the error message has already been printed by ST1ERR. The program may be able to

Fortran	ERROR=SG2ERR(IERR) or ERROR=TQG2ERR(IERR)	
C-interface	error=tq_sg2err(TC_INT* ierr);	

	handle the error to pass it on upwards. If no error the function value is .FALSE and IERR is zero. If the C-interface is used the value returned is of type: TC_ BOOL.
	
	EXAMPLE
	`LOGICAL SG2ERR`
	`...`
	`CALL TQCE(' ',IWSG,IWSE)`
	`IF(SG2ERR(IERR)) GOTO 900`
	`...`
	`900 RETURN`	

Arguments		
Name	**Type**	**Value set on call or returned**
IERR	Integer	Set to the error code

SG3ERR or TQG3ERR

This is a logical function.

Fortran	ERROR=SG3ERR(IERR, SUBR, MESS) or ERROR=TQG3ERR(IERR, SUBR, MESS)
C-interface	error=tq_sg3err(TC_INT* ierr,TC_STRING subr,TC_STRING_LENGTH strlen_subr,TC_STRING mess,TC_STRING_LENGTH strlen_mess);
Full name:	Get Error Code and Message.
Purpose:	This is a logical function which could be called after calling any TQ subroutine that can detect an error. If there is an error the function value is .TRUE and the appropriate error code is in IERR, the subroutine that detected the error in SUBR and the message in MESS. No printing on the error unit. This is useful if the calling program wants to print the message itself in an appropriate context.
Comments:	This should be used when the error testing subroutine wants to handle the printing of the error message itself. It is possible that the error message has

Fortran	**ERROR=SG3ERR(IERR, SUBR, MESS) or ERROR=TQG3ERR(IERR, SUBR, MESS)**	
C-interface	**error=tq_sg3err(TC_INT* ierr,TC_STRING subr,TC_STRING_LENGTH strlen_subr,TC_STRING mess,TC_STRING_LENGTH strlen_mess);**	
	already been printed by ST1ERR. If the C-interface is used the value returned is of type: TC_BOOL.	
Arguments		
Name	**Type**	**Value set on call or returned**
IERR	Integer	Return the error code.
SUBR	Character*6	Return the name of the subroutine detecting an error.
MESS	Character*72	Return the error message

RESERR or TQRSERR

Fortran	**RESERR or TQRSERR**
C-interface	**tq_reserr();**
Full name:	Reset Error Code and Message.
Purpose:	This subroutine resets the error code. A subsequent call to the SG* functions gives no error.
Comments:	This should be used when the error has been cleared so that execution can continue. Unless the error code is cleared by this subroutine the SG* functions continue to report the same error.
Arguments	None

TQSP3F

Fortran	**TQSP3F(FILE, IWSG, IWSE)**	
C-interface	**tq_sp3f(TC_STRING filename,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Save the workspaces on a POLY-3 file.	
Purpose:	This subroutine save the current workspaces of a POLY-3 file that can be read into the Thermo-Calc program to see what conditions are set.	
Arguments		
Name	**Type**	**Value set on call or returned**
FILE	Character*72	Set to file name to which workspaces should be saved.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

Extra Subroutines–Phase Properties

Purpose	Subroutine
Get Gibbs energy of a phase, Method A, B, and C*	TQGMA, TQGMB and TQGMC
Get 1st partial derivative of Gibbs energy w.r.t. site fractions.*	TQGMDY
Get mobility of a species in a phase.	TQGMOB
Set temperature and pressure for TQGMC, TQGMDY, and TQGMOB.	TQSTP
Set site fractions for TQGMB, TQGMC, TQGMDY, and TQGMOB.	TQSYF
Get index of a system species.	TQGSSPI
Check if Mobility data is available Method A and B	TQCMOBA and TQCMOBB†
Get 1st and 2nd partial derivative of Gibbs energy w.r.t. site fractions.*	TQDGYY
Get constitutional properties of a phase.*	TQGPHP
Convert mole fraction to site fraction for phases with no internal degree of freedom.*	TQX2Y
Convert 1st partial derivative of Gibbs energy w.r.t. site fractions to that w.r.t. mole fractions.*	TQGMDX
*in SI unit for one mole of formula unit.	† Logical function.

TQGMA, TQGMB and TQGMC

Fortran	**TQGMA(INDEXP, TP, YF, VAL, IWSG, IWSE)** **TQGMB(INDEXP, TP, VAL, IWSG, IWSE)** **TQGMC(INDEXP, VAL, IWSG, IWSE)**
C-interface	**tq_gma(TC_INT indexp,TC_FLOAT* tp,TC_FLOAT* yf,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);tq_gmb(TC_INT indexp,TC_FLOAT* tp,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);** **tq_gmc(TC_INT indexp,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);**
Full name:	Get Gibbs Energy – Method A, B, and C.
Purpose:	Getting Gibbs energy of a phase if temperature, pressure, and site fractions are given as arguments or by other subroutines shown.

Fortran	**TQGMA(INDEXP, TP, YF, VAL, IWSG, IWSE)** **TQGMB(INDEXP, TP, VAL, IWSG, IWSE)** **TQGMC(INDEXP, VAL, IWSG, IWSE)**
C-interface	**tq_gma(TC_INT indexp,TC_FLOAT* tp,TC_FLOAT* yf,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);tq_gmb(TC_INT indexp,TC_FLOAT* tp,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);** **tq_gmc(TC_INT indexp,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);**
Comments:	The returned value is in J/mole of formula unit. Remember this subroutine requires no action of setting condition and calculating equilibrium. It is for getting the Gibbs energy of a single phase with given temperature, pressure and atomic arrangements no matter if the phase is stable, metastable, or unstable in competition with other phases. The application program should take care of the phase stability or phase equilibrium if it is of interest.

Arguments

Name	Type	Value set on call or returned
INDEXP	Integer	Set to a phase index.
TP	Double precision array	Set to temperature and pressure values.
YF	Double precision array	Set to site fraction values in the index order of phase constituent.
VAL	Double precision	Return Gibbs energy value.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGMDY

Fortran	**TQGMDY(INDEXP, VARR, IWSG, IWSE)**
C-interface	**tq_gmdy(TC_INT indexp,TC_FLOAT* varr,TC_INT* iwsg,TC_INT* iwse);**
Full name:	Get Gibbs Energy and its partial Derivative w.r.t. y-fraction.
Purpose:	Getting Gibbs energy and its 1st partial derivatives with respect to site fractions

Fortran	TQGMDY(INDEXP, VARR, IWSG, IWSE)	
C-interface	**tq_gmdy(TC_INT indexp,TC_FLOAT* varr,TC_INT* iwsg,TC_INT* iwse);**	
	for a phase if temperature, pressure, and site fractions have been given by other subroutines shown.	
Comments:	The returned value is in J/mole of formula unit. Remember this subroutine requires no action of setting condition and calculating equilibrium. It is for getting the Gibbs energy and its 1st partial derivative w.r.t site fractions for a single phase with given temperature, pressure and atomic arrangements no matter if the phase is stable, metastable, or unstable in competition with other phases. The application program should take care of the phase stability or phase equilibrium if it is of interest.  This subroutine is demonstrated in Example 9.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index.
VARR	Double precision array	Return values of Gibbs energy and its 1st partial derivatives w.r.t. site fractions in the index order of phase constituents.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGMOB

Fortran	TQGMOB(INDEXP, ISP, VAL, IWSG, IWSE)
C-interface	**tq_gmob(TC_INT indexp,TC_INT isp,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);**
Full name:	Get Mobility
Purpose:	Getting mobility of a species in a phase with the temperature, pressure, and site fractions given by other subroutines shown.

Fortran	TQGMOB(INDEXP, ISP, VAL, IWSG, IWSE)	
C-interface	tq_gmob(TC_INT indexp,TC_INT isp,TC_FLOAT* val,TC_INT* iwsg,TC_INT* iwse);	
Comments:	Remember this subroutine requires no action of setting condition and calculating equilibrium. It is for getting the atomic or species mobility in a single phase with given temperature, pressure and atomic arrangements no matter if the phase is stable, metastable, or unstable in competition with other phases. The application program should take care of the phase stability or phase equilibrium if it is of interest.  The use of this subroutine is demonstrated in Example 9.	
Arguments		
Name	Type	Value set on call or returned
INDEXP	Integer	Set to a phase index.
ISP	Integer	Set to a system species index
VAL	Double precision	Return species or atomic mobility value.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSTP

Fortran	TQSTP(TP, IWSG, IWSE)
C-interface	tq_stp(TC_FLOAT* tp,TC_INT* iwsg,TC_INT* iwse);
Full name:	Set Temperature and Pressure
Purpose:	Setting temperature and pressure.
Comments:	This subroutine is used before calling TQGMC, TQGMDY, TQDGYY, and TQGMOB.  See Example 9.
Arguments	

Fortran	TQSTP(TP, IWSG, IWSE)	
C-interface	**tq_stp(TC_FLOAT* tp,TC_INT* iwsg,TC_INT* iwse);**	
Name	**Type**	**Value set on call or returned**
TP	Double precision array	Set temperature and pressure.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSYF

Fortran	TQSYF(INDEXP, YF, IWSG, IWSE)	
C-interface	**tq_syf(TC_INT indexp,TC_FLOAT* yf,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Set Site Fractions	
Purpose:	Setting site fractions for a phase.	
Comments:	This subroutine is used before calling TQGMB, TQGMC, TQGMDY, TQDGYY, and TQGMOB.  See Example 9.	
Arguments		
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index.
YF	Double precision array	Set to site fraction values in the index order of the phase constituents.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGSSPI

Fortran	TQGSSPI(SPN, ISP, IWSG, IWSE)	
C-interface	tq_gsspi(TC_STRING name,TC_INT* index,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get System Species Index	
Purpose:	Getting index of a system species with given name.	
Comments:	Useful if you want to use TQGMOB. See Example 9.	
Arguments		
Name	Type	Value set on call or returned
SPN	Character*24	Set to a system species name.
ISP	Integer	Return index value of the system species
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQCMOBA and TQCMOBB

These are logical functions.

Fortran	STATUS=TQCMOBA(INDEXP, ISP, IWSG, IWSE) STATUS=TQCMOBB(INDEXP, IWSG, IWSE)
C-interface	status=tq_cmoba(TC_INT indexp,TC_INT* iwsg,TC_INT* iwse); status=tq_cmobb(TC_INT indexp,TC_INT* iwsg,TC_INT* iwse);
Full name:	Check if Mobility data available – Method A and B
Purpose:	Check if mobility data have been appended into thermodynamic data file.
Comments:	If the C-interface is used the value returned is of type: TC_BOOL.

Fortran	STATUS=TQCMOBA(INDEXP, ISP, IWSG, IWSE) STATUS=TQCMOBB(INDEXP, IWSG, IWSE)	
C-interface	status=tq_cmoba(TC_INT indexp,TC_INT* iwsg,TC_INT* iwse); status=tq_cmobb(TC_INT indexp,TC_INT* iwsg,TC_INT* iwse);	
Arguments		
Name	Type	Value set on call or returned
INDEXP	Integer	Set to a phase index
ISP	Integer	Set to a system species index
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQDGYY

Fortran	TQDGYY(INDEXP, VARR1, VARR2, IWSG, IWSE)	
C-interface	tq_dgyy(TC_INT indexp,TC_FLOAT* varr1,TC_FLOAT* varr2,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Get Gibbs Energy and its 1st and 2nd Partial Derivative w.r.t. site-fractions.	
Purpose:	Getting Gibbs energy and its 1st and 2nd partial derivatives with respect to site fractions for a phase if temperature, pressure, and site fractions have been given by other subroutines shown below in this Section.	
Comments:	The returned value is in J/mole of formula unit. Remember this subroutine requires no action of setting condition and calculating equilibrium. It is for getting the Gibbs energy and its 1st and 2nd partial derivatives w.r.t site fractions for a single phase with given temperature, pressure and atomic arrangements no matter if the phase is stable, metastable, or unstable in competition with other phases. The application program should take care of the phase stability or phase equilibrium if it is of interest.	
Arguments		
Name	Type	Value set on call or returned

Fortran	TQDGYY(INDEXP, VARR1, VARR2, IWSG, IWSE)	
C-interface	**tq_dgyy(TC_INT indexp,TC_FLOAT* varr1,TC_FLOAT* varr2,TC_INT* iwsg,TC_INT* iwse);**	
INDEXP	Integer	Set to a phase index.
VARR1	Double precision array	Return values of Gibbs energy and its 1st partial derivatives w.r.t. site fractions in the index order of phase constituents.
VARR2	Double precision array	Return values of 2nd partial derivatives of Gibbs energy w.r.t. site fractions in the index order of IR: IR=J+I*(I-1)/2, I>=J; IR=I+J*(J-1)/2, I<J, where I and J are row and column indexes of phase constituents, respectively.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGPHP

Fortran	TQGPHP(INDEXP, NE, NCNV, NC, IWORK, WORK, IWSG, IWSE)	
C-interface	**tq_gphp(TC_INT indexp,TC_INT* ne,TC_INT* ncnv,TC_INT* nc,TC_INT* iwork,TC_FLOAT* work,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get phase constitution properties.	
Purpose:	Getting phase constitution properties such as number of components, number of constituents, number of constituents without counting vacancies, etc.	
Comments:	This subroutine is designed to speed up conversions of quantities involving mole fractions and site fractions in dynamic calculations where such operations are needed at each local time and space grid point. For each phase involved, one call of this subroutine is enough for subsequent conversions concerning this phases.  See Example 10.	
Arguments		
Name	**Type**	**Value set on call or returned**

Fortran	TQGPHP(INDEXP, NE, NCNV, NC, IWORK, WORK, IWSG, IWSE)	
C-interface	**tq_gphp(TC_INT indexp,TC_INT* ne,TC_INT* ncnv,TC_INT* nc,TC_INT* iwork,TC_FLOAT* work,TC_INT* iwsg,TC_INT* iwse);**	
INDEXP	Integer	Set to a phase index.
NE	Integer	Return number of components
NCNV	Integer	Return number of constituents without counting vacancies
NC	Integer	Return number of constituents
IWORK	Integer array	Return values needed in X to Y conversion, array size >= 4*NCNV
WORK	Double precision array	Return values needed in X to Y conversion, array size >= (NE+1)*NCNV
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQX2Y

Fortran	TQX2Y(INDEXP, NE, NCNV, NC, IWORK, WORK, XF, YF, IWSG, IWSE)
C-interface	**tq_x2y(TC_INT indexp,TC_INT ne,TC_INT ncnv,TC_INT nc,TC_INT* iwork,TC_FLOAT* work,TC_FLOAT* xf,TC_FLOAT* yf,TC_INT* iwsg,TC_INT* iwse);**
Full name:	Get Y-fraction given X-fraction.
Purpose:	Converting mole fractions to site fractions in a phase without internal degree of freedom.
Comments:	This subroutine uses the phase constitution properties obtained by TQGPHP as input.  See Example 10.
Arguments	

Fortran	TQX2Y(INDEXP, NE, NCNV, NC, IWORK, WORK, XF, YF, IWSG, IWSE)	
C-interface	tq_x2y(TC_INT indexp,TC_INT ne,TC_INT ncnv,TC_INT nc,TC_INT* iwork,TC_FLOAT* work,TC_FLOAT* xf,TC_FLOAT* yf,TC_INT* iwsg,TC_INT* iwse);	
Name	**Type**	**Value set on call or returned**
INDEXP	Integer	Set to a phase index
NE	Integer	Set to number of components
NCNV	Integer	Set to number of constituents without counting vacancies
NC	Integer	Set to number of constituents
IWORK	Integer array	Set to values needed in X to Y conversion
WORK	Double precision array	Set to values needed in X to Y conversion
XF	Double precision array	Set to mole fractions
YF	Double precision array	Return site fractions
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGMDX

Fortran	TQGMDX(IP, NE, NCNV, NC, IWORK, WORK, YF, VARR, GM, DGDX, XF, IWSG, IWSE)
C-interface	tq_gmdx(TC_INT indexp,TC_INT ne,TC_INT ncnv,TC_INT nc,TC_INT* iwork, TC_FLOAT* work,TC_FLOAT* yf,TC_FLOAT* varr,TC_FLOAT* gm,TC_FLOAT* dgdx,TC_FLOAT* xf,TC_INT* iwsg,TC_INT* iwse);
Full name:	Get Gibbs energy and its partial derivative w.r.t. X-fraction.
Purpose:	Converting Gibbs energy and its 1st partial derivatives with respect to site fractions (VARR obtained by calling TQGMDY) to that w.r.t mole fractions for a phase.
Comments:	Uses the phase constitution properties obtained by TQGPHP as input. Note

Fortran	**TQGMDX(IP, NE, NCNV, NC, IWORK, WORK, YF, VARR, GM, DGDX, XF, IWSG, IWSE)**
C-interface	**tq_gmdx(TC_INT indexp,TC_INT ne,TC_INT ncnv,TC_INT nc,TC_INT* iwork, TC_FLOAT* work,TC_FLOAT* yf,TC_FLOAT* varr,TC_FLOAT* gm,TC_FLOAT* dgdx,TC_FLOAT* xf,TC_INT* iwsg,TC_INT* iwse);**
	VARR obtained by calling TQGMDY is in unit of J/mole of formula unit. GM and DGDX in the present subroutine is in unit of J/mole of atoms.  For the use of this subroutine together with TQGPHP and TQX2Y, see Example 10.

Arguments

Name	Type	Value set on call or returned
IP	Integer	Set to a phase index.
NE	Integer	Set to number of components
NCNV	Integer	Set to number of constituents without counting vacancies
NC	Integer	Set to number of constituents
IWORK	Integer array	Set to values needed in X to Y conversion
WORK	Double precision array	Set to values needed in X to Y conversion
YF	Double precision array	Set to site fractions
VARR	Double precision array	Set to Gibbs energy and its first derivative with respect to site fractions
GM	Double precision	Return Gibbs energy
DGDX	Double precision array	Return Gibbs energy and its first derivative with respect to mole fractions
XF	Double precision array	Return mole fractions
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

Database Subroutines

See Example 12 .

Purpose	Subroutine
Get lists of database names	TQGDBN
Open or switch to a database	TQOPDB
List database elements	TQLIDE
Append a database	TQAPDB
Select an element	TQDEFEL
Reject a selected element	TQREJEL
Reject a phase or all phases	TQREJPH
Restore a phase	TQRESPH
List phases related to the selected element(s)	TQLISPH
List retained phases for the selected element(s)	TQLISSF
Get data from the selected database	TQGDAT
Reject defined system and reinitiate workspace	TQREJSY

TQGDBN

Fortran	**TQGDBN(DB_ARR, N, IWSG, IWSE)**	
C-interface	**tq_gdbn(tc_databases_strings* databases,TC_INT* n,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Database Names and Number.	
Purpose:	Get the names and total number of thermodynamic and kinetic databases listed in the database initiation file of Thermo-Calc: `tc_initd.tdb`.	
Comments:	IERR = 1001 is Failed to find the initiation file.	
Arguments		
Name	**Type**	**Value set on call or returned**

Fortran	TQGDBN(DB_ARR, N, IWSG, IWSE)	
C-interface	**tq_gdbn(tc_databases_strings* databases,TC_INT* n,TC_INT* iwsg,TC_INT* iwse);**	
DB_ARR	Character*24 array	Return database names.
N	Integer	Return total number of databases available.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQOPDB

Fortran	TQOPDB(TDB, IWSG, IWSE)	
C-interface	**tq_opdb(TC_STRING database,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Open Database.	
Purpose:	Open a thermodynamic or kinetic database.	
Comments:	IERR = 1001 Failed to find the initiation file. IERR = 1002 Database or its license not available.	
Arguments		
Name	**Type**	**Value set on call or returned**
TDB	Character*256	Set to the name of a database.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQLIDE

Fortran	**TQLIDE(EL_ARR, N, IWSG, IWSE)**	
C-interface	**tq_lide(tc_elements_strings* elements,TC_INT* num,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	List Database Elements.	
Purpose:	List all elements available in the chosen database.	
Arguments		
Name	**Type**	**Value set on call or returned**
EL_ARR	Character*2 array	Return the names of all elements.
N	Integer	Return the total number of elements.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQAPDB

Fortran	**TQAPDB(TDB, IWSG, IWSE)**	
C-interface	**tq_apdb(TC_STRING database,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Append Database.	
Purpose:	Append a thermodynamic or kinetic database.	
Comments:	IERR = 1002 Database or its license not available.	
Arguments		
Name	**Type**	**Value set on call or returned**
TDB	Character*256	Set to the name of a database.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQDEFEL

Fortran	TQDEFEL(ELNAM, IWSG, IWSE)	
C-interface	tq_defel(TC_STRING element,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Define Element.	
Purpose:	Define a system element.	
Comments:	IERR = 1011 Element not included in the chosen database. IERR = 1012 Element already defined.	
Arguments		
Name	Type	Value set on call or returned
ELNAM	Character*2	Set to the name of an element.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQREJEL

Fortran	TQREJEL(ELNAM, IWSG, IWSE)	
C-interface	tq_rejel(TC_STRING element,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Reject Element.	
Purpose:	Reject a defined system element.	
Comments:	IERR = 1013 Element not included in the chosen database. IERR = 1014 Element already rejected.	
Arguments		
Name	Type	Value set on call or returned
ELNAM	Character*2	Set to the name of an element.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQREJPH

Fortran	TQREJPH(PHNAM, IWSG, IWSE)	
C-interface	tq_rejph(TC_STRING phase,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Reject Phase.	
Purpose:	Reject a system phase.	
Comments:	IERR = 1017 Phase not included in the chosen database.IERR = 1018 Phase already rejected.	
Arguments		
Name	Type	Value set on call or returned
PHNAM	Character*24	Set to a phase name If * is used then all phases are rejected
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQRESPH

Fortran	TQRESPH(PHNAM, IWSG, IWSE)	
C-interface	tq_resph(TC_STRING phase,TC_INT* iwsg,TC_INT* iwse);	
Full name:	Restore Phase.	
Purpose:	Restore a rejected system phase.	
Comments:	IERR = 1015 Phase not included in the chosen database. IERR = 1016 Phase already restored.	
Arguments		
Name	Type	Value set on call or returned
PHNAM	Character*24	Set to a phase name

Fortran	TQRESPH(PHNAM, IWSG, IWSE)	
C-interface	tq_resph(TC_STRING phase,TC_INT* iwsg,TC_INT* iwse);	
		If * is used then all phases are rejected
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQLISPH

Fortran	TQLISPH(PH_ARR, N, IWSG, IWSE)	
C-interface	tq_lisph(tc_phases_strings* phases,TC_INT* num,TC_INT* iwsg,TC_INT* iwse);	
Full name:	List System Phase.	
Purpose:	List all phases (both rejected and restored) available for the defined system.	
Arguments		
Name	Type	Value set on call or returned
PH_ARR	Character*24 array	Return phase names.
N	Integer	Return the total number of phases
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQLISSF

Fortran	**TQLISSF(PH_ARR, N, IWSG, IWSE)**	
C-interface	**tq_lissf(tc_phases_strings* phases,TC_INT* num,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	List Selected System Phase.	
Purpose:	List phases not rejected for the defined system.	
Arguments		
Name	**Type**	**Value set on call or returned**
PH_ARR	Character*24 array	Return phase names.
N	Integer	Return the total number of phases
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQGDAT

Fortran	**TQGDAT(IWSG, IWSE)**	
C-interface	**tq_gdat(TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Get Data.	
Purpose:	Get data for the defined system from the chosen database.	
Arguments		
Name	**Type**	**Value set on call or returned**
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQREJSY

Fortran	**TQREJSY(IWSG, IWSE)**	
C-interface	**tq_rejsy(TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Reject system.	
Purpose:	Reject the defined system and reinitiate the workspace in order to do a completely new calculation for a different system selected from the same or a different database.	
Comments:	In any application programs, either TQINI or TQINI3 should be called only once. If there is a need to do a completely new calculation on a totally different system without exiting the application program, one should call TQREJS instead before going to (open a new database and) define a new system, get data, and make calculations.	
Arguments		
Name	**Type**	**Value set on call or returned**
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

Adaptive Interpolation Schemes

About Adaptive Interpolation Schemes

In order to perform a simulation using the scheme, the TQ-library must be initialized in the normal way using the routine TQINI and thermodynamic information must be loaded, usually with the TQRFIL routine.

The scheme is then initialized using the TQIPS_INIT_TOP routine and each branch in the calculation is initialized using the TQIPS_INIT_BRANCH routine. For each set of interpolated values which are to be defined and obtained from a certain branch of the scheme, the TQIPS_INIT_FUNCTION routine is called. The values for all functions defined in the branch are then returned using the TQIPS_GET_VALUE routine.

Purpose	Subroutine
Initiate the interpolation scheme	TQIPS_INIT_TOP
Initiate a branch in the interpolation scheme	TQIPS_INIT_BRANCH
Define a function or state variable to be interpolated	TQIPS_INIT_FUNCTION
Retrieve the interpolated value	TQIPS_GET_VALUE
Write the data of the interpolation scheme to file.	TQIPS_WRITE_IPS_DATA_TO_FILE
Read interpolation scheme data from file.	TQIPS_READ_IPS_DATA_FROM_FILE
Get statistics on the usage of the interpolation scheme.	TQIPS_GET_MEMORY_USAGE

TQIPS_INIT_TOP

Fortran	**TQIPS_INIT_TOP(IERR, IWSG, IWSE)**
C-interface	**tq_ips_init_top(TC_INT* err,TC_INT* iwsg,TC_INT* iwse)**
Full name:	Initiate the top structure of the adaptive interpolation scheme.
Purpose:	Initiates the top structure of the interpolation scheme which may contain several branches with different conditions, phases and values to be interpolated.
Comments:	IERR is returned with 0 if no error occurs.
Arguments	

Fortran	TQIPS_INIT_TOP(IERR, IWSG, IWSE)	
C-interface	**tq_ips_init_top(TC_INT* err,TC_INT* iwsg,TC_INT* iwse)**	
Name	**Type**	**Value set on call or returned**
IERR	Integer	Returns the error code.
IWSG	Integer array	Workspace.
IWSE	Integer array	Workspace.

TQIPS_INIT_BRANCH

Fortran	TQIPS_INIT_BRANCH(TISCOND, TISCNST, PISCOND, PISCNST, IDEPEL, IDISCRT, NSTEP, IPHSTA, T, TMIN, TMAX, P, PMIN, PMAX, RMEMFR, PHAMNT,XMIN, XMAX, IBRANCH, IERR IWSG, IWSE
C-interface	**tq_ips_init_branch(TC_BOOL t_is_condition, TC_BOOL t_is_constant, TC_BOOL p_is_condition, TC_BOOL p_is_constant, TC_BOOL* independent_elements,TC_INT dicretization_type, TC_INT nr_of_ steps, TC_INT* state_of_phases, TC_FLOAT t, TC_FLOAT tmin, TC_ FLOAT tmax,TC_FLOAT p,TC_FLOAT pmin, TC_FLOAT pmax, TC_FLOAT memory_fraction, TC_FLOAT* amount_of_phases, TC_FLOAT* xmin, TC_FLOAT* xmax, TC_INT* branch_nr, TC_INT* err, TC_INT* iwsg, TC_INT* iwse)**
Full name:	Initiate a branch of the adaptive interpolation scheme.
Purpose:	Initiates a branch of the interpolation scheme with a set of conditions, phases and values to be interpolated.
Comments:	The size of the arrays IDEPEL, XMIN and XMAX are defined as the number of all components supplied by TQGNC must be provided in the same order as supplied by TQGCOM.Composition conditions are set as the normalized number of moles for each component (N(c) =value).The size of the arrays IPHSTA and PHAMNT are defined as the number of all phases supplied by TQGNP must be provided in the same order as supplied by TQGPN.The allocation of memory to each branch is performed at the first time values are retrieved using TQIPS_GET_VALUE, therefore some considerations must be made when using several branches in order to allocate the same amount of memory to each branch.
Arguments	

Fortran	**TQIPS_INIT_BRANCH(TISCOND, TISCNST, PISCOND, PISCNST, IDEPEL, IDISCRT, NSTEP, IPHSTA, T, TMIN, TMAX, P, PMIN, PMAX, RMEMFR, PHAMNT,XMIN, XMAX, IBRANCH, IERR IWSG, IWSE**	
C-interface	**tq_ips_init_branch(TC_BOOL t_is_condition, TC_BOOL t_is_constant, TC_BOOL p_is_condition, TC_BOOL p_is_constant, TC_BOOL* independent_elements,TC_INT dicretization_type, TC_INT nr_of_ steps, TC_INT* state_of_phases, TC_FLOAT t, TC_FLOAT tmin, TC_ FLOAT tmax,TC_FLOAT p,TC_FLOAT pmin, TC_FLOAT pmax, TC_FLOAT memory_fraction, TC_FLOAT* amount_of_phases, TC_FLOAT* xmin, TC_FLOAT* xmax, TC_INT* branch_nr, TC_INT* err, TC_INT* iwsg, TC_INT* iwse)**	
Name	**Type**	**Value set on call or returned**
TISCOND	Logical	Set to TRUE if temperature is a condition in this branch.
TISCNST	Logical	Set to TRUE if temperature is constant in this branch.
PISCOND	Logical	Set to TRUE if pressure is a condition in this branch.
PISCNST	Logical	Set to TRUE if pressure is constant in this branch.
IDEPEL	Logical array	Set to TRUE for each element for which conditions are present.
IDISCRT	Integer	Indicates the type of discretization where: 1=linear2=logarithmic
NSTEP	Integer	Set to the logarithm (10 base) number of steps to be used to interpolate in the temperature / pressure / composition space.
IPHSTA	Integer array	Set to the status for the phases in this branch, where: 1=ENTERED, 2=SUSPENDED, 3=DORMANT, 4=FIXED
T	Double precision	Set to temperature if temperature is a condition, otherwise used as starting value.

Fortran	**TQIPS_INIT_BRANCH(TISCOND, TISCNST, PISCOND, PISCNST, IDEPEL, IDISCRT, NSTEP, IPHSTA, T, TMIN, TMAX, P, PMIN, PMAX, RMEMFR, PHAMNT,XMIN, XMAX, IBRANCH, IERR IWSG, IWSE**	
C-interface	**tq_ips_init_branch(TC_BOOL t_is_condition, TC_BOOL t_is_constant, TC_BOOL p_is_condition, TC_BOOL p_is_constant, TC_BOOL* independent_elements,TC_INT dicretization_type, TC_INT nr_of_ steps, TC_INT* state_of_phases, TC_FLOAT t, TC_FLOAT tmin, TC_ FLOAT tmax,TC_FLOAT p,TC_FLOAT pmin, TC_FLOAT pmax, TC_FLOAT memory_fraction, TC_FLOAT* amount_of_phases, TC_FLOAT* xmin, TC_FLOAT* xmax, TC_INT* branch_nr, TC_INT* err, TC_INT* iwsg, TC_INT* iwse)**	
TMIN	Double precision	Set to lower limit of temperature range.
TMAX	Double precision	Set to upper limit of temperature range.
P	Double precision	Set to pressure if pressure is a condition, otherwise used as starting value.
PMIN	Double precision	Set to lower limit of pressure range.
PMAX	Double Precision	Set to upper limit of pressure range.
RMEMFR	Double precision	Set to the fraction of the amount of free physical memory to be allocated to the interpolation scheme for this branch (value < 1.0). If a value larger than 1.0 if set, it is interpreted as the number of megabytes allocated to the branch.
PHAMNT	Double precision array	Set to the amount of the phase if defined as a fixed phase with IPHSTA.
XMIN	Double precision array	Set to the lower limit of the composition range of each component.
XMAX	Double precision array	Set to the upper limit of the composition range of each component.
IBRANCH	Integer	Set to branch number for which the variable in STRING is to be interpolated.
IERR	Integer	Returns error code.
IWSG	Integer array	Workspace.

Fortran	**TQIPS_INIT_BRANCH(TISCOND, TISCNST, PISCOND, PISCNST, IDEPEL, IDISCRT, NSTEP, IPHSTA, T, TMIN, TMAX, P, PMIN, PMAX, RMEMFR, PHAMNT,XMIN, XMAX, IBRANCH, IERR IWSG, IWSE**	
C-interface	**tq_ips_init_branch(TC_BOOL t_is_condition, TC_BOOL t_is_constant, TC_BOOL p_is_condition, TC_BOOL p_is_constant, TC_BOOL* independent_elements,TC_INT dicretization_type, TC_INT nr_of_ steps, TC_INT* state_of_phases, TC_FLOAT t, TC_FLOAT tmin, TC_ FLOAT tmax,TC_FLOAT p,TC_FLOAT pmin, TC_FLOAT pmax, TC_FLOAT memory_fraction, TC_FLOAT* amount_of_phases, TC_FLOAT* xmin, TC_FLOAT* xmax, TC_INT* branch_nr, TC_INT* err, TC_INT* iwsg, TC_INT* iwse)**	
IWSE	Integer array	Workspace

TQIPS_INIT_FUNCTION

Fortran	**TQIPS_INIT_FUNCTION(STRING, IBRANCH, IERR, IWSG, IWSE)**	
C-interface	**tq_ips_init_function(TC_STRING function_string, TC_INT branch_nr, TC_INT* err, TC_INT* iwsg, TC_INT* iwse);**	
Full name:	Initiates a function for a specific branch whose value(s) are to be retrieved from the adaptive interpolation scheme.	
Purpose:	Initiates a function or state variable for a specific branch whose value(s) are to be retrieved from the adaptive interpolation scheme.	
Arguments		
Name	**Type**	**Value set on call or returned**
STRING	Character*128	Set to the name of the function or state variable to be interpolated, wildcards (*) may be used in place of element and/or phase names.
IBRANCH	Integer	Set to branch number for which the variable in STRING is to be interpolated.
IERR	Integer	Returns the error code.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQIPS_GET_VALUE

Fortran	**TQIPS_GET_VALUE(IBRANCH, NOSCHEME, ARR, RESULT, IERR, ISHORT, IWSG, IWSE)**	
C-interface	**tq_ips_get_value(TC_INT branch_nr, TC_INT noscheme, TC_FLOAT* variable_values, TC_FLOAT* function_values, TC_INT* err, TC_INT* shortcut, TC_INT* iwsg,TC_INT* iwse);**	
Full name:	Retrieve interpolated value(s) from the adaptive interpolation scheme.	
Purpose:	Retrieves all the values defined by all TQIPS_INIT_FUNCTION defined for branch IBRANCH in sequential order.	
Arguments		
Name	**Type**	**Value set on call or returned**
IBRANCH	Integer	Set to branch number.
NOSCHEME	Integer	Set to 1 if the interpolation scheme is to be disabled.
ARR	Double precision array	Array set to the mole-fractions of all the components followed by the temperature and the pressure, if a component is dependent the value may be arbitrary. The same applies if the temperature or pressure is constant.
RESULT	Double precision array	Returns the interpolated values in the same order as they were defined in TQS_INIT_FUNCTION.
IERR	Integer	Returns the error code.
ISHORT	Integer	Set to the last returned value or zero, 0. Returns a shortcut to data pertaining to the grid point in virtual composition/temperature/pressure space for the values in ARR
IWSG	Integer array	Workspace.
IWSE	Integer array	Workspace.

TQIPS_WRITE_IPS_DATA_TO_FILE

Fortran	**TQIPS_WRITE_IPS_DATA_TO_FILE(FILENAME,IERR,IWSG,IWSE)**	
C-interface	**tq_ips_write_ips_data_to_file(TC_STRING filename, TC_INT* ierr, TC_INT* iwsg, TC_INT* iwse)**	
Full name:	Write the data of the interpolation scheme to file.	
Purpose:	To save all the data of the interpolation scheme in order to read them at a later time with routine tqips_read_ips_data_from_file.	
Arguments		
Name	**Type**	**Value set on call or returned**
FILENAME	Character*256	The name of the file to be saved
IERR	Integer	Returns the error code
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQIPS_READ_IPS_DATA_FROM_FILE

Fortran	**TQIPS_READ_IPS_DATA_FROM_FILE(FILENAME, MEMORY_FRACTION, IERR, IWSG, IWSE)**	
C-interface	**tq_ips_read_ips_data_from_file(TC_STRING filename, TC_FLOAT* memory_fraction, TC_INT* ierr, TC_INT* iwsg, TC_INT* iwse)**	
Full name:	Read interpolation scheme data from file.	
Purpose:	To read from file interpolation scheme data that has been saved previously with routine tqips_write_ips_data_to_file.	
Comments:	If memory_fraction has a value smaller than zero the amount of allocated memory will be determined by the value read from file. If memory_fraction is larger than zero it will be interpreted in the same way as argument RMEMFR of routine tqips_init_branch.	
Arguments		
Name	**Type**	**Value set on call or returned**

Fortran	**TQIPS_READ_IPS_DATA_FROM_FILE(FILENAME, MEMORY_FRACTION, IERR, IWSG, IWSE)**	
C-interface	**tq_ips_read_ips_data_from_file(TC_STRING filename, TC_FLOAT* memory_fraction, TC_INT* ierr, TC_INT* iwsg, TC_INT* iwse)**	
FILENAM	Character*256	The name of the file to be read
MEMORY_ FRACTION	double precision	See comment
IERR	Integer	Returns the error code
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQIPS_GET_MEMORY_USAGE

Fortran	**TQIPS_GET_MEMORY_USAGE(IBRANCH, FRACTION, ISLOTS, IUSEDSLOTS, ICALLS, IEQCALCS, IERR, IWSG, IWSE)**	
C-interface	**tq_ips_get_memory_usage(TC_INT branch_nr, TC_FLOAT* fraction,TC_INT* total_number_of_data_slots, TC_INT* number_of_ used_data_slots, TC_INT* total_number_of_calls, TC_INT* total_ number_of_equil_calcs, TC_INT* ierr,TC_INT* iwsg,TC_INT* iwse)**	
Full name:	Get statistics on the usage of the interpolation scheme.	
Purpose:	To get some statistics on the performance of the interpolation scheme.	
Arguments		
Name	**Type**	**Value set on call or returned**
IBRANCH	Integer	If IBRANCH>0 it is the branch number for which the data should be returned. If IBRANCH=0 then data is returned summed over all branches.
FRACTION	double precision	This is simply equal to IUSEDSLOTS/ISLOTS
ISLOTS	Integer	The total number of data slots allocated
IUSEDSLOTS	Integer	The number of used data slots

Fortran	**TQIPS_GET_MEMORY_USAGE(IBRANCH, FRACTION, ISLOTS, IUSEDSLOTS, ICALLS, IEQCALCS, IERR, IWSG, IWSE)**	
C-interface	**tq_ips_get_memory_usage(TC_INT branch_nr, TC_FLOAT* fraction,TC_INT* total_number_of_data_slots, TC_INT* number_of_used_data_slots, TC_INT* total_number_of_calls, TC_INT* total_number_of_equil_calcs, TC_INT* ierr,TC_INT* iwsg,TC_INT* iwse)**	
ICALLS	Integer	The number of calls to tqips_get_value
IEQCALCS	Integer	The number of equilibrium calculations performed by Thermo-Calc on behalf of the interpolation scheme
IERR	Integer	error code
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

Composition Set Reordering Routines

Purpose	Subroutine
Initialize IWSR workspace for reordering of CS in TQ.	TQROINIT
Set ideal composition in this phase	TQSETRX
Reorder CS in current EQ	TQORDER
List content of IWSR set by user.	TQLROX

TQROINIT

Fortran	**TQROINIT(NWSR, IWSR, IWSG, IWSE)**	
C-interface	**tq_roinit(TC_INT nwsr, TC_INT* iwsr,TC_INT* iwsg, TC_INT* iwse);**	
Full name:	Initialize IWSR workspace for reordering of CS in TQ.	
Purpose:	With this subroutine the application program initializes the Thermo-Calc package for use of the reordering subroutines. It must be called before using any of the subroutines TQSETRX, TQORDER, TQLROX.	
Comments:	NWSR=1000 should be enough for several composition sets	
Arguments		
Name	**Type**	**Value set on call or returned**
NWSR	Integer	On call set to size of the workspace IWSR.
IWSR	Integer array	Memory area for storage of data inside the package.
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQSETRX

Fortran	TQSETRX(PHASE, X, IWSR, IWSG, IWSE)	
C-interface	tq_setrx(TC_STRING phase, TC_FLOAT* x, TC_INT* iwsr, TC_INT* iwsg, TC_INT* iwse);	
Full name:	Set ideal composition in this phase	
Purpose:	Store composition of phase in IWSR for future use.	
Comments:	The order in the X array is the order of the components in the system	
Arguments		
Name	Type	Value set on call or returned
Phase	Character*24	Phase name (e.g. 'fcc#2')
X	Double precision array	On call set to the ideal composition in this composition set in this phase.
IWSR	Integer array	Workspace
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQORDER

Fortran	TQORDER(IWSR, IWSG, IWSE)
C-interface	tq_order(TC_INT* iwsr, TC_INT* iwsg,TC_INT* iwse);
Full name:	Reorder CS in current EQ
Purpose:	The ideal composition set by the user is used to reorder the CS in respective phase to minimize the distance compared to present eq.
Comments:	Calling routines more than once in a row should affect nothing. Routines minimize the distance between the set ideal composition and the composition found in the present equilibria, and reorder the CS in the equilibria to achieve the minima. This does not affect the properties of the equilibria.
Arguments	

Fortran	**TQORDER(IWSR, IWSG, IWSE)**	
C-interface	**tq_order(TC_INT* iwsr, TC_INT* iwsg,TC_INT* iwse);**	
Name	**Type**	**Value set on call or returned**
IWSR	Integer array	Workspace
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

TQLROX

Fortran	**TQLROX(IWSR, IWSG, IWSE)**	
C-interface	**tq_lrox(TC_INT* iwsr,TC_INT* iwsg,TC_INT* iwse);**	
Full name:	List content of IWSR set by user.	
Purpose:	List the ideal composition set in the output unit using TQSETRX in IWSR. It is for debugging.	
Arguments		
Name	**Type**	**Value set on call or returned**
IWSR	Integer array	Workspace
IWSG	Integer array	Workspace
IWSE	Integer array	Workspace

Compiler Settings

Programming Languages

In the compiler flag paths, *<libraryversion>* is the current name of the library that changes between software releases. Look through your operating system's file structure to determine the current name.

Compiling FORTRAN Code

There is different OS support for Windows and Linux as shown below.

Windows: Visual Studio 2010, Intel FORTRAN Composer 16

64-BIT CONFIGURATION

Compiler flags:

```
/integer_size:64
/real_size:64
/double_size:64
/iface:default
```

Example:

```
ifort /integer_size:64 /real_size:64 /double_size:64 /iface:default /c
tqex01.F
ifort/exe:tqex01.exe tqex01.obj libtq-win-x64-<libraryversion>.lib
```

Linux: GNU compiler version 4.4

64-BIT CONFIGURATION

Compiler flags:

```
-fdefault-real-8
-fdefault-double-8
-fdefault-integer-8
```

Example:

```
gfortran –c -fdefault-real-8 -fdefault-double-8 \fdefault-integer-8  tqex01.F
```

```
gfortran –o tqex01 tqex01.o libtq-linux-x86_64-gfortran44-<libraryversion>.so
```

Linux: Intel FORTRAN Compiler

64-BIT CONFIGURATION

Compiler flags:

```
-real-size 64
-double-size 64
-integer-size 64
```

Example:

```
ifort –c real-size 64 -double-size 64 \ integer-size 64 tqex01.F
ifort –o tqex01 tqex01.o libtq-linux-x86_64-ifort-<libraryversion>.so
```

Compiling C code

When compiling the C-code it is necessary to include the files **tqroot.h** and **tc_data_defs.h**, therefore the path to where these files are located must be specified.

Windows: Visual Studio 2010

C programs linked with TQ in Windows, must use release libraries (/MT or /MD) due to clashes in the memory allocation routines causing the global minimization procedure to fail if debug libraries are used.

64-BIT CONFIGURATION

Compiler flags:

```
/DWIN32
/DWIN64
/I..\tq\C\include
```

Example:

```
cl /c /DWIN32 /DWIN64 /I..\tq\C\include tqex01.c
link /OUT:tqex01.exe tqex01.obj libtq-win-x64-<libraryversion>.lib
```

Linux: GNU compiler version 4.4

64-BIT CONFIGURATION

Compiler flags:

```
-I../tq/C/include
```

Example:

```
gcc –c -I../tq/C/include tqex01.c
gcc –o tqex01 tqex01.o libtq-linux-x86_64-gfortran44-<libraryversion>.so
```