TC-Python Documentation

Release 2022a

Thermo-Calc Software AB

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CHAPTER ONE

INSTALLATION GUIDE

This guide helps you to get a working TC-Python API installation.

There is a PDF guide included with your installation. In the Thermo-Calc menu, select Help → Manuals Folder. Then double-click to open the Software Development Kits (SDKs) folder.

Note: A license is required to run TC-Python.

1.1 What type of installation should I choose?

There are two possibilities to install TC-Python:

1. *Using the Python-interpreter bundled to Thermo-Calc:* This interpreter has TC-Python preinstalled together with some popular Python-packages. This is the recommended option for new users to TC-Python, but it is limited to the preinstalled packages.

2. *Installing TC-Python into the Python-interpreter of your choice:* This is the recommended option for any more advanced usage and provides full flexibility.

1.2 Using the Python-interpreter bundled to Thermo-Calc

Note: A Python-interpreter is bundled to Thermo-Calc beginning with version 2021a.

1.2.1 Limitations

The bundled Python 3.7.2 interpreter is containing the following major packages:

<table>
<thead>
<tr>
<th>Package</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>matplotlib</td>
<td>3.3.2</td>
</tr>
<tr>
<td>numpy</td>
<td>1.19.2</td>
</tr>
<tr>
<td>scikit-learn</td>
<td>0.23.2</td>
</tr>
<tr>
<td>scipy</td>
<td>1.5.2</td>
</tr>
<tr>
<td>TC-Python</td>
<td>2022a</td>
</tr>
</tbody>
</table>
Please contact the Thermo-Calc support if you think that further packages might be useful in future releases.

**Note:** The following TC-Python examples are requiring additional packages that are not available in the bundled Python-interpretor, they can therefore not be run:

- pyex_M_01_Input_from_file.py
- pyex_M_02_Output_to_file.py

**Warning:** The Python-interpretor bundled to Thermo-Calc is also used for running the property models in Thermo-Calc. *Any changes to the interpreter packages can therefore break Thermo-Calc and should be avoided.* If the installation gets broken, it can be fixed by reinstalling Thermo-Calc after having removed it.

### 1.2.2 Step 1: Install an IDE (Integrated Development Environment)

Any editor can be used to write the Python code, but an IDE is recommended, e.g. PyCharm. These instructions are based on the use of PyCharm.

Use of an IDE will give you access to code completion, which is of great help when you use the API as it will give you the available methods on the objects you are working with.

2. Click to choose your OS and then click **Download**. You can use the **Community** version of PyCharm.
3. Follow the instructions. It is recommended you keep all the defaults.

**Note:** For Mac installations, you also need to set some environment variables as described below in *Mac OS: Setting Environment Variables*.

### 1.2.3 Step 2: Configure PyCharm to use the bundled Python-interpretor

Open PyCharm and configure the interpretor:

1. Go the menu **File**→**Settings**.
2. Navigate in the tree to **Project:** *YourProjectName* and choose **Project Interpreter**.
3. Click on the settings symbol close to the **Project Interpreter** dropdown menu and choose **Add**.
4. Now choose **System Interpreter** and add the bundled Thermo-Calc Python 3 interpretor. It is located in different places depending on the operating system:
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<table>
<thead>
<tr>
<th>Operating system</th>
<th>Path to the bundled Python-interpreter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>C:\Program Files\Thermo-Calc\2022a\python\python.exe</td>
</tr>
<tr>
<td>Linux</td>
<td>/home/UserName/Thermo-Calc/2022a/python/bin/python3</td>
</tr>
<tr>
<td>MacOS</td>
<td>/Applications/Thermo-Calc-2022a.app/Contents/Resources/python/bin/python3</td>
</tr>
</tbody>
</table>

5. Select your added interpreter and confirm.

### 1.2.4 Step 3: Run a TC-Python Example

Now you are ready to start working with TC-Python.

It is recommended that you open one or more of the included examples to both check that the installation has worked and to start familiarizing yourself with the code.

#### 1.2.4.1 Open the TC-Python Project in PyCharm

When you first open the TC-Python project and examples, it can take a few moments for the Pycharm IDE to index before some of the options are available.

1. Open PyCharm and then choose **File** → **Open**. The first time you open the project you will need to navigate to the path of the TC-Python installation:

<table>
<thead>
<tr>
<th>Operating system</th>
<th>Path to the TC-Python folder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>C:\Users\UserName\Documents\Thermo-Calc\2022a\SDK\TC-Python</td>
</tr>
<tr>
<td>Linux</td>
<td>/home/UserName/Thermo-Calc/2022a/SDK/TC-Python</td>
</tr>
<tr>
<td>MacOS</td>
<td>/Users/Shared/Thermo-Calc/2022a/SDK/TC-Python</td>
</tr>
</tbody>
</table>

2. Click on the **Examples** folder and then click **OK**.

3. From any subfolder:
   - Double-click to open an example file to examine the code.
   - Right-click an example and choose **Run**.

**Note:** If you are not following the recommended approach and create a new project (**File** → **New Project**...), you need to consider that by default the options to choose the interpreter are hidden within the **Create Project** window. So click on **Project Interpreter: New Virtual Environment** and in most cases choose your **System Interpreter** containing the Python bundled to Thermo-Calc instead of the default **New Virtual Environment**.
1.3 Installing TC-Python into the Python-interpreter of your choice

1.3.1 Step 1: Install a Python Distribution

If you already have a Python distribution installation, version 3.5 or higher, skip this step.

These instructions are based on using the Anaconda platform for the Python distribution. Install version 3.5 or higher to be able to work with TC-Python, although it is recommended that you use the most recent version.

1.3.1.1 Install Anaconda

2. Click to choose your OS (operating system) and then click Download. Follow the instructions. It is recommended you keep all the defaults.

1.3.2 Step 2: Install Thermo-Calc and the TC-Python SDK

Note: TC-Python is available starting with Thermo-Calc version 2018a.

1. Install Thermo-Calc
2. When the installation is complete, open the TC-Python folder that includes the *.whl file needed for the next step. There is also an file:Examples folder with Python files you can use in the IDE to understand and work with TC-Python.

1.3.3 Step 3: Install TC-Python

On Windows, it is recommended that you use the Python distribution prompt (i.e. Anaconda, ...), especially if you have other Python installations. Do not use Virtual Environments unless you have a good reason for that.

1. Open the command line. For example, in Anaconda on a Windows OS, go to Start → Anaconda → Anaconda Prompt.
2. At the command line, enter the following. Make sure there are no spaces at the end of the string or in the folder name or it will not run:

   pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl

Tip: Note that on Linux depending on the interpreter usually pip3 is used.

<table>
<thead>
<tr>
<th>Operating system</th>
<th>Path to the TC-Python folder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>C:\Users\UserName\Documents\Thermo-Calc\2022a\SDK\TC-Python</td>
</tr>
<tr>
<td>Linux</td>
<td>/home/UserName/Thermo-Calc/2022a/SDK/TC-Python</td>
</tr>
<tr>
<td>MacOS</td>
<td>/Users/Shared/Thermo-Calc/2022a/SDK/TC-Python</td>
</tr>
</tbody>
</table>
3. Press <Enter>. When the process is completed, there is a confirmation that TC-Python is installed.

**Note:** If your computer is located behind a proxy-server, the default pip-command will fail with a network connection error. In that case you need to install the dependencies of TC-Python in a special configuration:

```
pip install -proxy user:password@proxy_ip:port py4j jproperties
```

See “pip install” fails with “Failed to establish a new network connection” or similar for detailed information.

### 1.3.4 Step 4: Install an IDE (Integrated Development Environment)

Any editor can be used to write the Python code, but an IDE is recommended, e.g. PyCharm. These instructions are based on the use of PyCharm.

Use of an IDE will give you access to code completion, which is of great help when you use the API as it will give you the available methods on the objects you are working with.

2. Click to choose your OS and then click Download. You can use the Community version of PyCharm.
3. Follow the instructions. It is recommended you keep all the defaults.

**Note:** For Mac installations, you also need to set some environment variables as described below in Mac OS: Setting Environment Variables.

### 1.3.5 Step 5: Open the IDE and Run a TC-Python Example

After you complete all the software installations, you are ready to open the IDE to start working with TC-Python.

It is recommended that you open one or more of the included examples to both check that the installation has worked and to start familiarizing yourself with the code.

#### 1.3.5.1 Open the TC-Python Project in PyCharm

When you first open the TC-Python project and examples, it can take a few moments for the Pycharm IDE to index before some of the options are available.

1. Open PyCharm and then choose File→Open. The first time you open the project you will need to navigate to the path of the TC-Python installation.

<table>
<thead>
<tr>
<th>Operating system</th>
<th>Path to the TC-Python folder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>C:\Users\UserName\Documents\Thermo-Calc\2022a\SDK\TC-Python</td>
</tr>
<tr>
<td>Linux</td>
<td>/home/UserName/Thermo-Calc/2022a/SDK/TC-Python</td>
</tr>
<tr>
<td>MacOS</td>
<td>/Users/Shared/Thermo-Calc/2022a/SDK/TC-Python</td>
</tr>
</tbody>
</table>
2. Click on the Examples folder and then click OK.
3. From any subfolder:
   - Double-click to open an example file to examine the code.
   - Right-click an example and choose Run.

### 1.3.5.2 Fixing potential issues with the environment

In most cases you should run TC-Python within your global Python 3 interpreter and not use Virtual Environments unless you have a good reason to do so. A common problem on first usage of TC-Python is the error message “No module named tc_python”. You can resolve this and other problems with the interpreter settings as follows:

1. Go the menu File → Settings.
2. Navigate in the tree to Project: YourProjectName and choose Project Interpreter.
3. Click on the settings symbol close to the Project Interpreter dropdown menu and choose Add.
4. Now choose System Interpreter and add your existing Python 3 interpreter.
5. Select your added interpreter and confirm.

**Note:** If you are not following the recommended approach and create a new project (File → New Project…), you need to consider that by default the options to choose the interpreter are hidden within the Create Project window. So click on Project Interpreter: New Virtual Environment and in most cases choose your System Interpreter instead of the default New Virtual Environment.

**Note:** If you really need to use a Virtual Environment, please consider the hints given in the Python Virtual Environments chapter.

### 1.4 Updating to a newer version

When updating to a newer version of Thermo-Calc, you need to also install the latest version of TC-Python. This is not necessary if are using the bundled Python-interpreter that has it automatically installed. It is not sufficient to run the installer of Thermo-Calc:

```bash
pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl
```

**Tip:** Note that on Linux depending on the interpreter usually pip3 is used.

In case of problems you may wish to uninstall the previous version of TC-Python in advance:

```bash
pip uninstall TC-Python
pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl
```
However, that should normally not be required.

You can check the currently installed version of TC-Python by running:

```
pip show TC-Python
```
MAC OS: SETTING ENVIRONMENT VARIABLES

In order to use TC-Python on Mac you need to set some environment variables.

TC22A_HOME=/Applications/Thermo-Calc-2022a.app/Contents/Resources

If you use a license server:

LSHOST=<name-of-the-license-server>

If you have a node-locked license:

LSHOST=NO-Net
LSERVRC=/Users/Shared/Thermo-Calc/lservrc

In PyCharm, you can add environment variables in the configurations.

Select Run→Edit Configurations to open the Run/Debug Configurations window. Choose Templates and then Python. Enter the environment variable(s) by clicking the button to the right of the Environment Variables text field. Now the environment variables(s) will be set for each new configuration by default.

Note: Existing configurations need to be removed and recreated to obtain the environment variables in them.

The same way for configuring the environment variables can be used on other operating systems as if necessary.
CHAPTER
THREE

ARCHITECTURE OVERVIEW

TC-Python contains classes of these types:

- **TCPython** – this is where you start with general settings.
- **SystemBuilder** and **System** – where you choose database and elements etc.
- **Calculation** – where you choose and configure the calculation.
- **Result** – where you get the results from a calculation you have run.

### 3.1 TCPython

This is the starting point for all TC-Python usage.

You can think of this as the start of a “wizard”.

You use it to select databases and elements. That will take you to the next step in the wizard, where you configure the system.

**Example:**

```python
from tc_python import *

with TCPython() as start:
    start.select_database_and_elements(...
    # e.t.c
    # after with clause

# or like this
with TCPython():
    SetUp().select_database_and_elements(...
    # e.t.c
    # after with clause
```

**Tip:** If you use TC-Python from Jupyter Lab / Notebook, you should use TC-Python slightly different to be able to use multiple cells. See *Using TC-Python within a Jupyter Notebook or the Python console* for details.

**Note:** When your python script runs a row like this:

```python
with TCPython() as start:
```
a process running a calculation server starts. Your code, via TC-Python, uses socket communication to send and receive messages to and from that server.

When your Python script has run as far as this row:

```python
# after with clause
```

the calculation server automatically shuts down, and all temporary files are deleted. It is important to ensure that this happens by structuring your Python code using a `with()` clause as in the above example.

**Note:** To re-use results from previous calculations, set a folder where TC-Python saves results, and looks for previous results.

This is done with the function `set_cache_folder()`.

```python
from tc_python import *
with TCPython() as start:
    start.set_cache_folder("cache")
```

This folder can be a network folder and shared by many users. If a previous TC-Python calculation has run with the same cache_folder and EXACTLY the same system and calculation settings, the calculation is not re-run. Instead the result is automatically loaded from disk.

It is also possible to explicitly save and load results.

```python
from tc_python import *
with TCPython() as start:
    #... diffusion calculation (could be any calculation type)
    calculation_result.save_to_disk('path to folder')
    #...
    loaded_result = start.load_result_from_disk().diffusion('path to folder')
```

### 3.2 SystemBuilder and System

A **SystemBuilder** is returned when you have selected your database and elements in **TCPython**.

The **SystemBuilder** lets you further specify your system, for example the phases that should be part of your system.

**Example:**

```python
from tc_python import *
with TCPython() as start:
    start.select_database_and_elements("ALDEMO", ["Al", "Sc"])
    # e.t.c
```

When all configuration is done, you call `get_system()` which returns an instance of a `System` class. The `System` class is fixed and cannot be changed. If you later want to change the database, elements or something else, change the `SystemBuilder` and call `get_system()` again, or create a new `SystemBuilder` and call `get_system()`.

From the `System` you can create one or more calculations, which is the next step in the “wizard”.

---

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Note: You can use the same System object to create several calculations.

### 3.3 Calculation

The best way to see how a calculation can be used is in the TC-Python examples included with the Thermo-Calc installation.

Some calculations have many settings. Default values are used where it is applicable, and are overridden if you specify something different.

When you have configured your calculation you call `calculate()` to start the actual calculation. That returns a Result, which is the next step.

#### 3.3.1 Single equilibrium calculations

In single equilibrium calculations you need to specify the correct number of conditions, depending on how many elements your System contains.

You do that by calling `set_condition()`.

An important difference from other calculations is that single equilibrium calculations have two functions to get result values.

The `calculate()` method, which gives a SingleEquilibriumTempResult, is used to get actual values. This result is “temporary”, meaning that if you run other calculations or rerun the current one, the resulting object no longer gives values corresponding to the first calculation.

This is different from how other calculations work. If you want a Result that you can use after running other calculations, you need to call `calculate_with_state()`, which returns a SingleEquilibriumResult.

Note: `calculate()` is the recommended function and works in almost all situations. Also it has much better performance than `calculate_with_state()`.

Example:

```python
from tc_python import *

with TCPython() as start:
    gibbs_energy = {
        start.
            select_database_and_elements("FEDEMO", ["Fe", "Cr", "C"]).
            get_system().
            with_single_equilibrium_calculation().
                set_condition(ThermodynamicQuantity.temperature(), 2000.0).
                set_condition(ThermodynamicQuantity.mole_fraction_of_a_component("Cr →"), 0.1).
                set_condition(ThermodynamicQuantity.mole_fraction_of_a_component("C"), 0.01).
                calculate().
                get_value_of("G")
    }
```

3.3. Calculation
3.3.2 Batch equilibrium calculations

Batch equilibrium calculations are used when you want to do many single equilibrium calculations and it is known from the beginning which result values are required from the equilibrium. This is a vectorized type of calculation that can reduce the overhead from Python and TC-Python similar to the approach used in numpy-functions for example.

Tip: The performance of batch equilibrium calculations can be significantly better than looping and using single equilibrium calculations if the actual Thermo-Calc calculation is fast. There is little advantage if the Thermo-Calc equilibrium calculations take a long time (typically for large systems and databases).

Example:

```python
from tc_python import *

with TCPython() as start:
    calculation = (start
        .set_cache_folder(os.path.basename(__file__) + "_cache")
        .select_database_and_elements("NIDEMO", ["Ni", "Al", "Cr"])
        .get_system()
        .with_batch_equilibrium_calculation()
        .set_condition("T", 800.1)
        .set_condition("X(Al)", 1E-2)
        .set_condition("X(Cr)", 1E-2)
        .disable_global_minimization()
    )

list_of_x_Al = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
list_of_x_Cr = [3, 5, 7, 9, 11, 13, 15]
lists_of_conditions = []
for x_Al in list_of_x_Al:
    for x_Cr in list_of_x_Cr:
        lists_of_conditions.append([("X(Al)", x_Al / 100),
                                     ("X(Cr)", x_Cr / 100)])
    calculation.set_conditions_for_equilibria(lists_of_conditions)

results = calculation.calculate(['BM', 'VM'])

masses = results.get_values_of('BM')
volumes = results.get_values_of('VM')

print(masses)
print(volumes)
```
3.3.3 Precipitation calculations

All that can be configured in the Precipitation Calculator in Graphical Mode can also be done here in this calculation. However, you must at least enter a matrix phase, a precipitate phase, temperature, simulation time and compositions.

Example:

```python
from tc_python import *

with TCPython() as start:
    precipitation_curve = (
        start.
        select_thermodynamic_and_kinetic_databases_with_elements("ALDEMO", "MALDEMO", ["Al", "Sc"]).
        get_system().
        with_isothermal_precipitation_calculation().
        set_composition("Sc", 0.18).
        set_temperature(623.15).
        set_simulation_time(1e5).
        with_matrix_phase(MatrixPhase("FCC_A1").
            add_precipitate_phase(PrecipitatePhase("AL3SC"))).
        calculate()
    )
```

3.3.4 Scheil calculations

All Scheil calculations available in Graphical Mode or Console Mode can also be done here in this calculation. The minimum you need to specify are the elements and compositions. Everything else is set to a default value.

Example:

```python
from tc_python import *

with TCPython() as start:
    temperature_vs_mole_fraction_ofSolid = (
        start.
        select_database_and_elements("FEDEMO", ["Fe", "C"]).
        get_system().
        with_scheil_calculation().
        set_composition("C", 0.3).
        calculate().
        get_values_of(ScheilQuantity.temperature(),
            ScheilQuantity.mole_fraction_of_all_solid_phases())
    )
```

3.3.5 Property diagram calculations

For the property diagram (step) calculation, everything that you can configure in the Equilibrium Calculator when choosing Property diagram in Graphical Mode can also be configured in this calculation. In Console Mode the property diagram is created using the Step command. The minimum you need to specify are elements, conditions and the calculation axis. Everything else is set to default values, if you do not specify otherwise.

Example:
from tc_python import *

with TCPython() as start:
    property_diagram = {
        start.
            select_database_and_elements("FEDEMO", ["Fe", "C"]).
            get_system().
            with_property_diagram_calculation().
                with_axis(CalculationAxis(ThermodynamicQuantity.temperature()).
                    set_min(500).
                    set_max(3000)).
                set_condition(ThermodynamicQuantity.mole_fraction_of_a_component("C"),
                    0.01).
                calculate().
                get_values_grouped_by_stable_phases_of(ThermodynamicQuantity.
                    temperature(),                            ThermodynamicQuantity.volume_.
                    fraction_of_a_phase("ALL"))
    }

3.3.6 Phase diagram calculations

For the phase diagram (map) calculation, everything that you can configure in the Equilibrium Calculator when choosing Phase diagram in Graphical Mode can also be configured in this calculation. In Console Mode the phase diagram is created using the Map command. The minimum you need to specify are elements, conditions and two calculation axes. Everything else is set to default values, if you do not specify otherwise.

Example:

from tc_python import *

with TCPython() as start:
    phase_diagram = {
        start.
            select_database_and_elements("FEDEMO", ["Fe", "C"]).
            get_system().
            with_phase_diagram_calculation().
                with_first_axis(CalculationAxis(ThermodynamicQuantity.temperature()).
                    set_min(500).
                    set_max(3000)).
                with_second_axis(CalculationAxis(ThermodynamicQuantity.mole_fraction_of_a_component("C"))),
                    set_min(0).
                    set_max(1)).
                set_condition(ThermodynamicQuantity.mole_fraction_of_a_component("C"),
                    0.01).
                calculate().
                get_values_grouped_by_stable_phases_of(ThermodynamicQuantity.mass_.
                    fraction_of_a_component("C"),                            ThermodynamicQuantity.
                    temperature())
    }
3.3.7 Diffusion calculations

For diffusion calculations, everything that you can configure in the Diffusion Calculator can also be configured in this calculation. The minimum you need to specify are elements, temperature, simulation time, a region with a grid and width, a phase and an initial composition.

Example:

```
from tc_python import *

with TCPython() as start:
    diffusion_result = {
        start.
        select_thermodynamic_and_kinetic_databases_with_elements("FEDEMO", "MFEDEMO", ["Fe", "Ni"]).
        get_system().
        with_isothermal_diffusion_calculation().
        set_temperature(1400.0).
        set_simulation_time(108000.0).
        add_region(Region("Austenite").
            set_width(1E-4).
            with_grid(CalculatedGrid.linear().set_no_of_points(50)).
            with_composition_profile(CompositionProfile().
                add("Ni", ElementProfile.linear(10.0, 50.0))
            ).
            add_phase("FCC_A1")).
        calculate()
    }

    distance, ni_fraction = diffusion_result.get_mass_fraction_of_component_at_time("Ni", 108000.0)
```

3.3.8 Property Model calculations

For Property Model calculations, everything that you can configure in the Property Model Calculator in Graphical Mode can also be configured in this calculation. The minimum you need to specify are elements, composition and which Property Model you want to use.

Example:

```
from tc_python import *

with TCPython() as start:
    print("Available Property Models: ", format(start.get_property_models()))
    property_model = {
        start.
        select_database_and_elements("FEDEMO", ["Fe", "C"]).
        get_system().
        with_property_model_calculation("Driving force").
        set_composition("C", 1.0).
        set_argument("precipitate", "GRAPHITE")
    }

    print("Available arguments: ", format(property_model.get_arguments()))
    result = property_model.calculate()

    print("Available result quantities: ", format(result.get_result_quantities()))
    driving_force = result.get_value_of("normalizedDrivingForce")
```
3.3.9 Material to Material calculations

Material to Material calculations are generally regular single equilibrium, property diagram or phase diagram calculations but they are specialised to handle the mixture of two materials A and B. Everything that you can configure in the Material to Material Calculator in Graphical Mode can also be configured in this calculation. The minimum required configuration is shown below for a Property diagram calculation for varying amount of material B. The other calculators (single fraction of material B and phase diagram calculations) are configured in a similar way.

Example:

```python
from tc_python import *

with TCPython() as start:
    material_to_material_property_diagram = (start.
        select_database_and_elements("FEDEMO", ["Fe", "Cr", "Ni", "C"]).
        get_system().
        with_material_to_material().
        with_property_diagram_calculation().
        set_material_a({"Cr": 10.0, "Ni": 15.0}, "Fe").
        set_material_b({"Cr": 15.0, "Ni": 10.0}, "Fe").
        set_activities({"C": 0.1}).
        with_constant_condition(ConstantCondition.temperature(800 + 273.15)).
        with_axis(MaterialToMaterialCalculationAxis.fraction_of_material_b(from_
            fraction=0.0,
            to_
            fraction=1.0,
            start_
            fraction=0.5))
        )

    result = material_to_material_property_diagram.calculate()
    data = result.get_values_grouped_by_quantity_of(MATERIAL_B_FRACTION,
        ThermodynamicQuantity.volume_
        fraction_of_a_phase(ALL_PHASES))

    for group in data.values():
        fractions_of_b = group.x
        volume_fractions_of_phase = group.y
        phase_name = group.label
```

3.4 Result

All calculations have a method called calculate() that starts the calculations and when finished, returns a Result. The Result classes have very different methods, depending on the type of calculation. The Result is used to get numerical values from a calculation that has run. The Result can be saved to disk by the method save_to_disk(). Previously saved results can be loaded by the method load_result_from_disk() on the SetUp class.

Example:
# code above sets up the calculation
r = calculation.calculate()
time, meanRadius = r.get_mean_radius_of("AL3SC")

The Result objects are completely independent from calculations done before or after they are created. The objects return valid values corresponding to the calculation they were created from, for their lifetime. The only exception is if you call calculate() and not calculate_with_state() on a single equilibrium calculation.

As in the following example you can mix different calculations and results, and use old results after another calculation has run.

Example:

```python
# ...
# some code to set up a single equilibrium calculation
# ...

single_eq_result = single_eq_calculation.calculate_with_state()
# ...
# some code to set up a precipitation calculation
# ...

prec_result = precipitation_calculation.calculate()
# ...
# some code to set up a Scheil calculation
# ...

scheil_result = scheil_calculations.calculate()

# now it is possible to get results from the single equilibrium calculation, without having to re-run it (because it has been calculated with saving of the state)
gibbs = single_eq_result.get_value_of("G")
```

### 3.4.1 DiffusionResult

The DiffusionResult class, that is returned when calling calculate() on any DiffusionCalculation, has the possibility to create a ContinuedDiffusionCalculation, in addition to the “normal” functionality for results. This makes it possible to run a diffusion calculation and then, depending on the result, change some settings and continue.

Example:

```python
# ...
# some code to set up a Diffusion calculation
# ...

first_diffusion_result = diffusion_calculation.calculate()

continued_calculation = first_diffusion_result.with_continued_calculation()

continued_calculation.set_simulation_time(110000.0)
continued_calculation.with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element('C', 1.0))
second_result = continued_calculation.calculate()
```

(continues on next page)
# Property Model Framework

The Python Property Model SDK extends the Thermo-Calc software to enable you to create your own Property Models. A Property Model is a Python-based calculation that can use any TC-Python functionality (including diffusion and precipitation calculations) but is usable through the Graphical User Interface (UI) of Thermo-Calc in a more simple way. It is typically used to model material properties but by no means limited to that. Examples of Property Models provided by Thermo-Calc include Martensite and Pearlite formation in steel.

The Property Model Framework uses standard Python 3 beginning with Thermo-Calc 2021a and can access all TC-Python functionality and any Python package including numpy, scipy, tensorflow, etc. The actual calculation code is nearly identical, regardless if called from within a Property Model or from standard Python.

This is a complete rewrite of the original version of the framework that was based on Jython 2.7 and therefore had a number of limitations. Property models written with the old Property Model Framework before Thermo-Calc 2021a are not compatible with the new framework. However, the migration should be relatively easy because the syntax was changed as little as possible.

### 3.5.1 Property models vs. TC-Python

The main difference between a Property Model and regular TC-Python code is that a Property Model is directly integrated into the UI of Thermo-Calc via a plugin architecture while TC-Python code can only be accessed by programs and scripts written in Python.

The user should develop a Property Model if the functionality needs to be available from the Thermo-Calc UI, especially if it should be applied by other users not familiar to programming languages. Otherwise it is preferable to implement the functionality directly in a TC-Python program. If required, Property Models can as well be accessed from within TC-Python.

### 3.5.2 Architecture

Every Property Model needs to contain a class that implements the interface `tc_python.propertymodel_sdk.PropertyModel`. There are naming conventions that must to be fulfilled: the file name is required to follow the the pattern `XYPythonModel.py` and the name of the class needs to match this. Additionally the file must be placed in a directory named `XYPython` within the Property Model directory. The content of the placeholder `XY` can be freely chosen.

A simple complete Property Model, saved in a file called `SimplePythonModel.py` in the directory `SimplePython`, looks like this:

```python
from tc_python import *

class SimplePythonModel(PropertyModel):
    def provide_model_category(self) -> List[str]:
        return ["Demo"]
```

(continues on next page)
def provide_model_name(self) -> str:
    return "My Demo Model"

def provide_model_description(self) -> str:
    return "This is a demo model."

def provide_ui_panel_components(self) -> List[UIComponent]:
    return [UIBooleanComponent("CHECKBOX", "Should this be checked?", "Simple checkbox", setting=False)]

def provide_calculation_result_quantities(self) -> List[ResultQuantity]:
    return [create_general_quantity("RESULT", "A result")]

def evaluate_model(self, context: CalculationContext):
    if context.get_ui_boolean_value("CHECKBOX"):
        self.logger.info("The checkbox is checked")

        # obtain the entered values from the GUI
        composition_as_mass_fraction = context.get_mass_fractions()
        temp_in_k = context.get_temperature()
        calc = context.system.with_single_equilibrium_calculation()

        # continue with a TC-Python calculation now ...
        context.set_result_quantity_value("RESULT", 5.0)  # the value would normally have been calculated

The basic building blocks of the Property Model API are:

- `tc_python.propertymodel_sdk.ResultQuantity`: Defines a calculation result of a Property Model that will be provided to the UI after each model evaluation

- `tc_python.propertymodel_sdk.CalculationContext`: Provides access to the data from the UI (such as the entered composition and temperature) and to the current TC-Python system object which is the entrypoint for using TC-Python from within the Property Model

- `tc_python.propertymodel_sdk.UIComponent`: These are the UI-components that create the user interface of the Property Model within the model panel of the Thermo-Calc application UI. Different components are available (for example checkboxes, text fields and lists).

### 3.5.3 Property Model directory

The Property Model `py`-files need to be located within subdirectories of the `Property Model directory`, e.g. `PropertyModelDir/XYPython/XYPythonModel.py`. The default Property Model directory can be changed in the menu `Tools -> Options` in the graphical user interface.

<table>
<thead>
<tr>
<th>Operating system</th>
<th>Default Property Model directory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>C:\Users\UserName\Documents\Thermo-Calc\2022a\PropertyModels</td>
</tr>
<tr>
<td>Linux</td>
<td>/home/UserName/Thermo-Calc/2022a/PropertyModels</td>
</tr>
<tr>
<td>MacOS</td>
<td>/Users/Shared/Thermo-Calc/2022a/PropertyModels</td>
</tr>
</tbody>
</table>
4.1 Re-use of the single equilibrium calculation state

The Thermo-Calc core keeps an internal state containing the data from previously performed calculations (such as composition of sublattices, previously formed phases, ...). This will be used for start values of future calculations (if not explicitly overwritten) and can strongly influence their convergence and calculation time. It can be useful to save and restore later the core-state in advanced use cases, these include:

- Improving the convergence speed in case of very complicated equilibria if a similar equilibrium had been calculated already before. Similarity refers here primarily to composition, temperature and entered phase set. This case can occur for example with the Nickel-database TCNi.

- Convenient and fast switching between states that have changed a lot (for example regarding suspended phases, numerical settings, ...)

The mechanism of saving and restoring the state is called bookmarking and is controlled with the two methods `tc_python.single_equilibrium.SingleEquilibriumCalculation.bookmark_state()` and `tc_python.single_equilibrium.SingleEquilibriumCalculation.set_state_to_bookmark()`. The following short example demonstrates how to switch between two different states easily in practice:

```python
from tc_python import *

with TCPython() as session:
    calc = (session.
        select_database_and_elements("FEDEMO", ["Fe", "C"]).
        get_system().
        with_single_equilibrium_calculation().
        set_condition(ThermodynamicQuantity.temperature(), 2000.0).
        set_condition("X(C)", 0.01))

    calc.calculate()
    bookmark_temp_condition = calc.bookmark_state()

    calc.set_phase_to_fixed("BCC", 0.5)
    calc.remove_condition(ThermodynamicQuantity.temperature())
    bookmark_fixed_phase_condition = calc.bookmark_state()

    result_temp = calc.set_state_to_bookmark(bookmark_temp_condition)
    print("Conditions do contain temperature: {}".format(result_temp.get_conditions()))
    # this calculation had already been performed
    print("Stable phases (do not contain BCC): {}".format(result_temp.get_stable_phases()))
```

(continues on next page)
4.2 Re-use and saving of results

Before a calculation is run in TC-Python, a check is made to see if the exact same calculation has run before, and if that is the case, the result from the calculation can be loaded from disk instead of being re-calculated. This functionality is always enabled within a script running TC-Python, but you can make it work the same way when re-running a script, or even when running a completely different script.

To use results from previous calculations, set a folder where TC-Python saves results, and looks for previous results. This is controlled by the method `tc_python.server.SetUp.set_cache_folder()`.

```python
from tc_python import *

with TCPython() as start:
    start.set_cache_folder("cache")
```

This folder can be a network folder and shared by many users. The calculation is not re-run if there is a previous TC-Python calculation with the same cache folder and exactly the same settings; the result is instead loaded from disk.

Another possibility is to explicitly save the result to disk and reload it later:

```python
from tc_python import *

with TCPython() as start:
    # ... the system and calculator are set up and the calculation is performed
    result = calculator.calculate()
    result.save_to_disk("./result_dir")
```

You can then load the result again in another session:

```python
from tc_python import *

with TCPython() as start:
    result = SetUp().load_result_from_disk().diffusion("./result_dir")
    x, frac = result.get_mole_fraction_of_component_at_time("Cr", 1000.0)
```
4.3 All TC-Python objects are non-copyable

Never create a copy of an instance of a class in TC-Python, neither by using the Python built-in function `deepcopy()` nor in any other way. All classes in TC-Python are proxies for classes in the underlying calculation server and normally hold references to result files. A copied class object in Python would consequently point to the same classes and result files in the calculation server.

Instead of making a copy, always create a new instance:

```python
from tc_python import *

with TCPython() as start:
    system = start.select_database_and_elements("FEDEMO", ["Fe", "Cr"]).get_system()
    calculator = system.with_single_equilibrium_calculation()

    # *do not* copy the 'calculator' object, create another one instead
    calculator_2 = system.with_single_equilibrium_calculation()

    # now you can use both calculators for different calculations ...
```

4.4 Python Virtual Environments

A Python installation can have several virtual environments. You can think of a virtual environment as a collection of third party packages that you have access to in your Python scripts. `tc_python` is such a package.

To run TC-Python, you need to install it into the same virtual environment as your Python scripts are running in. If your scripts fail on `import tc_python`, you need to execute the following command in the terminal of the same Python environment as your script is running in:

```bash
pip install TC_Python-<version>-py3-none-any.whl
```

If you use the PyCharm IDE, you should do that within the `Terminal` built into the IDE. This `Terminal` runs automatically within your actual (virtual) environment.

To prevent confusion, it is recommend in most cases to install TC-Python within your global interpreter, for example by running the `pip install` command within your default Anaconda prompt.

4.5 Using `with TCPython()` efficiently

Normally you should call `with TCPython()` only once within each process.

**Note:** When leaving the `with`-clause, the Java backend engine process is stopped and all temporary data is deleted. Finally when entering the next `with`-clause a new Java process is started. This can take several seconds.

If appropriate, it is safe to run `with TCPython()` in a loop. **Due to the time it takes this only makes sense if the calculation time per iteration is longer than a minute.**

To prevent calling `with TCPython()` multiple times and cleaning up temporary data, you can use the following pattern.

**Example:**
from tc_python import *
#

def calculation(calculator):
    # you could also pass the 'session' or 'system' object if more appropriate
    calculator.set_condition("W(Cr)", 0.1)
    # further configuration ...

    result = calculator.calculate()
    # ...
    result.invalidate()  # if the temporary data needs to be cleaned up immediately

if __name__ == '__main__':
    with TCPython() as session:
        system = session.select_database_and_elements("FEDEMO", ["Fe", "Cr"]).get_
        →
        system()
        calculator = system.with_single_equilibrium_calculation()

        for i in range(50):
            calculation(calculator)

4.6 Parallel calculations

It is possible to perform parallel calculations with TC-Python using multi-processing.

Note: Please note that multi-threading is not suitable for parallelization of computationally intensive tasks in Python. Additionally the Thermo-Calc core is not thread-safe. Using suitable Python frameworks it is also possible to dispatch the calculations on different computers of a cluster.

A general pattern that can be applied is shown below. This code snippet shows how to perform single equilibrium calculations for different compositions in parallel. In the same way all other calculators of Thermo-Calc can be used or combined. For performance reasons in a real application, probably numpy arrays instead of Python arrays should be used.

Example:

import concurrent.futures
from tc_python import *

def do_perform(parameters):
    # this function runs within an own process
    with TCPython() as start:
        elements = ["Fe", "Cr", "Ni", "C"]
        calculation = (start.select_database_and_elements("FEDEMO", elements).
                       get_system().
                       with_single_equilibrium_calculation().
                       set_condition("T", 1100).
                       set_condition("W(C)", 0.1 / 100).
                       set_condition("W(Ni)", 2.0 / 100))

(continues on next page)
phase_fractions = []
    cr_contents = range(parameters["cr_min"],
                        parameters["cr_max"],
                        parameters["delta_cr"])
    for cr in cr_contents:
        result = (calculation.set_condition("W(Cr)", cr / 100).
                  calculate())
        phase_fractions.append(result.get_value_of("NPM(BCC_A2)"))
    return phase_fractions

if __name__ == "__main__":
    parameters = [
        {"index": 0, "cr_min": 10, "cr_max": 15, "delta_cr": 1},
        {"index": 1, "cr_min": 15, "cr_max": 20, "delta_cr": 1}]
    bcc_phase_fraction = []
    num_processes = 2
    with concurrent.futures.ProcessPoolExecutor(num_processes) as executor:
        for result_from_process in zip(parameters, executor.map(do_perform, parameters)):
            params, phase_fractions_from_process = result_from_process
            bcc_phase_fraction.extend(phase_fractions_from_process)

4.7 Handling crashes of the calculation engine

In some cases the Thermo-Calc calculation engine can crash. If batch calculations are performed, this brings down the complete batch. To handle this situation there is an exception you can use.

UnrecoverableCalculationException

That exception is thrown if the calculation server enters a state where no further calculations are possible. You should catch that exception outside of the with TCPython() clause and continue within a new with-clause.

Example:

from tc_python import *

for temperature in range(900, 1100, 10):
    try:
        with TCPython() as start:
            diffusion_result = (start.
                                 select_thermodynamic_and_kinetic_databases_with_elements("FEDEMO",
                               "MFEDEMO", ["Fe", "Ni"])).
(continues on next page)
get_system().
with_isothermal_diffusion_calculation().
  set_temperature(temperature).
  set_simulation_time(108000.0).
  add_region(Region("Austenite").
    set_width(1E-4).
    with_grid(CalculatedGrid.linear().set_no_of_points(50)).
    with_composition_profile(CompositionProfile().
      add("Ni", ElementProfile.linear(10.0, 50.0)))
 ).
  add_phase("FCC_A1")).
  calculate()

distance, ni_fraction = diffusion_result.get_mass_fraction_of_component_ 
  at_time("Ni", 108000.0)
  print(ni_fraction)

except UnrecoverableCalculationException as e:
  print('Could not calculate. Continuing with next...')

4.8 Using TC-Python within a Jupyter Notebook or the Python console

TC-Python can also be used from within an interactive Jupyter Notebook and a Python console as well as similar products. The main difference from a regular Python program is that it is not recommended to use a `with`-clause to manage the TC-Python resources. That is only possible within a single Jupyter Notebook cell. Instead the standalone functions `tc_python.server.start_api_server()` and `tc_python.server.stop_api_server()` should be used for manually managing the resources.

**Note:** The resources of TC-Python are primarily the Java-process running on the backend side that performs the actual calculations and the temporary-directory of TC-Python that can grow to a large size over time, especially if precipitation calculations are performed. If a `with`-clause is used, these resources are automatically cleared after use.

You need to make sure that you execute the two functions `tc_python.server.start_api_server()` and `tc_python.server.stop_api_server()` exactly once within the Jupyter Notebook session. If not stopping TC-Python, extra Java-processes might be present and the temporary disk-space is not cleared. However, these issues can be resolved manually.

The temporary directories of TC-Python are named, for example, TC_TMP4747588488953835507 that has a random ID. The temporary directory on different operating systems varies according to the pattern shown in the table.

<table>
<thead>
<tr>
<th>Operating system</th>
<th>Temporary directory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>C:\Users[UserName]\AppData\Local\Temp\TC_TMP4747588488953835507</td>
</tr>
<tr>
<td>MacOS</td>
<td>/var/folders/g7/7du81ti_b7mm84n184fn3k9100001g/T/TC_TMP4747588488953835507</td>
</tr>
<tr>
<td>Linux</td>
<td>/tmp/TC_TMP4747588488953835507</td>
</tr>
</tbody>
</table>

In a Jupyter Notebook some features of an IDE such as auto-completion (`TAB-key`), available method lookup (press `.` and then `TAB`) and parameter lookup (set the cursor within the method-parenthesis and press `SHIFT + TAB` or `SHIFT + TAB + TAB` for the whole docstring) are also available.
4.9 Property Model Framework

4.9.1 Debugging Property Model code

You can debug property models while running them from Thermo-Calc.

- Start Thermo-Calc and create a Property Model calculator.
- Select the model you want to debug and check the debug checkbox in the lower right corner of the Python code tab.

Now the model that you want to debug has been updated with code needed to connect with Thermo-Calc.

- Start debugging the model in the IDE of your choice.

**Note:** You must use a Python interpreter where TC-Python is installed.

In PyCharm it looks like this:
Note: When your IDE and Thermo-Calc have successfully connected, you will see this in the Thermo-Calc log:

```
10:34:42,170 INFO Waiting for developer(!) to start Python process in debugger...
10:34:42,171 INFO Connected successfully to the Python process for the model 'DrivingForcePythonModel' in DEBUG mode
```

You can stop the debug session in your IDE, change the model code, and start debugging again. The changes you made will take effect in Thermo-Calc without the need to restart. If you for instance changed the method `evaluate_model()`, the change will take effect the next time you press `Perform`.

It is also possible to start the models from TC-Python. The workflow is exactly the same as described above, except instead of starting Thermo-Calc graphical user interface, you start a Python script and use the parameter `debug_model=True` when selecting your model.

```
from tc_python import *

with TCPython() as start:
    property_model = {
        start.
        select_database_and_elements("FEDEMO", ["Fe", "C"]).
        get_system().
        with_property_model_calculation("my own Driving Force", debug_model=True).
        set_composition("C", 1.0).
    }
    property_model.calculate()
...
```
4.9.2 Developing Property Models in several files

You can split your Property Model code in several .py files, and there are two ways of doing that:

- side-by-side modules
- common modules

Side-by-side modules are Python files located in the same folder as the Property Model. Common modules are Python files located in a folder outside of the Property Model folder, which makes it possible to share them with several models as a common library.

4.9.2.1 side-by-side modules

You are required to:

- Add a __init__.py file to your Property Model folder
- Add all imports of side-by-side modules in your main Property Model Python file also to the __init__.py file

Example:

CriticalTemperaturesPythonModel.py (The main Property Model file):

```python
from CriticalTemperaturesPython import CriticalTemperatures
from tc_python import *
import numpy as np
class CriticalTemperaturesPythonModel(PropertyModel):
...
```

__init__.py:

```python
from CriticalTemperaturesPython.critical_temperatures_library import CriticalTemperatures
```

If you are using PyCharm, the package name of the Property Model might be highlighted as an error, in this case you can mark the Property Model directory (i.e. the root of the present model directory) by right-clicking on it in the project window of PyCharm and marking it as Sources Root:

critical_temperatures_library.py:

```python
from tc_python import *
import numpy as np
from scipy import optimize
from enum import Enum
class CriticalTemperatures(object):
...
```
Note: Modules installed in the Python interpreter such as `numpy`, `scipy`, etc can be imported as normal. This only concerns files imported as *side-by-side* modules.

4.9.2.2 *common* modules

*common* modules work very similar to *side-by-side* modules except the import statements are done in the “main” `_init__.py` file in *Property Model directory*.

You are required to:

- Add a `_init__.py` file to your property model folder.
- Add all imports of *common* modules in your main property model python file also to both the `_init__.py` file in *Property Model directory* AND the `_init__.py` of the property model.

Example:

CriticalTemperaturesPythonModel.py (The main Property Model file):

```python
from PropertyModels import Martensite
from tc_python import *

class CriticalTemperaturesPythonModel(PropertyModel):
...
```

`_init__.py` (The init file located in the property model folder)

```python
from PropertyModels import Martensite
```

`_init__.py` (The init file located in *Property Model directory*)

```python
from PropertyModels.common.martensite_library import Martensite
```

The file `critical_temperatures_library.py` should in this example be located in a folder called *common* in the *Property Model directory*.

`critical_temperatures_library.py`:

```python
from tc_python import *
import numpy as np
from scipy import optimize
from enum import Enum

class CriticalTemperatures(object):
...
```

Note: *common* modules don’t have to be located in folder called *common*. It can be any name, as long as the imports match the folder name.

Note: In this example the *Property Model directory* is called ‘PropertyModels’. If you use a different directory for your property model, your imports have to match that.
4.9.3 Alternative Python for Property Models

4.9.3.1 Default bundled Python interpreter

Thermo-Calc is by default using a Python 3.7.2 interpreter bundled to the software for running the property models. It is containing the following major packages:

<table>
<thead>
<tr>
<th>Package</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>matplotlib</td>
<td>3.3.2</td>
</tr>
<tr>
<td>numpy</td>
<td>1.19.2</td>
</tr>
<tr>
<td>scikit-learn</td>
<td>0.23.2</td>
</tr>
<tr>
<td>scipy</td>
<td>1.5.2</td>
</tr>
<tr>
<td>TC-Python</td>
<td>2022a</td>
</tr>
</tbody>
</table>

**Warning:** Any changes to the interpreter packages can therefore break Thermo-Calc and should be avoided. If the installation gets broken, it can be fixed by reinstalling Thermo-Calc after having removed it.

Please contact the Thermo-Calc support if you think that further packages might be useful in future releases. If these packages are insufficient for you, it is possible to use another Python-interpreter: Configuring another Python interpreter.

The interpreter is located in different places depending on the platform:

<table>
<thead>
<tr>
<th>Operating system</th>
<th>Path to the bundled Python-interpreter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>C:\Program Files\Thermo-Calc\2022a\python\python.exe</td>
</tr>
<tr>
<td>Linux</td>
<td>/home/UserName/Thermo-Calc/2022a/python/bin/python3</td>
</tr>
<tr>
<td>MacOS</td>
<td>/Applications/Thermo-Calc-2022a.app/Contents/Resources/python/bin/python3</td>
</tr>
</tbody>
</table>

4.9.3.2 Configuring another Python interpreter

If you require additional Python-packages or prefer to use your own interpreter installed on your system, you can change the interpreter used by Thermo-Calc to run the property models. Select Tools → Options in the Thermo-Calc GUI and modify the path to that of your Python 3 interpreter of choice:
5.1 Calculations

5.1.1 Module “single_equilibrium”

```python
class tc_python.single_equilibrium.AbstractSingleEquilibriumCalculation(calculator)
    Bases: tc_python.abstract_base.AbstractCalculation

Abstract configuration required for a single equilibrium calculation.

Note: This is an abstract class that cannot be used directly.

    abstract calculate() \rightarrow tc_python.single_equilibrium.SingleEquilibriumTempResult

    disable_global_minimization()
    Turns the global minimization completely off.

    Returns This `SingleEquilibriumCalculation` object

    enable_global_minimization()
    Turns the global minimization on (using the default settings).

    Returns This `SingleEquilibriumCalculation` object

    get_components() \rightarrow List[str]
    Returns a list of components in the system (including all components auto-selected by the database(s)).

    Returns The components

    get_gibbs_energy_addition_for(phase: str) \rightarrow float
    Used to get the additional energy term (always being a constant) of a given phase. The value given is added
to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface
tension, elastic energy, etc.

    It is not composition-, temperature- or pressure-dependent.

    Parameters phase – Specify the name of the (stoichiometric or solution) phase with the addition

    Returns Gibbs energy addition to G per mole formula unit.

    get_system_data() \rightarrow tc_python.abstract_base.SystemData
    Returns the content of the database for the currently loaded system. This can be used to modify the param-
eters and functions and to change the current system by using `with_system_modifications()`.
```
Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

**run_poly_command** *(command: str)*
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

*Parameters* `command` – The Thermo-Calc Console Mode command

*Returns* This `SingleEquilibriumCalculation` object

**set_component_to_entered** *(component: str)*
Sets the specified component to the status ENTERED, that is the default state.

*Parameters* `component` – The component name or `ALL_COMPONENTS`

*Returns* This `SingleEquilibriumCalculation` object

**set_component_to_suspended** *(component: str, reset_conditions: bool = False)*
Sets the specified component to the status SUSPENDED, i.e. it is ignored in the calculation.

*Parameters*

- `reset_conditions` – if ‘True’ also remove composition conditions for the component if they are defined
- `component` – The component name or `ALL_COMPONENTS`

*Returns* This `SingleEquilibriumCalculation` object

**set_gibbs_energy_addition_for** *(phase: str, gibbs_energy: float)*
Used to specify the additional energy term (always being a constant) of a given phase. The value (`gibbs_energy`) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

*Parameters*

- `phase` – Specify the name of the (stoichiometric or solution) phase with the addition
- `gibbs_energy` – Addition to G per mole formula unit

*Returns* This `SingleEquilibriumCalculation` object

**set_phase_to_dormant** *(phase: str)*
Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

*Parameters* `phase` – The phase name or `ALL_PHASES` for all phases

*Returns* This `SingleEquilibriumCalculation` object
**set_phase_to_entered** *(phase: str, amount: float = 1.0)*

Sets the phase to the status ENTERED, that is the default state.

**Parameters**

- **phase** – The phase name or ALL_PHASES for all phases
- **amount** – The phase fraction (between 0.0 and 1.0)

**Returns** This `SingleEquilibriumCalculation` object

**set_phase_to_fixed** *(phase: str, amount: float)*

Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

**Parameters**

- **phase** – The phase name
- **amount** – The fixed phase fraction (between 0.0 and 1.0)

**Returns** This `SingleEquilibriumCalculation` object

**set_phase_to_suspended** *(phase: str)*

Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters**

- **phase** – The phase name or ALL_PHASES for all phases

**Returns** This `SingleEquilibriumCalculation` object

**with_options** *(options: tc_python.single_equilibrium.SingleEquilibriumOptions)*

Sets the simulation options.

**Parameters**

- **options** – The simulation options

**Returns** This `SingleEquilibriumCalculation` object

**with_reference_state** *(component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)*

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

**Parameters**

- **component** – The name of the element must be given.
- **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
• **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.

• **pressure** – The Pressure (in Pa) for the reference state.

**Returns** This SingleEquilibriumCalculation object

**with_system_modifications** *(system_modifications: tc_python.abstract_base.SystemModifications)*

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

**Note:** This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb*-file.

**Parameters** system_modifications – The system modification to be performed

**Returns** This SingleEquilibriumCalculation object

### class tc_python.single_equilibrium.SingleEquilibriumCalculation*(calculator)*

Bases: tc_python.single_equilibrium.AbstractSingleEquilibriumCalculation

Configuration for a single equilibrium calculation.

**Note:** Specify the conditions and possibly other settings, the calculation is performed with `calculate()`.

**bookmark_state** *(bookmark_id: str = '')* → str

Puts a “bookmark” on the current calculation-state of the calculator allowing the program to return to this state later as needed.

By bookmarking a state, you can simplify the convergence of equilibria when they strongly depend on the starting conditions (i.e. the state). Also use it to improve performance by running a calculation, then bookmarking it, and later returning to it for other equilibria whose conditions are “close” to the bookmarked equilibrium.

This method is used in combination with the method `set_state_to_bookmark()`.

**Parameters** bookmark_id – The bookmark id. If omitted a generated id is used and returned

**Returns** The bookmark id

**calculate** () → tc_python.single_equilibrium.SingleEquilibriumTempResult

Performs the calculation and provides a temporary result object that is only valid until something gets changed in the calculation state. The method `calculate()` is the default approach and should be used in most cases.

**Returns** A new SingleEquilibriumTempResult object which can be used to get specific values from the calculated result. It is undefined behavior to use that object after the state of the calculation has been changed.

**Warning:** If the result object should be valid for the whole program lifetime, use `calculate_with_state()` instead.

**calculate_with_state** () → tc_python.single_equilibrium.SingleEquilibriumResult

Performs the calculation and provides a result object that reflects the present state of the calculation during the whole lifetime of the object.
Note: Because this method has performance and temporary disk space overhead (i.e. it is resource heavy), only use it when it is necessary to access the result object after the state is changed. In most cases you should use the method \texttt{calculate()}.

\textbf{Returns} A new \texttt{SingleEquilibriumResult} object which can be used later at any time to get specific values from the calculated result.

disable\_global\_minimization()  
Turns the global minimization completely off.

\textbf{Returns} This \texttt{SingleEquilibriumCalculation} object

enable\_global\_minimization()  
Turns the global minimization on (using the default settings).

\textbf{Returns} This \texttt{SingleEquilibriumCalculation} object

get\_components() $\rightarrow$ \texttt{List[str]}  
Returns a list of components in the system (including all components auto-selected by the database(s)).

\textbf{Returns} The components

get\_gibbs\_energy\_addition\_for(phase: str) $\rightarrow$ float  
Used to get the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

\textbf{Parameters} \texttt{phase} – Specify the name of the (stoichiometric or solution) phase with the addition

\textbf{Returns} Gibbs energy addition to \( G \) per mole formula unit.

get\_interfacial\_energy(matrix\_phase: str, precipitate\_phases: \texttt{List[str]}, zero\_volume\_elements: \texttt{List[str]} = ['C', 'N']) $\rightarrow$ \texttt{Dict[str, float]}  
Estimates 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.

\textbf{Default}: elements with no contribution to volume are C and N.

\textbf{Parameters}

\begin{itemize}
  \item \texttt{matrix\_phase} – The matrix phase.
  \item \texttt{precipitate\_phases} – The list of precipitate phases for which interfacial energy between them and the matrix phase is to be calculated.
  \item \texttt{zero\_volume\_elements} – The elements that are assumed to not contribute to the volume.
\end{itemize}

\textbf{Returns} A dictionary containing interfacial energy per precipitate phase.

get\_system\_data() $\rightarrow$ \texttt{tc\_python.abstract\_base.SystemData}  
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using \texttt{with\_system\_modifications()}.

\textbf{Note}: Parameters can only be read from unencrypted (i.e. \texttt{user}) databases loaded as \*.tdb-file.
Returns The system data

remove_all_conditions()
Removes all set conditions.

Returns This SingleEquilibriumCalculation object

remove_condition (quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str])
Removes the specified condition.

Parameters quantity – the thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example “X(Cr)”)  

Returns This SingleEquilibriumCalculation object

run_poly_command (command: str)
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

Parameters command – The Thermo-Calc Console Mode command

Returns This SingleEquilibriumCalculation object

Note: It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

Warning: As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

set_component_to_entered (component: str)
Sets the specified component to the status ENTERED, that is the default state.

Parameters component – The component name or ALL_COMPONENTS

Returns This SingleEquilibriumCalculation object

set_component_to_suspended (component: str, reset_conditions: bool = False)
Sets the specified component to the status SUSPENDED, i.e. it is ignored in the calculation.

Parameters
• reset_conditions – if ‘True’ also remove composition conditions for the component if they are defined
• component – The component name or ALL_COMPONENTS

Returns This SingleEquilibriumCalculation object

set_condition (quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], value: float)
Sets the specified condition.

Parameters
• quantity – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example “X(Cr)”)  

• value – The value of the condition

Returns This SingleEquilibriumCalculation object
**set_gibbs_energy_addition_for** *(phase: str, gibbs_energy: float)*

Used to specify the additional energy term (always being a constant) of a given phase. The value *(gibbs_energy)* given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

**Parameters**

- **phase** – Specify the name of the (stoichiometric or solution) phase with the addition
- **gibbs_energy** – Addition to G per mole formula unit

**Returns** This *SingleEquilibriumCalculation* object

**set_phase_to_dormant** *(phase: str)*

Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

**Parameters**

- **phase** – The phase name or *ALL_PHASES* for all phases

**Returns** This *SingleEquilibriumCalculation* object

**set_phase_to_entered** *(phase: str, amount: float = 1.0)*

Sets the phase to the status ENTERED, that is the default state.

**Parameters**

- **phase** – The phase name or *ALL_PHASES* for all phases
- **amount** – The phase fraction (between 0.0 and 1.0)

**Returns** This *SingleEquilibriumCalculation* object

**set_phase_to_fixed** *(phase: str, amount: float)*

Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

**Parameters**

- **phase** – The phase name
- **amount** – The fixed phase fraction (between 0.0 and 1.0)

**Returns** This *SingleEquilibriumCalculation* object

**set_phase_to_suspended** *(phase: str)*

Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters**

- **phase** – The phase name or *ALL_PHASES* for all phases

**Returns** This *SingleEquilibriumCalculation* object

**set_state_to_bookmark** *(bookmark_id: str)* → *tc_python.single_equilibrium.SingleEquilibriumTempResult*

Resets the calculation state to a previously bookmarked state.

After calling this method, the calculation behaves exactly as it would after the bookmarked calculation ran.

This method is used in combination with the method *bookmark_state()*.

**Parameters**

- **bookmark_id** – The bookmark id of the state to return to.

**Returns** A new *SingleEquilibriumTempResult* object which can be used to get specific values from the calculated result. It is undefined behavior to use that object after the state of the calculation has been changed.
with_options (options: tc_python.single_equilibrium.SingleEquilibriumOptions)
Sets the simulation options.

Parameters  options – The simulation options

Returns  This SingleEquilibriumCalculation object

with_reference_state (component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)
The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

Parameters

• component – The name of the element must be given.
• phase – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
• temperature – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
• pressure – The Pressure (in Pa) for the reference state.

Returns  This SingleEquilibriumCalculation object

with_system_modifications (system_modifications: tc_python.abstract_base.SystemModifications)
Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Parameters  system_modifications – The system modification to be performed

Returns  This SingleEquilibriumCalculation object

Note:  This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb-file.

class tc_python.single_equilibrium.SingleEquilibriumOptions
Bases: object

General simulation conditions for the thermodynamic calculations.
disable_approximate_driving_force_for_metastable_phases()
Disables the approximation of the driving force for metastable phases.

Default: Enabled

**Note:** When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, use disable_approximate_driving_force_for_metastable_phases() to force the calculation to converge for the metastable phases.

Returns This SingleEquilibriumOptions object

disable_control_step_size_during_minimization()
Disables stepsize control during minimization (non-global).

Default: Enabled

Returns This SingleEquilibriumOptions object

disable_force_positive_definite_phase_hessian()
Disables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

Default: Enabled

Returns This SingleEquilibriumOptions object

enable_approximate_driving_force_for_metastable_phases()
Enables the approximation of the driving force for metastable phases.

Default: Enabled

**Note:** When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, use disable_approximate_driving_force_for_metastable_phases() to force the calculation to converge for the metastable phases.

Returns This SingleEquilibriumOptions object

enable_control_step_size_during_minimization()
Enables stepsize control during normal minimization (non-global).

Default: Enabled

Returns This SingleEquilibriumOptions object

enable_force_positive_definite_phase_hessian()
Enables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

Default: Enabled

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Returns This `SingleEquilibriumOptions` object

`set_global_minimization_max_grid_points` *(max_grid_points: int = 2000)*
Sets the maximum number of grid points in global minimization. **Only applicable if global minimization is actually used.**

**Default:** 2000 points

**Parameters** `max_grid_points` – The maximum number of grid points

**Returns** This `SingleEquilibriumOptions` object

`set_max_no_of_iterations` *(max_no_of_iterations: int = 500)*
Sets the maximum number of iterations.

**Default:** max. 500 iterations

**Note:** As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

**Parameters** `max_no_of_iterations` – The max. number of iterations

**Returns** This `SingleEquilibriumOptions` object

`set_required_accuracy` *(accuracy: float = 1e-06)*
Sets the required relative accuracy.

**Default:** 1.0E-6

**Note:** This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

**Parameters** `accuracy` – The required relative accuracy

**Returns** This `SingleEquilibriumOptions` object

`set_smallest_fraction` *(smallest_fraction: float = 1e-12)*
Sets the smallest fraction for constituents that are unstable.

It is normally only in the gas phase that you can find such low fractions.

The **default value** for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.

**Parameters** `smallest_fraction` – The smallest fraction for constituents that are unstable

**Returns** This `SingleEquilibriumOptions` object

---

**class** `tc_python.single_equilibrium.SingleEquilibriumResult` *(result)*

**Bases:** `tc_python.abstract_base.AbstractResult`

Result of a single equilibrium calculation, it can be evaluated using a Quantity or Console Mode syntax.

`change_pressure` *(pressure: float)*
Change the pressure and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with higher performance. The properties are calculated at the new pressure using the phase amount,
temperature and composition of phases from the initial equilibrium. Use \texttt{get\_value\_of()}
to obtain them.

**Parameters** **\texttt{pressure}** – The pressure [Pa]

**Returns** This \texttt{SingleEquilibriumCalculation} object

**\texttt{change\_temperature(temperature: float)}**
Change the temperature and re-evaluate the results from the equilibrium without minimizing Gibbs energy,
i.e. with high performance. The properties are calculated at the new temperature using the phase amount,
pressure and composition of phases from the initial equilibrium. Use \texttt{get\_value\_of()}
to obtain them.

**Note:** This is typically used when calculating room temperature properties (e.g. density) for a material
when it is assumed that the equilibrium phase amount and composition freeze-in at a higher temperature
during cooling.

**Parameters** **\texttt{temperature}** – The temperature [K]

**Returns** This \texttt{SingleEquilibriumCalculation} object

**\texttt{get\_components()}** → List[str]
Returns the names of the components selected in the system (including any components auto-selected by
the database(s)).

**Returns** The names of the selected components

**\texttt{get\_conditions()}** → List[str]
Returns the conditions.

**Returns** The selected conditions

**\texttt{get\_phases()}** → List[str]
Returns the phases present in the system due to its configuration. It also contains all phases that
have been automatically added during the calculation, this is the difference to the method \texttt{System.}
\texttt{get\_phases\_in\_system()}.

**Returns** The names of the phases in the system including automatically added phases

**\texttt{get\_stable\_phases()}** → List[str]
Returns the stable phases (i.e. the phases present in the current equilibrium).

**Returns** The names of the stable phases

**\texttt{get\_value\_of(quantity: Union[tc\_python.quantity\_factory.ThermodynamicQuantity, str])}** → float
Returns a value from a single equilibrium calculation.

**Parameters** **\texttt{quantity}** – The thermodynamic quantity to get the value of; a Console Mode
syntax strings can be used as an alternative (for example “NPM(FCC\_A1)”)

**Returns** The requested value

**\texttt{run\_poly\_command(command: str)}**
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine. This
affects only the state of the result object.

**Parameters** **\texttt{command}** – The Thermo-Calc Console Mode command

**Returns** This \texttt{SingleEquilibriumCalculation} object
**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

```python
def save_to_disk(path: str) -> str:
    """Saves the result to disk. Note that the result is a folder, containing potentially many files. The result can later be loaded with load_result_from_disk()."
    Parameters:
    path -- the path to the folder you want the result to be saved in. It can be relative or absolute.
    Returns:
    This SingleEquilibriumResult object
```

```python
class SingleEquilibriumTempResult:
    """Result of a single equilibrium calculation that is only valid until something gets changed in the calculation state. It can be evaluated using a Quantity or Console Mode syntax."
    Warning:
    Note that it is undefined behavior to use that object after something has been changed in the state of the calculation, this will result in an InvalidResultStateException exception being raised.
    change_pressure(pressure: float)
    Change the pressure and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with higher performance. The properties are calculated at the new pressure using the phase amount, temperature and composition of phases from the initial equilibrium. Use get_value_of() to obtain them.
    Parameters:
    pressure -- The pressure [Pa]
    Returns:
    This SingleEquilibriumCalculation object
    change_temperature(temperature: float)
    Change the temperature and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with high performance. The properties are calculated at the new temperature using the phase amount, pressure and composition of phases from the initial equilibrium. Use get_value_of() to obtain them.
    Note:
    This is typically used when calculating room temperature properties (e.g. density) for a material when it is assumed that the equilibrium phase amount and composition freeze-in at a higher temperature during cooling.
    Parameters:
    temperature -- The temperature [K]
    Returns:
    This SingleEquilibriumCalculation object
```

```python
def get_components() -> List[str]:
    """Returns the names of the components selected in the system (including any components auto-selected by the database(s))."
    Returns:
    The names of the selected components
```
Raises `InvalidResultStateException` – If something has been changed in the state of
the calculation since that result object has been created

`get_conditions()` → `List[str]`

Returns the conditions.

Returns List containing the selected conditions

Raises `InvalidResultStateException` – If something has been changed in the state of
the calculation since that result object has been created

`get_phases()` → `List[str]`

Returns the phases present in the system due to its configuration. It also contains all phases that
have been automatically added during the calculation, this is the difference to the method `System.get_phases_in_system()`.

Returns The names of the phases in the system including automatically added phases

Raises `InvalidResultStateException` – If something has been changed in the state of
the calculation since that result object has been created

`get_stable_phases()` → `List[str]`

Returns the stable phases (i.e. the phases present in the current equilibrium).

Returns The names of the stable phases

Raises `InvalidResultStateException` – If something has been changed in the state of
the calculation since that result object has been created

`get_value_of(quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) → float`

Returns a value from a single equilibrium calculation.

Parameters `quantity` – The thermodynamic quantity to get the value of; a Console Mode
syntax strings can be used as an alternative (for example “NPM(FCC_A1)"

Returns The requested value

Raises `InvalidResultStateException` – If something has been changed in the state of
the calculation since that result object has been created

`run_poly_command(command: str)`

Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

Parameters `command` – The Thermo-Calc Console Mode command

Returns This `SingleEquilibriumCalculation` object

---

**Note:** It should not be necessary for most users to use this method, try to use the corresponding method
implemented in the API instead.

---

**Warning:** As this method runs raw Thermo-Calc commands directly in the engine, it may hang the
program in case of spelling mistakes (e.g. forgotten equals sign).
5.1.2 Module “batch_equilibrium”

```python
class tc_python.batch_equilibrium.BatchEquilibriumCalculation(calculator):
    Bases: tc_python.abstract_base.AbstractCalculation

    Configuration for a series of single equilibrium calculations performed in a vectorized fashion.

    Note: Specify the conditions and call `calculate()`.
```

**Tip:** The performance of batch equilibrium calculations can be significantly better than looping and using `SingleEquilibriumCalculation` if the actual Thermo-Calc calculation is fast. There is little advantage if the Thermo-Calc equilibrium calculations take a long time (typically for large systems and databases).

```python
calculate(quantities: List[Union[tc_python.quantity_factory.ThermodynamicQuantity, str]],
          logging_frequency: int = 10) -> tc_python.batch_equilibrium.BatchEquilibriumResult
```

Runs the batch equilibrium calculation. The calculated `BatchEquilibriumResult` can then be queried for the values of the quantities specified.

**Example:**

```python
>>> quantities = ['G', 'X(BCC)']
```

**Parameters**

- **logging_frequency** – Determines how often logging should be done.

**Returns**

A `BatchEquilibriumResult` which later can be used to get specific values from the calculated result.

```python
disable_global_minimization()
```

Turns the global minimization completely off.

**Returns**

This `BatchEquilibriumCalculation` object

```python
enable_global_minimization()
```

Turns the global minimization on (using the default settings).

**Returns**

This `BatchEquilibriumCalculation` object

```python
get_components() -> List[str]
```

Returns a list of components in the system (including all components auto-selected by the database(s)).

**Returns**

The components

```python
get_gibbs_energy_addition_for(phase: str) -> float
```

Used to get the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

**Parameters**

- **phase** – Specify the name of the (stoichiometric or solution) phase with the addition

**Returns**

Gibbs energy addition to G per mole formula unit.

```python
get_system_data() -> tc_python.abstract_base.SystemData
```

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.
**Note:** Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb*-file.

**Returns** The system data

```python
remove_all_conditions()
```
Removes all set conditions.

**Returns** This `BatchEquilibriumCalculation` object

```python
remove_condition(quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str])
```
Removes the specified condition.

**Parameters**
- `quantity` – the thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example “X(Cr)”)

**Returns** This `BatchEquilibriumCalculation` object

```python
run_poly_command(command: str)
```
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

**Parameters**
- `command` – The Thermo-Calc Console Mode command

**Returns** This `BatchEquilibriumCalculation` object

**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

```python
set_component_to_entered(component: str)
```
Sets the specified component to the status ENTERED, that is the default state.

**Parameters**
- `component` – The component name or `ALL_COMPONENTS`

**Returns** This `BatchEquilibriumCalculation` object

```python
set_component_to_suspended(component: str, reset_conditions: bool = False)
```
Sets the specified component to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters**
- `reset_conditions` – if ‘True’ also remove composition conditions for the component if they are defined
- `component` – The component name or `ALL_COMPONENTS`

**Returns** This `BatchEquilibriumCalculation` object

```python
set_condition(quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], value: float)
```
Sets the specified condition.

**Parameters**
- `quantity` – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example “X(Cr)”)

5.1. Calculations
• value – The value of the condition

Returns This BatchEquilibriumCalculation object

set_conditions_for_equilibria(equilibria: List[List[Tuple[Union[tc_python.quantity_factory.ThermodynamicQuantity, str], float]]])
Set the conditions of the equilibria to be calculated.
This is done by sending a list of equilibria at once.
Each equilibrium itself is a list of conditions that will be changed for that equilibrium.
A condition is described by a tuple containing:
1. A Console Mode syntax string or a ThermodynamicQuantity instance,
2. A float value specifying the value of the condition.
Example:

```python
>>> [[('T', 800), ('X(Cr)', 0.1)], [('T', 850), ('X(Cr)', 0.11)]
```

You can use ThermodynamicQuantity instead of a Console Mode syntax string when specifying type of condition.
Example:

```python
>>> [[(ThermodynamicQuantity.temperature(), 800), (ThermodynamicQuantity.mole_fraction_of_a_component('Cr'), 0.1)], [(ThermodynamicQuantity.temperature(), 850), (ThermodynamicQuantity.mole_fraction_of_a_component('Cr'), 0.15)]
```

Parameters equilibria – The list of equilibria

Returns This BatchEquilibriumCalculation object

set_gibbs_energy_addition_for(phase: str, gibbs_energy: float)
Used to specify the additional energy term (always being a constant) of a given phase. The value (gibbs_energy) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

Parameters

• phase – Specify the name of the (stoichiometric or solution) phase with the addition

• gibbs_energy – Addition to G per mole formula unit

Returns This BatchEquilibriumCalculation object

set_phase_to_dormant(phase: str)
Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

Parameters phase – The phase name or ALL_PHASES for all phases

Returns This BatchEquilibriumCalculation object

set_phase_to_entered(phase: str, amount: float = 1.0)
Sets the phase to the status ENTERED, that is the default state.

Parameters

• phase – The phase name or ALL_PHASES for all phases
• **amount** – The phase fraction (between 0.0 and 1.0)

**Returns** This `BatchEquilibriumCalculation` object

**set_phase_to_fixed**(phase: str, amount: float)

Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

**Parameters**

• **phase** – The phase name

• **amount** – The fixed phase fraction (between 0.0 and 1.0)

**Returns** This `BatchEquilibriumCalculation` object

**set_phase_to_suspended**(phase: str)

Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters**

• **phase** – The phase name or ALL_PHASES for all phases

**Returns** This `BatchEquilibriumCalculation` object

**with_options**(options: tc_python.single_equilibrium.SingleEquilibriumOptions)

Sets the simulation options.

**Parameters**

• **options** – The simulation options

**Returns** This `BatchEquilibriumCalculation` object

**with_reference_state**(component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

**Parameters**

• **component** – The name of the element must be given.

• **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.

• **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.

• **pressure** – The Pressure (in Pa) for the reference state.
**Returns**

This *BatchEquilibriumCalculation* object

**with_system_modifications** *(system_modifications: tc_python.abstract_base.SystemModifications)*

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

**Note:** This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb*-file.

**Parameters**

- **system_modifications** – The system modification to be performed

**Returns**

This *BatchEquilibriumCalculation* object

**class** *tc_python.batch_equilibrium.BatchEquilibriumResult*(result)*

Bases: object

Result of a batch equilibrium calculation. This can be used to query for specific values.

**get_values_of** *(quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) → List[float]*

Returns values from a batch equilibrium calculation.

**Warning:** The quantity must be one of the quantities specified for the *BatchEquilibriumCalculation* object that created the result object.

**Example:**

```python
>>> batch_result = batch_calculation.calculate(quantities = ['G', 'X(BCC)'])
>>> batch_result.get_values_of('G')
```

**Parameters**

- **quantity** – the thermodynamic quantity to get the value of; a Console Mode syntax strings can be used as an alternative (for example “NPM(FCC_A1)”)

**invalidate()**

Invalidates the object and frees the disk space used by it.

**Note:** This is only required if the disk space occupied by the object needs to be released during the calculation. No data can be retrieved from the object afterwards.

### 5.1.3 Module “precipitation”

**class** *tc_python.precipitation.FixedGrainSize*(grain_radius: float = 0.0001)*

Bases: tc_python.precipitation.GrainGrowthModel

**set_grain_aspect_ratio** *(grain_aspect_ratio: float = 1.0)*

Enter a numerical value. **Default:** 1.0.

**Parameters**

- **grain_aspect_ratio** – The grain aspect ratio [-]

**class** *tc_python.precipitation.GrainGrowth*(grain_size_distribution: tc_python.precipitation.GrainSizeDistribution)*

Bases: tc_python.precipitation.GrainGrowthModel
disable_zener_pinning()
Disables Zener pinning to ignore the particle pinning effect on the grain growth. Zener pinning is by default disabled when no grain size distribution is defined, i.e. a single constant grain size is used. The setting is by default enabled when a grain size distribution is defined.

Returns This GrainSizeDistribution object

enable_zener_pinning()
Enables Zener pinning to simulate the particle pinning effect on the grain growth. The setting is by default enabled when a grain size distribution is defined.

Returns This GrainSizeDistribution object

set_grain_boundary_energy(energy: float = 0.5)
Sets the energy of the grain boundary.

Parameters energy – The grain boundary energy [J/m2]

Returns This GrainSizeDistribution object

set_grain_boundary_mobility_activation_energy(activation_energy: float = 242000.0)
Sets the grain boundary mobility activation energy where the mobility is defined by an Arrhenius type of equation.

Parameters activation_energy – The mobility activation energy [J/mol]

Returns This GrainSizeDistribution object

set_grain_boundary_mobility_pre_factor(pre_factor: float = 0.004)
Sets the grain boundary mobility prefactor where the mobility is defined by an Arrhenius type of equation.

Parameters pre_factor – The grain boundary mobility prefactor [m^4/(J s)]

Returns This GrainSizeDistribution object

class tc_python.precipitation.GrainGrowthModel
Bases: object

Factory class providing objects representing a grain growth model.

classmethod fixed_grain_size(grain_radius: float = 0.0001)
Fixed grain radius size. Default: 1.0E-4 m

Parameters grain_radius – The grain radius / size [m]

classmethod grain_growth(grain_size_distribution: tc_python.precipitation.GrainSizeDistribution)
Sets the initial grain size distribution for the matrix. Default: If the initial grain size distribution is not explicitly provided, a constant average grains size will be used and no grain growth evaluated during the simulation.

Tip: Use this option if you want to study the further evolution of an existing microstructure.

Parameters grain_size_distribution – grain size distribution

class tc_python.precipitation.GrainSizeDistribution
Bases: object

Represents the grain size distribution at a certain time.

add_radius_and_number_density(radius: float, number_density: float)
Adds a radius and number density pair to the grain size distribution.
Parameters

- `radius` – The radius [m]
- `number_density` – The number of grains per unit volume per unit length [m^-4]

**Returns**

This `GrainSizeDistribution` object

class tc_python.precipitation.GrowthRateModel(value)
Bases: enum.Enum

Choice of the used growth rate model for a precipitate.

The most efficient model is the *Simplified model*, which is the default and applicable to most alloy systems under the assumption that either the supersaturation is small, or the alloying elements have comparable diffusivity. If all alloying elements are substitutional but they have remarkable diffusivity difference, e.g. in Al-Zr system, or if the diffusivity is strongly composition-dependent, the *General model* is preferred. If the supersaturation is high, and meanwhile there are fast-diffusing interstitial elements such as C, the *Advanced model* is more appropriate to capture the NPLE mechanism.

**ADVANCED = 3**

The advanced model has been proposed by *Chen, Jeppsson, and Ågren (CJA) (2008)* and calculates the velocity of a moving phase interface in multicomponent systems by identifying the operating tie-line from the solution of the flux-balance equations. This model can treat both high supersaturation and cross-diffusion rigorously. Spontaneous transitions between different modes (LE and NPLE) of phase transformation can be captured without any ad-hoc treatment.

**Note:** Since it is not always possible to solve the flux-balance equations and it takes time, usage of a less rigorous but simple and efficient model is preferred if possible.

**GENERAL = 5**

The general model is based on the *Morral-Purdy* model, which follows the same quasi-steady state approximation as the *Simplified model*, but improves it by taking the cross-diffusion into account.

**NPLE = 11**

The Non-Partitioning Local Equilibrium (NPLE) growth rate model is only available for alloy systems where Fe is the major element and at least one interstitial element partitions into the precipitate phase. *This model is specifically designed to deal with the fast diffusion of interstitial elements (C, N, etc.) in Fe alloys.* Based on the *Simplified growth model*, it still holds a local equilibrium condition at the migrating interface. It chooses a tie-line under NPLE condition so that the u-fractions of all substitutional elements and minor interstitial elements in the precipitate phase are the same as those in the far-field matrix phase (i.e. the overall instantaneous matrix composition).

**PARA_EQ = 10**

The para-equilibrium model is only available for alloy systems where Fe is the major element and C is the only interstitial element, which also partitions into the precipitate phase. The interstitial elements, e.g. C, N, etc., usually have remarkably faster diffusion rate than the substitutional elements. Meanwhile, they are assumed to have negligible volume contribution, and as a result the composition variables are replaced by u-fractions when interstitial elements are included in the system. *This model is specifically designed to address the fast diffusion of C in Fe alloys.* Based on the *Simplified growth rate model* it holds a para-equilibrium condition at the migrating interface. Contrary to the regular ortho-equilibrium condition state that assumes that all alloying elements are in equilibrium at the interface, the para-equilibrium assumes only equilibrium for C. The substitutional elements are immobile and thus have the same compositions (u-fractions) across the interface.

**SIMPLIFIED = 2**

The simplified model is based on the advanced model but avoids the difficulty of finding the operating tie-line and uses instead the tie-line across the bulk composition. *This is the default growth rate model.*
class tc_python.precipitation.MatrixPhase(matrix_phase_name: str)
    Bases: object

    The matrix phase in a precipitation calculation

    add_precipitate_phase (precipitate_phase: tc_python.precipitation.PrecipitatePhase)
        Adds a precipitate phase.

            Parameters precipitate_phase – The precipitate phase

    set_dislocation_density (dislocation_density: float = 5000000000000.0)
        Enter a numerical value. Default: 5.0E12 m^-2.

            Parameters dislocation_density – The dislocation density [m^-2]

    set_grain_aspect_ratio (grain_aspect_ratio: float = 1.0)
        Enter a numerical value. Default: 1.0.

Note: Deprecated in version 2022a: Use with_grain_growth_model() instead. This method will be removed in release 2023a.

    Parameters grain_aspect_ratio – The grain aspect ratio [-]

    set_grain_radius (grain_radius: float = 0.0001)
        Sets grain radius / size. Default: 1.0E-4 m

Note: Deprecated in version 2022a: Use with_grain_growth_model() instead. This method will be removed in release 2023a.

    Parameters grain_radius – The grain radius / size [m]

    set_mobility_enhancement_activation_energy (mobility_enhancement_activation_energy: float = 0.0)
        A value that adds to the activation energy of mobility data from the database. Default: 0.0 J/mol

            Parameters mobility_enhancement_activation_energy – The value that adds to the activation energy of mobility data from the database [J/mol].

    set_mobility_enhancement_prefactor (mobility_enhancement_prefactor: float = 1.0)
        A parameter that multiplies to the mobility data from database. Default: 1.0

            Parameters mobility_enhancement_prefactor – The mobility enhancement factor [-]

    set_molar_volume (volume: float)
        Sets the molar volume of the phase.

            Default: If not set, the molar volume is taken from the thermodynamic database (or set to 7.0e-6 m^3/mol if the database contains no molar volume information).

            Parameters volume – The molar volume [m^3/mol]

    with_elastic_properties_cubic (c11: float, c12: float, c44: float)
        Sets the elastic properties to “cubic” and specifies the elastic stiffness tensor components. Default: if not chosen, the default is DISREGARD

            Parameters
                • c11 – The stiffness tensor component c11 [GPa]
• **c12** – The stiffness tensor component c12 [GPa]
• **c44** – The stiffness tensor component c44 [GPa]

**with_elastic_properties_disregard()**
Set to disregard to ignore the elastic properties. **Default:** This is the default option

**with_elastic_properties_isotropic**(shear_modulus: float, poisson_ratio: float)
Sets elastic properties to isotropic. **Default:** if not chosen, the default is DISREGARD

**Parameters**

- **shear_modulus** – The shear modulus [GPa]
- **poisson_ratio** – The Poisson’s ratio [-]

**with_grain_growth_model**(grain_growth_model: tc_python.precipitation.GrainGrowthModel)
Sets the model for grain growth. Either fixed size or with a starting distribution

**Default:** Fixed grain radius size 1.0E-4 m

**Parameters**

**grain_growth_model** – the grain growth model

**class tc_python.precipitation.NumericalParameters**
**Bases:** object

Numerical parameters

**set_max_overall_volume_change**(max_overall_volume_change: float = 0.001)
This defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step.

**Default:** 0.001

**Parameters**

**max_overall_volume_change** – The maximum absolute (not ratio) change of the volume fraction allowed during one time step [-]

**set_max_radius_points_per_magnitude**(max_radius_points_per_magnitude: float = 200.0)
Sets the maximum number of grid points over one order of magnitude in radius.

**Default:** 200.0

**Parameters**

**max_radius_points_per_magnitude** – The maximum number of grid points over one order of magnitude in radius [-]

**set_max_rel_change_critical_radius**(max_rel_change_critical_radius: float = 0.1)
Used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step.

**Default:** 0.1

**Parameters**

**max_rel_change_critical_radius** – The maximum relative change of the critical radius [-]

**set_max_rel_change_nucleation_rate_log**(max_rel_change_nucleation_rate_log: float = 0.5)
This parameter ensures accuracy for the evolution of effective nucleation rate.

**Default:** 0.5

**Parameters**

**max_rel_change_nucleation_rate_log** – The maximum logarithmic relative change of the nucleation rate [-]

**set_max_rel_radius_change**(max_rel_radius_change: float = 0.01)
The maximum value allowed for relative radius change in one time step.

**Default:** 0.01

**Parameters**

**max_rel_radius_change** – The maximum relative radius change in one time step [-]

**set_max_rel_solute_composition_change**(max_rel_solute_composition_change: float = 0.01)
Set a limit on the time step by controlling solute depletion or saturation, especially at isothermal stage.

**Default:** 0.01
Parameters `max_rel_solute_composition_change` – The limit for the relative solute composition change [\text{-}]

`set_max_time_step`( `max_time_step`: `float = 0.1`)  
The maximum time step allowed for time integration as fraction of the simulation time. **Default:** 0.1

Parameters `max_time_step` – The maximum time step as fraction of the simulation time [\text{-}]

`set_max_time_step_during_heating`( `max_time_step_during_heating`: `float = 1.0`)  
The upper limit of the time step that has been enforced in the heating stages. **Default:** 1.0 s

Parameters `max_time_step_during_heating` – The maximum time step during heating [s]

`set_max_volume_fraction_dissolve_time_step`( `max_volume_fraction_dissolve_time_step`: `float = 0.01`)  
Sets the maximum volume fraction of subcritical particles allowed to dissolve in one time step. **Default:** 0.01

Parameters `max_volume_fraction_dissolve_time_step` – The maximum volume fraction of subcritical particles allowed to dissolve in one time step [\text{-}]

`set_min_radius_nucleus_as_particle`( `min_radius_nucleus_as_particle`: `float = 5e-10`)  
The cut-off lower limit of precipitate radius. **Default:** 5.0E-10 m

Parameters `min_radius_nucleus_as_particle` – The minimum radius of a nucleus to be considered as a particle [m]

`set_min_radius_points_per_magnitude`( `min_radius_points_per_magnitude`: `float = 100.0`)  
Sets the minimum number of grid points over one order of magnitude in radius. **Default:** 100.0

Parameters `min_radius_points_per_magnitude` – The minimum number of grid points over one order of magnitude in radius [\text{-}]

`set_radius_points_per_magnitude`( `radius_points_per_magnitude`: `float = 150.0`)  
Sets the number of grid points over one order of magnitude in radius. **Default:** 150.0

Parameters `radius_points_per_magnitude` – The number of grid points over one order of magnitude in radius [\text{-}]

`set_rel_radius_change_class_collision`( `rel_radius_change_class_collision`: `float = 0.5`)  
Sets the relative radius change for avoiding class collision. **Default:** 0.5

Parameters `rel_radius_change_class_collision` – The relative radius change for avoiding class collision [\text{-}]

class `tc_python.precipitation.ParticleSizeDistribution`  
Bases: `object`

Represents the state of a microstructure evolution at a certain time including its particle size distribution, composition and overall phase fraction.

`add_radius_and_number_density`( `radius`: `float`, `number_density`: `float`)  
Adds a radius and number density pair to the particle size distribution.

Parameters

- `radius` – The radius [m]
- `number_density` – The number of particles per unit volume per unit length [m^\text{-}4]

Returns This `ParticleSizeDistribution` object

`set_initial_composition`( `element_name`: `str`, `composition_value`: `float`)  
Sets the initial precipitate composition.

5.1. Calculations
Parameters

- **element_name** – The name of the element
- **composition_value** – The composition value [composition unit defined for the calculation]

**Returns** This `ParticleSystemDistribution` object


Sets the type of the phase fraction or percentage. **Default**: By default volume fraction is used.

**Parameters**

- **volume_fraction_of_phase_type_enum** – Specifies if volume percent or fraction is used

**Returns** This `ParticleSystemDistribution` object

`set_volume_fraction_of_phase_value(value: float)`

Sets the overall volume fraction of the phase (unit based on the setting of `set_volume_fraction_of_phase_type()`).

**Parameters**

- **value** – The volume fraction 0.0 - 1.0 or percent value 0 - 100

**Returns** This `ParticleSystemDistribution` object

```python
class tc_python.precipitation.PrecipitateElasticProperties
Bases: object
```

Represents the elastic transformation strain of a certain precipitate class.

---

**Note:** This class is only relevant if the option `TransformationStrainCalculationOption.USER_DEFINED` has been chosen using `PrecipitatePhase.set_transformation_strain_calculation_option()`.

The elastic strain can only be considered for non-spherical precipitates.

```python
set_e11(e11: float)
```

Sets the elastic strain tensor component e11. **Default**: 0.0

**Parameters**

- **e11** – The elastic strain tensor component e11

**Returns** This `PrecipitateElasticProperties` object

```python
set_e12(e12: float)
```

Sets the strain tensor component e12. **Default**: 0.0

**Parameters**

- **e12** – The elastic strain tensor component e12

**Returns** This `PrecipitateElasticProperties` object

```python
set_e13(e13: float)
```

Sets the elastic strain tensor component e13. **Default**: 0.0

**Parameters**

- **e13** – The elastic strain tensor component e13

**Returns** This `PrecipitateElasticProperties` object

```python
set_e22(e22: float)
```

Sets the elastic strain tensor component e22. **Default**: 0.0

**Parameters**

- **e22** – The elastic strain tensor component e22

**Returns** This `PrecipitateElasticProperties` object

```python
set_e23(e23: float)
```

Sets the elastic strain tensor component e23. **Default**: 0.0
Parameters e23 – The elastic strain tensor component e23

Returns This PrecipitateElasticProperties object

def set_e33(e33: float)
Sets the elastic strain tensor component e33. Default: 0.0

Parameters e33 – The elastic strain tensor component e33

Returns This PrecipitateElasticProperties object

class tc_python.precipitation.PrecipitateMorphology(value)
Bases: enum.Enum

Available precipitate morphologies.

CUBOID = 3
Cuboidal precipitates, only available for bulk nucleation.

NEEDLE = 1
Needle-like precipitates, only available for bulk nucleation.

PLATE = 2
Plate-like precipitates, only available for bulk nucleation.

SPHERE = 0
Spherical precipitates, this is the default morphology.

class tc_python.precipitation.PrecipitatePhase(precipitate_phase_name: str)
Bases: object

Represents a certain precipitate class (i.e. a group of precipitates with the same phase and settings).

def disable_calculate_aspect_ratio_from_elastic_energy()
Disables the automatic calculation of the aspect ratio from the elastic energy of the phase.

Returns This PrecipitatePhase object

Note: If you use this method, you are required to set the aspect ratio explicitly using the method
set_aspect_ratio_value().

Default: This is the default setting (with an aspect ratio of 1.0).

def disable_driving_force_approximation()
Disables driving force approximation for this precipitate class. Default: Driving force approximation is
disabled.

Returns This PrecipitatePhase object

def enable_calculate_aspect_ratio_from_elastic_energy()
Enable the automatic calculation of the aspect ratio from the elastic energy of the phase. Default: The
aspect ratio is set to a value of 1.0.

Returns This PrecipitatePhase object

def enable_driving_force_approximation()
Enables driving force approximation for this precipitate class. This approximation is often required when
simulating precipitation of multiple particles that use the same phase description. E.g. simultaneous
precipitation of a Metal-Carbide(MC) and Metal-Nitride(MN) if configured as different composition sets
of the same phase FCC_A1. Default: Driving force approximation is disabled.

Returns This PrecipitatePhase object

5.1. Calculations
Tip: Use this if simulations with several compositions sets of the same phase cause problems.

set_alias (alias: str)
Sets an alias string that can later be used to get values from a calculated result. Typically used when having the same phase for several precipitates, but with different nucleation sites. For example two precipitates of the phase M7C3 with nucleation sites in ‘Bulk’ and at ‘Dislocations’. The alias can be used instead of the phase name when retrieving simulated results.

Parameters alias – The alias string for this class of precipitates

Returns This PrecipitatePhase object

Note: Typically used when having the same precipitate phase, but with different settings in the same calculation.

set_aspect_ratio_value (aspect_ratio_value: float)
Sets the aspect ratio of the phase. Default: An aspect ratio of 1.0.

Parameters aspect_ratio_value – The aspect ratio value

Returns This PrecipitatePhase object

Note: Only relevant if disable_calculate_aspect_ratio_from_elastic_energy() is used (which is the default).

set_gibbs_energy_addition (gibbs_energy_addition: float)
Sets a Gibbs energy addition to the Gibbs energy of the phase. Default: 0.0 J/mol

Parameters gibbs_energy_addition – The Gibbs energy addition [J/mol]

Returns This PrecipitatePhase object

set_interfacial_energy (interfacial_energy: float)
Sets the interfacial energy. Default: If the interfacial energy is not set, it is automatically calculated using a broken-bond model.

Parameters interfacial_energy – The interfacial energy [J/m^2]

Returns This PrecipitatePhase object

Note: The calculation of the interfacial energy using a broken-bond model is based on the assumption of an interface between a bcc- and a fcc-crystal structure with (110) and (111) lattice planes regardless of the actual phases.

set_interfacial_energy_estimation_prefactor (interfacial_energy_estimation_prefactor: float)
Sets the interfacial energy prefactor. Default: Prefactor of 1.0 (only relevant if the interfacial energy is automatically calculated).

Parameters interfacial_energy_estimation_prefactor – The prefactor for the calculated interfacial energy

Returns This PrecipitatePhase object
Note: The interfacial energy prefactor is an amplification factor for the automatically calculated interfacial energy. Example: \( \text{interfacial}_\text{energy}_\text{estimation}_\text{prefactor} = 2.5 \Rightarrow 2.5 \times \text{calculated interfacial energy} \)

**set_molar_volume** *(volume: float)*  
Sets the molar volume of the precipitate phase. **Default**: The molar volume obtained from the database. If no molar volume information is present in the database, a value of 7.0e-6 m\(^3\)/mol is used.  

**Parameters**  
- **volume** – The molar volume [m\(^3\)/mol]  

**Returns** This *PrecipitatePhase* object

**set_nucleation_at_dislocations** *(number_density=- 1)*  
Activates nucleation at dislocations for this class of precipitates. Calling the method overrides any other nucleation setting for this class of precipitates. **Default**: If not set, by default bulk nucleation is chosen.  

**Parameters**  
- **number_density** – Number density of nucleation sites. If not set, the value is calculated based on the matrix settings (grain size, dislocation density) [m\(^-3\)].  

**Returns** This *PrecipitatePhase* object

**set_nucleation_at_grain_boundaries** *(wetting_angle: float = 90.0, number_density: float = - 1)*  
Activates nucleation at grain boundaries for this class of precipitates. Calling the method overrides any other nucleation setting for this class of precipitates. **Default**: If not set, by default bulk nucleation is chosen.  

**Parameters**  
- **wetting_angle** – If not set, a default value of 90 degrees is used  
- **number_density** – Number density of nucleation sites. If not set, the value is calculated based on the matrix settings (grain size) [m\(^-3\)].  

**Returns** This *PrecipitatePhase* object

**set_nucleation_at_grain_corners** *(wetting_angle: float = 90, number_density: float = - 1)*  
Activates nucleation at grain corners for this class of precipitates. Calling the method overrides any other nucleation setting for this class of precipitates. **Default**: If not set, by default bulk nucleation is chosen.  

**Parameters**  
- **wetting_angle** – If not set, a default value of 90 degrees is used  
- **number_density** – Number density of nucleation sites. If not set, the value is calculated based on the matrix settings (grain size) [m\(^-3\)].  

**Returns** This *PrecipitatePhase* object

**set_nucleation_at_grain_edges** *(wetting_angle=90, number_density=- 1)*  
Activates nucleation at the grain edges for this class of precipitates. Calling the method overrides any other nucleation setting for this class of precipitates. **Default**: If not set, by default bulk nucleation is chosen.  

**Parameters**  
- **wetting_angle** – If not set, a default value of 90 degrees is used  
- **number_density** – Number density of nucleation sites. If not set, the value is calculated based on the matrix settings (grain size) [m\(^-3\)].  

**Returns** This *PrecipitatePhase* object

**set_nucleation_in_bulk** *(number_density: float = - 1.0)*  
Activates nucleation in the bulk for this class of precipitates. Calling the method overrides any other
nucleation setting for this class of precipitates. **Default**: This is the default setting (with an automatically calculated number density).

**Parameters**

- `number_density` – Number density of nucleation sites. If not set, the value is calculated based on the matrix settings (molar volume) \([\text{m}^{-3}]\).

**Returns**

This `PrecipitatePhase` object

---

**set_phase_boundary_mobility** *(phase_boundary_mobility: float)*

Sets the phase boundary mobility. **Default**: 10.0 \([\text{m}^4/(\text{Js})]\).

**Parameters**

- `phase_boundary_mobility` – The phase boundary mobility \([\text{m}^4/(\text{Js})]\).

**Returns**

This `PrecipitatePhase` object

---

**set_precipitate_morphology** *(precipitate_morphology_enum: tc_python.precipitation.PrecipitateMorphology)*

Sets the precipitate morphology. **Default**: `PrecipitateMorphology.SPHERE`

**Parameters**

- `precipitate_morphology_enum` – The precipitate morphology

**Returns**

This `PrecipitatePhase` object

---

**set_transformation_strain_calculation_option** *(transformation_strain_calculation_option_enum: tc_python.precipitation.TransformationStrainCalculationOption)*

Sets the transformation strain calculation option. **Default**: `TransformationStrainCalculationOption.DISREGARD`.

**Parameters**

- `transformation_strain_calculation_option_enum` – The chosen option

**Returns**

This `PrecipitatePhase` object

---

**with_elastic_properties** *(elastic_properties: tc_python.precipitation.PrecipitateElasticProperties)*

Sets the elastic properties. **Default**: The elastic transformation strain is disregarded by default.

**Parameters**

- `elastic_properties` – The elastic properties object

**Returns**

This `PrecipitatePhase` object

---

**Note:** This method has only an effect if the option `TransformationStrainCalculationOption.USER_DEFINED` is chosen using the method `set_transformation_strain_calculation_option()`.

---

**with_growth_rate_model** *(growth_rate_model_enum: tc_python.precipitation.GrowthRateModel)*

Sets the growth rate model for the class of precipitates. **Default**: `GrowthRateModel.SIMPLIFIED`

**Parameters**

- `growth_rate_model_enum` – The growth rate model

**Returns**

This `PrecipitatePhase` object

---

**with_particle_size_distribution** *(particle_size_distribution: tc_python.precipitation.ParticleSizeDistribution)*

Sets the initial particle size distribution for this class of precipitates. **Default**: If the initial particle size distribution is not explicitly provided, the simulation will start from a supersaturated matrix.

**Parameters**

- `particle_size_distribution` – The initial particle size distribution object

**Returns**

This `PrecipitatePhase` object

---

**Tip:** Use this option if you want to study the further evolution of an existing microstructure.
class tc_python.precipitation.PrecipitationCCTCalculation(calculation)
    Bases: tc_python.abstract_base.AbstractCalculation

Configuration for a Continuous-Cooling-Time (CCT) precipitation calculation.

calculate() \rightarrow tc_python.precipitation.PrecipitationCalculationTTTorCCTResult
    Runs the CCT diagram calculation.

    Returns A PrecipitationCalculationTTTorCCTResult which later can be used to get specific values from the calculated result

get_system_data() \rightarrow tc_python.abstract_base.SystemData
    Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

    Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

    Returns The system data

set_composition(element_name: str, value: float)
    Sets the composition of the elements. The unit for the composition can be changed using set_composition_unit(). Default: Mole percent (CompositionUnit.MOLE_PERCENT)

    Parameters
        • element_name – The element
        • value – The composition (fraction or percent depending on the composition unit)

    Returns This PrecipitationCCTCalculation object

set_composition_unit(unit_enum: tc_python.utils.CompositionUnit)
    Sets the composition unit. Default: Mole percent (CompositionUnit.MOLE_PERCENT).

    Parameters unit_enum – The new composition unit

    Returns This PrecipitationCCTCalculation object

set_cooling_rates(cooling_rates: List[float])
    Sets all cooling rates for which the CCT diagram should be calculated.

    Parameters cooling_rates – A list of cooling rates [K/s]

    Returns This PrecipitationCCTCalculation object

set_max_temperature(max_temperature: float)
    Sets maximum temperature of the CCT diagram.

    Parameters max_temperature – the maximum temperature [K]

    Returns This PrecipitationCCTCalculation object

set_min_temperature(min_temperature: float)
    Sets the minimum temperature of the CCT diagram.

    Parameters min_temperature – the minimum temperature [K]

    Returns This PrecipitationCCTCalculation object

stop_at_volume_fraction_of_phase(stop_criterion_value: float)
    Sets the stop criterion as a volume fraction of the phase. This setting is applied to all phases.
Parameters **stop_criterion_value** – the volume fraction of the phase (a value between 0 and 1)

Returns This *PrecipitationCCTCalculation* object

**with_matrix_phase** *(matrix_phase: tc_python.precipitation.MatrixPhase)*

Sets the matrix phase.

Parameters **matrix_phase** – The matrix phase

Returns This *PrecipitationCCTCalculation* object

**with_numerical_parameters** *(numerical_parameters: tc_python.precipitation.NumericalParameters)*

Sets the numerical parameters. If not specified, reasonable defaults are be used.

Parameters **numerical_parameters** – The parameters

Returns This *PrecipitationCCTCalculation* object

**with_system_modifications** *(system_modifications: tc_python.abstract_base.SystemModifications)*

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Note: This is only possible if the system has been read from unencrypted (i.e. *user*) databases loaded as a *.tdb*-file.

Parameters **system_modifications** – The system modification to be performed

Returns This *PrecipitationCCTCalculation* object

---

**class tc_python.precipitation.PrecipitationCalculationResult**(result)

*Based: tc_python.abstract_base.AbstractResult*

Result of a precipitation calculation. This can be used to query for specific values.

**save_to_disk**(path: str)

Saves the result to disc. Note that a result is a folder, containing potentially many files. The result can later be loaded with *load_result_from_disk()*

Parameters **path** – the path to the folder you want the result to be saved in. It can be relative or absolute.

Returns this *PrecipitationCalculationResult* object

**class tc_python.precipitation.PrecipitationCalculationSingleResult**(result)

*Based: tc_python.precipitation.PrecipitationCalculationCalculationResult*

Result of a isothermal or non-isothermal precipitation calculation. This can be used to query for specific values.

Search the Thermo-Calc help for definitions of the axis variables, e.g. search *isothermal variables* or *non-isothermal variables*.

**get_aspect_ratio_distribution_for_particle_length_of**(precipitate_id: str, time: float) → [typing.List[float], typing.List[float]]

Returns the aspect ratio distribution of a precipitate in dependency of its mean particle length at a certain time.

Only available if the morphology is set to *PrecipitateMorphology.NEEDLE* or *PrecipitateMorphology.PLATE*. 

Parameters

- **time** – The time [s]
- **precipitate_id** – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (mean particle length [m], aspect ratio)

get_aspect_ratio_distribution_for_radius_of \( (\text{precipitate}\_\text{id}: \text{str}, \text{time}: \text{float}) \rightarrow [\text{typing.List[float]}, \text{typing.List[float]}] \)

Returns the aspect ratio distribution of a precipitate in dependency of its mean radius at a certain time.

Only available if the morphology is set to \text{PrecipitateMorphology.NEEDLE} or \text{PrecipitateMorphology.PLATE}.

Parameters

- **time** – The time [s]
- **precipitate_id** – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (mean radius [m], aspect ratio)

get_critical_radius_of \( (\text{precipitate}\_\text{id}: \text{str}) \rightarrow [\text{typing.List[float]}, \text{typing.List[float]}] \)

Returns the critical radius of a precipitate in dependency of the time.

Parameters **precipitate_id** – The id of a precipitate can either be the phase name or alias

Returns A tuple of two lists of floats (time [s], critical radius [m])

get_cubic_factor_distribution_for_particle_length_of \( (\text{precipitate}\_\text{id}: \text{str}, \text{time}: \text{float}) \rightarrow [\text{typing.List[float]}, \text{typing.List[float]}] \)

Returns the cubic factor distribution of a precipitate in dependency of its mean particle length at a certain time.

Only available if the morphology is set to \text{PrecipitateMorphology.CUBOID}.

Parameters

- **time** – The time in seconds
- **precipitate_id** – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (particle length [m], cubic factor)

get_cubic_factor_distribution_for_radius_of \( (\text{precipitate}\_\text{id}: \text{str}, \text{time}: \text{float}) \rightarrow [\text{typing.List[float]}, \text{typing.List[float]}] \)

Returns the cubic factor distribution of a precipitate in dependency of its mean radius at a certain time.

Only available if the morphology is set to \text{PrecipitateMorphology.CUBOID}.

Parameters

- **time** – The time [s]
- **precipitate_id** – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (radius [m], cubic factor)

get_driving_force_of \( (\text{precipitate}\_\text{id}: \text{str}) \rightarrow [\text{typing.List[float]}, \text{typing.List[float]}] \)

Returns the (by \( R \times T \)) normalized driving force of a precipitate in dependency of the time.

Parameters **precipitate_id** – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], normalized driving force)
get_grain_critical_radius() → [typing.List[float], typing.List[float]]
Returns the critical radius of grains in dependency of the time.

Returns A tuple of two lists of floats (time [s], critical radius [m])

get_grain_mean_radius() → [typing.List[float], typing.List[float]]
Returns the mean grain size of the matrix phase in dependency of the time.

Returns A tuple of two lists of floats (time [s], mean radius [m])

get_grain_number_density() → [typing.List[float], typing.List[float]]
Returns the grain number density in dependency of the time.

Returns A tuple of two lists of floats (time [s], grain number density [m^-3])

get_grain_number_density_distribution_for_length(time: float) → [typing.List[float], typing.List[float]]
Returns the number density distribution of grains in dependency of its mean particle length at a certain time.

Parameters time – The time [s]

Returns A tuple of two lists of floats (grain length[m], number of grains per unit volume per unit length [m^-4])

get_grain_number_density_distribution_for_radius(time: float) → [typing.List[float], typing.List[float]]
Returns the number density distribution of a grains in dependency of its mean radius at a certain time.

Parameters time – The time [s]

Returns A tuple of two lists of floats (radius [m], number of grains per unit volume per unit length [m^-4])

get_grain_size_distribution(time: float) → [typing.List[float], typing.List[float]]
Returns the size distribution of the matrix phase in dependency of its grain radius length at a certain time.

Parameters time – The time [s]

Returns A tuple of two lists of floats (grain radius[m], number density of grains[m^-3])

get_matrix_composition_in_mole_fraction_of(element_name: str) → [typing.List[float], typing.List[float]]
Returns the matrix composition (as mole fractions) of a certain element in dependency of the time.

Parameters element_name – The element

Returns A tuple of two lists of floats (time [s], mole fraction)

get_matrix_composition_in_weight_fraction_of(element_name: str) → [typing.List[float], typing.List[float]]
Returns the matrix composition (as weight fraction) of a certain element in dependency of the time.

Parameters element_name – The element

Returns A tuple of two lists of floats (time [s], weight fraction)

get_mean_aspect_ratio_of( precipitate_id: str) → [typing.List[float], typing.List[float]]
Returns the mean aspect ratio of a precipitate in dependency of the time.

Only available if the morphology is set to PrecipitateMorphology.NEEDLE or PrecipitateMorphology.PLATE.
Parameters `precipitate_id` – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], mean aspect ratio)

`get_mean_cubic_factor_of(precipitate_id: str) → [typing.List[float], typing.List[float]]`

Returns the mean cubic factor of a precipitate in dependency of the time. Only available if the morphology is set to `PrecipitateMorphology.CUBOID`.

Parameters `precipitate_id` – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], mean cubic factor)

`get_mean_particle_length_of(precipitate_id: str) → [typing.List[float], typing.List[float]]`

Returns the mean particle length of a precipitate in dependency of the time.

Only available if the morphology is set to `PrecipitateMorphology.NEEDLE` or `PrecipitateMorphology.PLATE`.

Parameters `precipitate_id` – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], mean particle length [m])

`get_mean_radius_of(precipitate_id: str) → [typing.List[float], typing.List[float]]`

Returns the mean radius of a precipitate in dependency of the time.

Parameters `precipitate_id` – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], mean radius [m])

`get_normalized_grain_size_distribution(time: float) → [typing.List[float], typing.List[float]]`

Returns the normalized number density distribution of a grains at a certain time.

Parameters `time` – The time [s]

Returns A tuple of two lists of floats (Normalized size, Frequency)

`get_normalized_number_density_distribution_of(precipitate_id: str, time: float) → [typing.List[float], typing.List[float]]`

Returns the normalized number density distribution of a precipitate at a certain time.

Parameters

- `time` – The time [s]
- `precipitate_id` – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (Normalized size, Frequency)

`get_nucleation_rate_of(precipitate_id: str) → [typing.List[float], typing.List[float]]`

Returns the nucleation rate of a precipitate in dependency of the time.

Parameters `precipitate_id` – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], nucleation rate [m^-3 s^-1])

`get_number_density_distribution_for_particle_length_of(precipitate_id: str, time: float) → [typing.List[float], typing.List[float]]`

Returns the number density distribution of a precipitate in dependency of its mean particle length at a
certain time.

**Parameters**

- **time** – The time [s]
- **precipitate_id** – The id of a precipitate can either be the phase name or an alias

**Returns** A tuple of two lists of floats (particle length[m], number of particles per unit volume per unit length [m^-4])

get_number_density_distribution_for_radius_of (precipitate_id: str, time: float) → [typing.List[float], typing.List[float]]

Returns the number density distribution of a precipitate in dependency of its mean radius at a certain time.

**Parameters**

- **time** – The time [s]
- **precipitate_id** – The id of a precipitate can either be the phase name or an alias

**Returns** A tuple of two lists of floats (radius [m], number of particles per unit volume per unit length [m^-4])

get_number_density_of (precipitate_id: str) → [typing.List[float], typing.List[float]]

Returns the particle number density of a precipitate in dependency of the time.

**Parameters**

- **precipitate_id** – The id of a precipitate can either be phase name or alias

**Returns** A tuple of two lists of floats (time [s], particle number density [m^-3])

get_precipitate_composition_in_mole_fraction_of (precipitate_id: str, element_name: str) → [typing.List[float], typing.List[float]]

Returns the precipitate composition (as mole fractions) of a certain element in dependency of the time.

**Parameters**

- **precipitate_id** – The id of a precipitate can either be phase name or alias
- **element_name** – The element

**Returns** A tuple of two lists of floats (time [s], mole fraction)

get_precipitate_composition_in_weight_fraction_of (precipitate_id: str, element_name: str) → [typing.List[float], typing.List[float]]

Returns the precipitate composition (as weight fraction) of a certain element in dependency of the time.

**Parameters**

- **precipitate_id** – The id of a precipitate can either be phase name or alias
- **element_name** – The element

**Returns** A tuple of two lists of floats (time [s], weight fraction)

get_size_distribution_for_particle_length_of (precipitate_id: str, time: float) → [typing.List[float], typing.List[float]]

Returns the size distribution of a precipitate in dependency of its mean particle length at a certain time.

**Parameters**

- **time** – The time [s]
- **precipitate_id** – The id of a precipitate can either be the phase name or an alias
Returns A tuple of two lists of floats (particle length [m], number of particles per unit volume per unit length [m^-4])

get_size_distribution_for_radius_of (precipitate_id: str, time: float) \(\rightarrow\) [typing.List[float], typing.List[float]]
Returns the size distribution of a precipitate in dependency of its mean radius at a certain time.

Parameters
・ time – The time [s]
・ precipitate_id – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (radius [m], number of particles per unit volume per unit length [m^-4])

get_volume_fraction_of (precipitate_id: str) \(\rightarrow\) [typing.List[float], typing.List[float]]
Returns the volume fraction of a precipitate in dependency of the time.

Parameters precipitate_id – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], volume fraction)

class tc_python.precipitation.PrecipitationCalculationTTToCCTResult (result)
Bases: tc_python.precipitation.PrecipitationCalculationResult
Result of a TTT or CCT precipitation calculation.

get_result_for_precipitate (precipitate_id: str) \(\rightarrow\) [typing.List[float], typing.List[float]]
Returns the calculated data of a TTT or CCT diagram for a certain precipitate.

Parameters precipitate_id – The id of a precipitate can either be the phase name or an alias

Returns A tuple of two lists of floats (time [s], temp [K])

class tc_python.precipitation.PrecipitationIsoThermalCalculation (calculation)
Bases: tc_python.abstract_base.AbstractCalculation
Configuration for an isothermal precipitation calculation.

calculate () \(\rightarrow\) tc_python.precipitation.PrecipitationCalculationSingleResult
Runs the isothermal precipitation calculation.

Returns A PrecipitationCalculationSingleResult which later can be used to get specific values from the calculated result

get_system_data () \(\rightarrow\) tc_python.abstract_base.SystemData
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

set_composition (element_name: str, value: float)
Sets the composition of the elements. The unit for the composition can be changed using set_composition_unit (). Default: Mole percent (CompositionUnit.MOLE_PERCENT)

Parameters
・ element_name – The element
• **value** – The composition (fraction or percent depending on the composition unit)

**Returns** This *PrecipitationIsoThermalCalculation* object

**set_composition_unit**( `unit_enum: tc_python.utils.CompositionUnit = <CompositionUnit.MOLE_PERCENT: 1>` )

Sets the composition unit. **Default:** Mole percent (CompositionUnit.MOLE_PERCENT).

**Parameters**
- **unit_enum** – The new composition unit

**Returns** This *PrecipitationIsoThermalCalculation* object

**set_simulation_time**( `simulation_time: float` )

Sets the simulation time.

**Parameters**
- **simulation_time** – The simulation time [s]

**Returns** This *PrecipitationIsoThermalCalculation* object

**set_temperature**( `temperature: float` )

Sets the temperature for the isothermal simulation.

**Parameters**
- **temperature** – the temperature [K]

**Returns** This *PrecipitationIsoThermalCalculation* object

**with_matrix_phase**( `matrix_phase: tc_python.precipitation.MatrixPhase` )

Sets the matrix phase.

**Parameters**
- **matrix_phase** – The matrix phase

**Returns** This *PrecipitationIsoThermalCalculation* object

**with_numerical_parameters**( `numerical_parameters: tc_python.precipitation.NumericalParameters` )

Sets the numerical parameters. If not specified, reasonable defaults are be used.

**Parameters**
- **numerical_parameters** – The parameters

**Returns** This *PrecipitationIsoThermalCalculation* object

**with_system_modifications**( `system_modifications: tc_python.abstract_base.SystemModifications` )

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

**Note:** This is only possible if the system has been read from unencrypted (i.e. *user*) databases loaded as a *.tdb*-file.

**Parameters**
- **system_modifications** – The system modification to be performed

**Returns** This *PrecipitationIsoThermalCalculation* object

**class tc_python.precipitation.PrecipitationNonIsoThermalCalculation**( `calculation` )

**Bases:** tc_python.abstract_base.AbstractCalculation

Configuration for a non-isothermal precipitation calculation.

**calculate**( ) → tc_python.precipitation.PrecipitationCalculationSingleResult

Runs the non-isothermal precipitation calculation.

**Returns** A *PrecipitationCalculationSingleResult* which later can be used to get specific values from the calculated result
get_system_data() → tc_python.abstract_base.SystemData
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

set_composition(element_name: str, value: float)
Sets the composition of the elements. The unit for the composition can be changed using set_composition_unit(). Default: Mole percent (CompositionUnit.MOLE_PERCENT)

Parameters
  • element_name – The element
  • value – The composition (fraction or percent depending on the composition unit)

Returns This PrecipitationIsoThermalCalculation object

set_composition_unit(unit_enum: tc_python.utils.CompositionUnit)
Sets the composition unit. Default: Mole percent (CompositionUnit.MOLE_PERCENT).

Parameters unit_enum – The new composition unit

Returns This PrecipitationIsoThermalCalculation object

set_simulation_time(simulation_time: float)
Sets the simulation time.

Parameters simulation_time – The simulation time [s]

Returns This PrecipitationNonThermalCalculation object

with_matrix_phase(matrix_phase: tc_python.precipitation.MatrixPhase)
Sets the matrix phase.

Parameters matrix_phase – The matrix phase

Returns This PrecipitationIsoThermalCalculation object

with_numerical_parameters(numerical_parameters: tc_python.precipitation.NumericalParameters)
Sets the numerical parameters. If not specified, reasonable defaults are be used.

Parameters numerical_parameters – The parameters

Returns This PrecipitationIsoThermalCalculation object

with_system_modifications(system_modifications: tc_python.abstract_base.SystemModifications)
Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Note: This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb-file.

Parameters system_modifications – The system modification to be performed

Returns This PrecipitationNonThermalCalculation object
with_temperature_profile(temperature_profile: tc_python.utils.TemperatureProfile)
Sets the temperature profile to use with this calculation.

Parameters temperature_profile – the temperature profile object (specifying time / temperature points)

Returns This PrecipitationNonThermalCalculation object

class tc_python.precipitation.PrecipitationTTTCalculation(calculation)
Bases: tc_python.abstract_base.AbstractCalculation

Configuration for a TTT (Time-Temperature-Transformation) precipitation calculation.

calculate() \rightarrow tc_python.precipitation.PrecipitationCalculationTTTorCCTResult
Runs the TTT diagram calculation.

Returns A PrecipitationCalculationTTTorCCTResult which later can be used to get specific values from the calculated result.

get_system_data() \rightarrow tc_python.abstract_base.SystemData
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

set_composition(element_name: str, value: float)
Sets the composition of the elements. The unit for the composition can be changed using set_composition_unit(). Default: Mole percent (CompositionUnit.MOLE_PERCENT)

Parameters

• element_name – The element
• value – The composition (fraction or percent depending on the composition unit)

Returns This PrecipitationTTTCalculation object

set_composition_unit(unit_enum: tc_python.utils.CompositionUnit)
Sets the composition unit. Default: Mole percent (CompositionUnit.MOLE_PERCENT).

Parameters unit_enum – The new composition unit

Returns This PrecipitationTTTCalculation object

set_max_annealing_time(max_annealing_time: float)
Sets the maximum annealing time, i.e. the maximum time of the simulation if the stopping criterion is not reached.

Parameters max_annealing_time – the maximum annealing time [s]

Returns This PrecipitationTTTCalculation object

set_max_temperature(max_temperature: float)
Sets the maximum temperature for the TTT diagram.

Parameters max_temperature – the maximum temperature [K]

Returns This PrecipitationTTTCalculation object

set_min_temperature(min_temperature: float)
Sets the minimum temperature for the TTT diagram.
Parameters `min_temperature` – the minimum temperature [K]

Returns This `PrecipitationTTTCalculation` object

`set_temperature_step` *(temperature_step: float)*
Sets the temperature step for the TTT diagram. If not set, the default value is 10 K.

Parameters `temperature_step` – the temperature step [K]

Returns This `PrecipitationTTTCalculation` object

`stop_at_percent_of_equilibrium_fraction` *(percentage: float)*
Sets the stop criterion to a percentage of the overall equilibrium phase fraction, alternatively a required volume fraction can be specified (using `stop_at_volume_fraction_of_phase()`).

Parameters `percentage` – the percentage to stop at (value between 0 and 100)

Returns This `PrecipitationTTTCalculation` object

`stop_at_volume_fraction_of_phase` *(volume_fraction: float)*
Sets the stop criterion as a volume fraction of the phase, alternatively a required percentage of the equilibrium phase fraction can be specified (using `stop_at_percent_of_equilibria_fraction()`). Stopping at a specified volume fraction is the default setting.

This setting is applied to all phases.

Parameters `volume_fraction` – the volume fraction to stop at (a value between 0 and 1)

Returns This `PrecipitationTTTCalculation` object

`with_matrix_phase` *(matrix_phase: tc_python.precipitation.MatrixPhase)*
Sets the matrix phase.

Parameters `matrix_phase` – The matrix phase

Returns This `PrecipitationTTTCalculation` object

`with_numerical_parameters` *(numerical_parameters: tc_python.precipitation.NumericalParameters)*
Sets the numerical parameters. If not specified, reasonable defaults are be used.

Parameters `numerical_parameters` – The parameters

Returns This `PrecipitationTTTCalculation` object

`with_system_modifications` *(system_modifications: tc_python.abstract_base.SystemModifications)*
Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Note: This is only possible if the system has been read from unencrypted (i.e. *user*) databases loaded as a *.tdb*-file.

Parameters `system_modifications` – The system modification to be performed

Returns This `PrecipitationTTTCalculation` object

```python
class tc_python.precipitation.TransformationStrainCalculationOption(value)
    Bases: enum.Enum

Options for calculating the transformation strain.

CALCULATE_FROM_MOLAR_VOLUME = 2
    Calculates the transformation strain from the molar volume, obtains a purely dilatational strain.
```
DISREGARD = 1
    Ignores the transformation strain, **this is the default setting.**

USER_DEFINED = 3
    Transformation strain to be specified by the user.

class tc_python.precipitation.VolumeFractionOfPhaseType(value)
    Bases: enum.Enum

    Unit of the volume fraction of a phase.

    VOLUME_FRACTION = 6
        Volume fraction (0 - 1), **this is the default.**

    VOLUME_PERCENT = 5
        Volume percent (0% - 100%).

5.1.4 Module “scheil”

class tc_python.scheil.CalculateSecondaryDendriteArmSpacing
    Bases: tc_python.scheil.ScheilBackDiffusion

    Configures a secondary dendrite arm spacing calculation used by Scheil with back diffusion. The used equation is \( c \times \text{cooling\_rate}^{-n} \) with \( c \) and \( n \) being provided either by the user or taken from the defaults.

    set_c(c: float = 5e-05)
        Sets the scaling factor \( c \) in the governing equation \( c \times \text{cooling\_rate}^{-n} \).

        Default: 50 µm

        Parameters
        c – The scaling factor [m]

        Returns
        This CalculateSecondaryDendriteArmSpacing object

    set_cooling_rate(cooling_rate: float = 1.0)
        Sets the cooling rate.

        Default: 1.0 K/s

        An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.

        Parameters
        cooling_rate – The cooling rate [K/s]

        Returns
        This CalculateSecondaryDendriteArmSpacing object

    set_fast_diffusing_elements(element_names: List[str])
        Sets elements as fast diffusing. This allows redistribution of these elements in both the solid and liquid parts of the alloy.

        Default: No fast-diffusing elements.

        Parameters
        element_names – The elements

        Returns
        This CalculateSecondaryDendriteArmSpacing object

    set_n(n: float = 0.33)
        Sets the exponent \( n \) in the governing equation \( c \times \text{cooling\_rate}^{-n} \).

        Default: 0.33

        Parameters
        n – The exponent [-]

        Returns
        This CalculateSecondaryDendriteArmSpacing object
**set_primary_phasename** *(primary_phase_name: str = 'AUTOMATIC')*

Sets the name of the primary phase.

The primary phase is the phase where the back diffusion takes place. If AUTOMATIC is selected, the program tries to find the phase which will give the most back diffusion. That behavior can be overridden by selecting a specific primary phase.

**Default:** AUTOMATIC

**Parameters**

- **primary_phase_name** – The phase name (or AUTOMATIC)

**Returns**

This CalculateSecondaryDendriteArmSpacing object

class tc_python.scheil.ConstantSecondaryDendriteArmSpacing *(secondary_dendrite_arm_spacing: float = 5e-05)*

Bases: tc_python.scheil.ScheilBackDiffusion

Configures a constant secondary dendrite arm spacing used by Scheil with back diffusion. The secondary dendrite arm spacing can either be provided by the user or taken from the defaults.

**set_cooling_rate** *(cooling_rate: float = 1.0)*

Sets the cooling rate.

**Default:** 1.0 K/s

An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.

**Parameters**

- **cooling_rate** – The cooling rate [K/s]

**Returns**

This ConstantSecondaryDendriteArmSpacing object

**set_fast_diffusing_elements** *(element_names: List[str])*

Sets elements as fast diffusing. This allows redistribution of these elements in both the solid and liquid parts of the alloy.

**Default:** No fast-diffusing elements.

**Parameters**

- **element_names** – The elements

**Returns**

This ConstantSecondaryDendriteArmSpacing object

**set_primary_phasename** *(primary_phase_name: str = 'AUTOMATIC')*

Sets the name of the primary phase.

The primary phase is the phase where the back diffusion takes place. If AUTOMATIC is selected, the program tries to find the phase which will give the most back diffusion. That behavior can be overridden by selecting a specific primary phase.

**Default:** AUTOMATIC

**Parameters**

- **primary_phase_name** – The phase name (or AUTOMATIC)

**Returns**

This ConstantSecondaryDendriteArmSpacing object

class tc_python.scheil.ScheilBackDiffusion

Bases: tc_python.scheil.ScheilCalculationType

Configuration for back diffusion in the solid primary phase.

**Warning:** This feature has only effect on systems with diffusion data (typically a mobility database). If used for a system without diffusion data, a normal Scheil calculation is done.
classmethod `calculate_secondary_dendrite_arm_spacing()`  
Calculate the secondary dendrite arm spacing based on the following equation: $c \times cooling\_rate^{-n}$ with $c$ and $n$ being provided either by the user or taken from the defaults.

Use the methods provide by `CalculateSecondaryDendriteArmSpacing` to configure the parameters.

**Returns** A `CalculateSecondaryDendriteArmSpacing`  

classmethod `constant_secondary_dendrite_arm_spacing(secondary_dendrite_arm_spacing: float = 5e-05)`  
Assuming constant secondary dendrite arm spacing, provided either by the user or taken from the defaults.

**Default:** 50 µm  
**Parameters** `secondary_dendrite_arm_spacing` – The dendrite arm spacing [m]  
**Returns** A `ConstantSecondaryDendriteArmSpacing`  

class `tc_python.scheil.ScheilCalculation(calculator)`  
Bases: `tc_python.abstract_base.AbstractCalculation`  
Configuration for a Scheil solidification calculation.

**Note:** Specify the settings, the calculation is performed with `calculate()`.

`calculate()` → `tc_python.scheil.ScheilCalculationResult`  
Runs the Scheil calculation.

**Warning:** Scheil calculations do not support the GAS phase being selected, this means the GAS phase must always be deselected in the system if it is present in the database.

**Returns** A `ScheilCalculationResult` which later can be used to get specific values from the simulation.

disable_global_minimization()  
Disables global minimization.

**Default:** Enabled  
**Note:** When enabled, a global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

**Returns** This `ScheilCalculation` object  

enable_global_minimization()  
Enables global minimization.

**Default:** Enabled  
**Note:** When enabled, a global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

**Returns** This `ScheilCalculation` object
get_system_data() → tc_python.abstract_base.SystemData
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

set_composition(component_name: str, value: float)
Sets the composition of a component. The unit for the composition can be changed using set_composition_unit().

Default: Mole percent (CompositionUnit.MOLE_PERCENT)

Parameters
- component_name – The component
- value – The composition value [composition unit defined for the calculation]

Returns This ScheilCalculation object

set_composition_unit(unit_enum: tc_python.utils.CompositionUnit = <CompositionUnit.MOLE_PERCENT: 1>)
Sets the composition unit.

Default: Mole percent (CompositionUnit.MOLE_PERCENT).

Parameters unit_enum – The new composition unit

Returns This ScheilCalculation object

set_fast_diffusing_elements(element_names: List[str])
Sets elements as fast diffusing. This allows redistribution of these elements in both the solid and liquid parts of the alloy.

Note: Deprecated in version 2021b: This method has been moved into the class ScheilCalculationType, which is used with the method with_calculation_type(). It will be removed in release 2022b.

Default: No fast-diffusing elements.

Parameters element_names – The elements

Returns This ScheilCalculation object

set_start_temperature(temperature_in_kelvin: float = 2500.0)
Sets the start temperature.

Warning: The start temperature needs to be higher than the liquidus temperature of the alloy.

Default: 2500.0 K

Parameters temperature_in_kelvin – The temperature [K]

Returns This ScheilCalculation object
with_back_diffusion (scheil_back_diffusion: tc_python.scheil.ScheilBackDiffusion)

Enables back diffusion in the solid primary phase.

Note: Deprecated in version 2021b: Use with_calculation_type() instead. This method will be removed in release 2022b.

Warning: This feature has only effect on systems with diffusion data (typically a mobility database). If used for a system without diffusion data, a normal Scheil calculation is performed.

Parameters scheil_back_diffusion – an instance of a ScheilBackDiffusion class, where the options for back diffusion can be specified.

Returns This ScheilCalculation object

with_calculation_type (scheil_calculation_type: tc_python.scheil.ScheilCalculationType)

Chooses a specific Scheil calculation. ClassicScheil for only setting fast diffusers, ScheilBackDiffusion enables back diffusion in the solid primary phase and optionally fast diffusers in all solid phases, and ScheilSoluteTrapping enables solute trapping in the solid primary phase. :param scheil_type: Type of Scheil calculation, either ClassicScheil, BackDiffusion or SoluteTrapping :return: This ScheilCalculation object

with_options (options: tc_python.scheil.ScheilOptions)

Sets the Scheil simulation options.

Parameters options – The Scheil simulation options

Returns This ScheilCalculation object

with_system_modifications (system_modifications: tc_python.abstract_base.SystemModifications)

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Note: This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb-file.

Parameters system_modifications – The system modification to be performed

Returns This ScheilCalculation object

class tc_python.scheil.ScheilCalculationResult (result)
Bases: tc_python.abstract_base.AbstractResult

Result of a Scheil calculation.

get_values_grouped_by_quantity_of (x_quantity: Union[tc_python.quantity_factory.ScheilQuantity, str], y_quantity: Union[tc_python.quantity_factory.ScheilQuantity, str], sort_and_merge: bool = True) → Dict[str, tc_python.utils.ResultValueGroup]

Returns x-y-line data grouped by the multiple datasets of the specified quantities (for example in dependency of phases or components). Use get_values_of() instead if you need no separation. The available quantities can be found in the documentation of the factory class ScheilQuantity.
**Note:** The different datasets might contain NaN-values between different subsections and might not be sorted **even if the flag 'sort_and_merge' has been set** (because they might be unsortable due to their nature).

**Parameters**

- **x_quantity** – The first Scheil quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example “T”)
- **y_quantity** – The second Scheil quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example “NV”)
- **sort_and_merge** – If True, the data will be sorted and merged into as few subsections as possible (divided by NaN)

**Returns**

Containing the ResultValueGroup dataset objects with their *quantity labels* as keys

```python
get_values_grouped_by_stable_phases_of(x_quantity: Union[tc_python.quantity_factory.ScheilQuantity, str],
                                       y_quantity: Union[tc_python.quantity_factory.ScheilQuantity, str],
                                       sort_and_merge: bool = True) -> Dict[str, tc_python.utils.ResultValueGroup]
```

Returns x-y-line data grouped by the sets of “stable phases” (for example “LIQUID” or “LIQUID + FCC_A1”). Use `get_values_of()` instead if you need no separation. The available quantities can be found in the documentation of the factory class ScheilQuantity.

**Note:** The different datasets might contain NaN-values between different subsections and might not be sorted **even if the flag 'sort_and_merge' has been set** (because they might be unsortable due to their nature).

**Parameters**

- **x_quantity** – The first Scheil quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example “T”)
- **y_quantity** – The second Scheil quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example “NV”)
- **sort_and_merge** – If True, the data will be sorted and merged into as few subsections as possible (divided by NaN)

**Returns**

Containing the ResultValueGroup dataset objects with their “stable phases” labels as keys

```python
get_values_of(x_quantity: Union[tc_python.quantity_factory.ScheilQuantity, str],
              y_quantity: Union[tc_python.quantity_factory.ScheilQuantity, str]) -> [typing.List[float], typing.List[float]]
```

Returns sorted x-y-line data without any separation. Use `get_values_grouped_by_quantity_of()` or `get_values_grouped_by_stable_phases_of()` instead if you need such a separation. The available quantities can be found in the documentation of the factory class ScheilQuantity.

**Note:** This method will always return sorted data without any NaN-values. In case of ambiguous quantities (for example: CompositionOfPhaseAsWeightFraction(“FCC_A1”, “All”)) that can give data that is
hard to interpret. In such a case you need to choose the quantity in another way or use one of the other methods.

Parameters

- **x_quantity** – The first Scheil quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example “T”)
- **y_quantity** – The second Scheil quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example “NV”)

Returns A tuple containing the x- and y-data in lists

```python
def save_to_disk(path: str)
    # Saves the result to disc. Note that a result is a folder, containing potentially many files. The result can later be loaded with load_result_from_disk()

    Parameters path – the path to the folder you want the result to be saved in.

    Returns this `ScheilCalculationResult` object
```

class tc_python.scheil.ScheilCalculationType
    Bases: object

    Specific configuration for the different Scheil calculation types

    classmethod scheil_back_diffusion()
        Configuration for back diffusion in the solid primary phase.

        Warning: This feature has only effect on systems with diffusion data (typically a mobility database). If used for a system without diffusion data, a normal Scheil calculation is done. :return: A `ScheilBackDiffusion` object

    classmethod scheil_classic()
        Configuration for Classic Scheil with fast diffusers. :return: A `ScheilClassic` object

    classmethod scheil_solute_trapping()
        Configures the Scheil solute trapping settings. The used solidification speed equation is `Scanning speed * cos(angle)` with `Scanning speed` and `angle` being provided either by the user or taken from the defaults. :return: A `ScheilSoluteTrapping` object

```python
class tc_python.scheil.ScheilClassic
    Bases: tc_python.scheil.ScheilCalculationType

    Configuration for Classic Scheil with fast diffusers.

    set_fast_diffusing_elements(element_names: List[str])
        Sets elements as fast diffusing. This allows redistribution of these elements in both the solid and liquid parts of the alloy.

        Default: No fast-diffusing elements.

        Parameters element_names – The elements

        Returns This `ScheilClassic` object
```

class tc_python.scheil.ScheilOptions
    Bases: object

    Options for the Scheil simulation.
**calculate_from_liquidus()**

Solidification calculation starting from the liquidus temperature. Liquid properties between start temperature and liquidus are not obtainable.

**Default:** Calculation starts from liquidus temperature.

**Returns** This `ScheilOptions` object

**calculate_from_start_temperature()**

Calculation of equilibria from start temperature at 50 K intervals until liquidus temperature is reached. This option makes it possible to obtain properties of the liquid phase before the solidification starts.

**Default:** Calculation starts from liquidus temperature.

**Returns** This `ScheilOptions` object

**disable_approximate_driving_force_for_metastable_phases()**

Disables the approximation of the driving force for metastable phases.

**Default:** Enabled

**Note:** When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, use `disable_approximate_driving_force_for_metastable_phases()` to force the calculation to converge for the metastable phases.

**Returns** This `ScheilOptions` object

**disable_control_step_size_during_minimization()**

Disables stepsize control during minimization (non-global).

**Default:** Enabled

**Returns** This `ScheilOptions` object

**disable_equilibrium_solidification_calculation()**

Skips the property (one axis) diagram calculation of solidification under equilibrium conditions, before the Scheil solidification calculation starts.

In general it is not necessary to perform this calculation.

**Default:** Disabled. The equilibrium solidification calculation is skipped.

**Returns** This `ScheilOptions` object

**disable_force_positive_definite_phase_hessian()**

Disables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

**Default:** Enabled

**Returns** This `ScheilOptions` object

**enable_approximate_driving_force_for_metastable_phases()**

Enables the approximation of the driving force for metastable phases.

**Default:** Enabled
Note: When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, use `disable_approximate_driving_force_for_metastable_phases()` to force the calculation to converge for the metastable phases.

**Returns** This `ScheilOptions` object

### enable_control_step_size_during_minimization()

Enables stepsize control during normal minimization (non-global).

**Default:** Enabled

**Returns** This `ScheilOptions` object

### enable_equilibrium_solidification_calculation()

Performs a property (one axis) diagram calculation of solidification under equilibrium conditions, before the Scheil solidification calculation starts, in the same way as is typically done in graphical and console mode.

In general it is not necessary to perform this calculation.

**Default:** Disabled. The equilibrium solidification calculation is skipped.

**Returns** This `ScheilOptions` object

### enable_force_positive_definite_phase_hessian()

Enables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

**Default:** Enabled

**Returns** This `ScheilOptions` object

### set_global_minimization_max_grid_points(max_grid_points: int = 2000)

Sets the maximum number of grid points in global minimization. ** Only applicable if global minimization is actually used**.

**Default:** 2000 points

**Parameters** `max_grid_points` – The maximum number of grid points

**Returns** This `ScheilOptions` object

### set_global_minimization_test_interval(global_test_interval: int = 10)

Sets the interval for the global test.

**Default:** 10

**Parameters** `global_test_interval` – The global test interval

**Returns** This `ScheilOptions` object

### set_liquid_phase(phase_name: str = ‘LIQUID’)

Sets the phase used as the liquid phase.

**Default:** The phase “LIQUID”.

**Parameters** `phase_name` – The phase name

**Returns** This `ScheilOptions` object
**set_max_no_of_iterations** *(max_no_of_iterations: int = 500)*
Set the maximum number of iterations.

**Default:** max. 500 iterations

**Note:** As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

**Parameters** `max_no_of_iterations` – The max. number of iterations

**Returns** This `ScheilOptions` object

**set_required_accuracy** *(accuracy: float = 1e-06)*
Sets the required relative accuracy.

**Default:** 1.0E-6

**Note:** This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

**Parameters** `accuracy` – The required relative accuracy

**Returns** This `ScheilOptions` object

**set_smallest_fraction** *(smallest_fraction: float = 1e-12)*
Sets the smallest fraction for constituents that are unstable.

It is normally only in the gas phase that you can find such low fractions.

The **default value** for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.

**Parameters** `smallest_fraction` – The smallest fraction for constituents that are unstable

**Returns** This `ScheilOptions` object

**set_temperature_step** *(temperature_step_in_kelvin: float = 1.0)*
Sets the temperature step. Decreasing the temperature step increases the accuracy, but the default value is usually adequate.

**Default step:** 1.0 K

**Parameters** `temperature_step_in_kelvin` – The temperature step [K]

**Returns** This `ScheilOptions` object

**terminate_on_fraction_of_liquid_phase** *(fraction_to_terminate_at: float = 0.01)*
Sets the termination condition to a specified remaining fraction of liquid phase.

**Default:** Terminates at 0.01 fraction of liquid phase.

**Note:** Either the termination criterion is set to a temperature or fraction of liquid limit, both together are not possible.
Parameters **fraction_to_terminate_at** – the termination fraction of liquid phase (value between 0 and 1)

**Returns** This *ScheilOptions* object

**terminate_on_temperature** *(temperature_in_kelvin: float)*
Sets the termination condition to a specified temperature.

**Default**: Terminates at 0.01 fraction of liquid phase, i.e. not at a specified temperature.

**Note**: Either the termination criterion is set to a temperature or fraction of liquid limit, both together are not possible.

Parameters **temperature_in_kelvin** – the termination temperature [K]

**Returns** This *ScheilOptions* object

### class `tc_python.scheil.ScheilSoluteTrapping`

**Bases**: `tc_python.scheil.ScheilCalculationType`

Configures the Scheil solute trapping settings. The used solidification speed equation is *Scanning speed * \(\cos(\text{angle})\) with *Scanning speed* and *angle* being provided either by the user or taken from the defaults.

**set_angle** *(alpha: float = 45.0)*
Sets the transformation angle alpha between the solid/liquid boundary and laser scanning direction.

**Default**: 45.0

**Parameters** **alpha** – The transformation angle [degree]

**Returns** This *ScheilSoluteTrapping* object

**set_primary_phasename** *(primary_phase_name: str = 'AUTOMATIC')*
Sets the name of the primary phase.

The primary phase is the phase where solute trapping takes place. A necessary condition for this phase is that the phase definition contains all of the elements that are chosen in the system. When *AUTOMATIC* is selected, the program tries to find a suitable primary phase that fills this condition.

**Default**: *AUTOMATIC*

**Parameters** **primary_phase_name** – The phase name (or *AUTOMATIC*)

**Returns** This *ScheilSoluteTrapping* object

**set_scanning_speed** *(scanning_speed: float = 1.0)*
Sets the scanning speed.

**Default**: 1 m/s

**Parameters** **scanning_speed** – The scaling factor [m/s]

**Returns** This *ScheilSoluteTrapping* object
5.1.5 Module “step_or_map_diagrams”

```python
class tc_python.step_or_map_diagrams.AbstractAxisType
    Bases: object
    The abstract base class for all axis types.

class tc_python.step_or_map_diagrams.AbstractPhaseDiagramCalculation(calculator)
    Bases: tc_python.abstract_base.AbstractCalculation
    Abstract configuration required for a property diagram calculation.

Note: This is an abstract class that cannot be used directly.
```

add_initial_equilibrium(initial_equilibrium: tc_python.step_or_map_diagrams.InitialEquilibrium) →
Add initial equilibrium start points from which a phase diagram is calculated.
Scans along the axis variables and generates start points when the scan procedure crosses a phase boundary.
It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the core remembers all node points and subsequently stops calculations along a line when it finds a known node point.
It is also possible to create a sequence of start points from one initial equilibria.

**Parameters**

- initial_equilibrium — The initial equilibrium

**Returns**

- This `PhaseDiagramCalculation` object

```python
abstract calculate(keep_previous_results: bool = False) →
tc_python.step_or_map_diagrams.PhaseDiagramResult
```

```python
disable_global_minimization() →
Disables global minimization.

**Default:** Enabled

- Returns This `PhaseDiagramCalculation` object

```python
dont_keep_default_equilibria() →
Do not keep the initial equilibria added by default.
This is only relevant in combination with `add_initial_equilibrium()`.
This is the default behavior.

- Returns This `PhaseDiagramCalculation` object

```python
enable_global_minimization() →
Enables global minimization.

**Default:** Enabled

- Returns This `PhaseDiagramCalculation` object

get_components() → List[str]
Returns the names of the components in the system (including all components auto-selected by the database(s)).

- Returns The component names

```python
get_gibbs_energy_addition_for(phase: str) → float
Used to get the additional energy term (always being a constant) of a given phase. The value given is added
```
to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

**Parameters** phase – Specify the name of the (stoichiometric or solution) phase with the addition

**Returns** Gibbs energy addition to G per mole formula unit.

**get_system_data() → tc_python.abstract_base.SystemData**

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

**Note:** Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

**Returns** The system data

**keep_default_equilibria()**

Keep the initial equilibria added by default. This is only relevant in combination with `add_initial_equilibrium()`.

Default behavior is to not keep default equilibria.

**Returns** This `PhaseDiagramCalculation` object

**remove_all_initial_equilibria()**

Removes all previously added initial equilibria.

**Returns** This `PhaseDiagramCalculation` object

**run_poly_command(command: str)**

Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

**Parameters** command – The Thermo-Calc Console Mode command

**Returns** This `PhaseDiagramCalculation` object

**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

**set_gibbs_energy_addition_for(phase: str, gibbs_energy: float)**

Used to specify the additional energy term (always being a constant) of a given phase. The value (gibbs_energy) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

**Parameters**

- **phase** – Specify the name of the (stoichiometric or solution) phase with the addition

- **gibbs_energy** – Addition to G per mole formula unit

**Returns** This `PhaseDiagramCalculation` object
set_phase_to_dormant (phase: str)
Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

Parameters phase – The phase name or ALL_PHASES for all phases

Returns This PhaseDiagramCalculation object

set_phase_to_entered (phase: str, amount: float = 1.0)
Sets the phase to the status ENTERED, that is the default state.

Parameters

• phase – The phase name or ALL_PHASES for all phases

• amount – The phase fraction (between 0.0 and 1.0)

Returns This PhaseDiagramCalculation object

set_phase_to_fixed (phase: str, amount: float)
Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

Parameters

• phase – The phase name

• amount – The fixed phase fraction (between 0.0 and 1.0)

Returns This PhaseDiagramCalculation object

set_phase_to_suspended (phase: str)
Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

Parameters phase – The phase name or ALL_PHASES for all phases

Returns This PhaseDiagramCalculation object

with_options (options: tc_python.step_or_map_diagrams.PhaseDiagramOptions)
Sets the simulation options.

Parameters options – The simulation options

Returns This PhaseDiagramCalculation object

with_reference_state (component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)
The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.
If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

**Parameters**

- **component** – The name of the element must be given.
- **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
- **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
- **pressure** – The Pressure (in Pa) for the reference state.

**Returns** This PhaseDiagramCalculation object

**with_system_modifications** (system_modifications: tc_python.abstract_base.SystemModifications)

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

---

**Note:** This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb*-file.

---

**Parameters** system_modifications – The system modification to be performed

**Returns** This PhaseDiagramCalculation object

**class** tc_python.step_or_map_diagrams.AbstractPropertyDiagramCalculation (calculator)

**Bases:** tc_python.abstract_base.AbstractCalculation

Abstract configuration required for a property diagram calculation.

---

**Note:** This is an abstract class that cannot be used directly.

**abstract calculate** (keep_previous_results: bool = False)

Disables global minimization.

**Default:** Enabled

**Returns** This PropertyDiagramCalculation object

**disable_global_minimization** ()

Disables step separate phases. This is the default setting.

**Returns** This PropertyDiagramCalculation object

**enable_global_minimization** ()

Enables global minimization.

**Default:** Enabled

**Returns** This PropertyDiagramCalculation object

**disable_step_separate_phases** ()

Enables step separate phases.

**Default:** By default separate phase stepping is disabled

**enable_step_separate_phases** ()

Enables step separate phases.

**Default:** By default separate phase stepping is disabled
Note: This is an advanced option, it is used mostly to calculate how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIGMA-phase, G-phase, MU-phase, etc.).

Returns This PropertyDiagramCalculation object

get_components() → List[str]
Returns the names of the components in the system (including all components auto-selected by the database(s)).

Returns The component names

get_gibbs_energy_addition_for(phase: str) → float
Used to get the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

Parameters phase – Specify the name of the (stoichiometric or solution) phase with the addition

Returns Gibbs energy addition to G per mole formula unit.

get_system_data() → tc_python.abstract_base.SystemData
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

run_poly_command(command: str)
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

Parameters command – The Thermo-Calc Console Mode command

Returns This PropertyDiagramCalculation object

Note: It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

Warning: As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

set_gibbs_energy_addition_for(phase: str, gibbs_energy: float)
Used to specify the additional energy term (always being a constant) of a given phase. The value (gibbs_energy) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.
Parameters

- **phase** – Specify the name of the (stoichiometric or solution) phase with the addition

- **gibbs_energy** – Addition to G per mole formula unit

Returns This `PropertyDiagramCalculation` object

`set_phase_to_dormant(phase: str)`

Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

Parameters **phase** – The phase name or `ALL_PHASES` for all phases

Returns This `PropertyDiagramCalculation` object

`set_phase_to_entered(phase: str, amount: float = 1.0)`

Sets the phase to the status ENTERED, that is the default state.

Parameters

- **phase** – The phase name or `ALL_PHASES` for all phases
- **amount** – The phase fraction (between 0.0 and 1.0)

Returns This `PropertyDiagramCalculation` object

`set_phase_to_fixed(phase: str, amount: float)`

Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

Parameters

- **phase** – The phase name
- **amount** – The fixed phase fraction (between 0.0 and 1.0)

Returns This `PropertyDiagramCalculation` object

`set_phase_to_suspended(phase: str)`

Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

Parameters **phase** – The phase name or `ALL_PHASES` for all phases

Returns This `PropertyDiagramCalculation` object

`with_options(options: tc_python.step_or_map_diagrams.PropertyDiagramOptions)`

Sets the simulation options.

Parameters **options** – The simulation options

Returns This `PropertyDiagramCalculation` object

`with_reference_state(component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)`

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set
as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

**Parameters**

- **component** – The name of the element must be given.
- **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
- **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
- **pressure** – The Pressure (in Pa) for the reference state.

**Returns**

This `PropertyDiagramCalculation` object

**with_system_modifications** *(system_modifications: tc_python.abstract_base.SystemModifications)*

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

**Note:** This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb*-file.

**Parameters system_modifications** – The system modification to be performed

**Returns**

This `PropertyDiagramCalculation` object

**class** `tc_python.step_or_map_diagrams.AxisType`

**Bases:** `tc_python.step_or_map_diagrams.AbstractAxisType`

Factory class providing objects for configuring a logarithmic or linear axis by using `AxisType.linear()` or `AxisType.logarithmic()`.

**classmethod linear()**

Creates an object for configuring a linear calculation axis.

**Default:** A minimum number of 40 steps.

**Note:** The returned object can be configured regarding the maximum step size or the minimum number of steps on the axis.

**Returns**

A new `Linear` object

**classmethod logarithmic()**

Creates an object for configuring a logarithmic calculation axis.

**Default:** A scale factor of 1.1
Note: The returned object can be configured regarding the scale factor.

Returns A new Logarithmic object

class tc_python.step_or_map_diagrams.CalculationAxis(quantity:
    Union[tc_python.quantity_factory.ThermodynamicQuantity,
    str])

Bases: object

A calculation axis used for property and phase diagram calculations.

Note: A calculation axis is defining the varied condition and the range of variation. It is the same concept as in Thermo-Calc Graphical Mode or Console Mode.

Default: A Linear axis with a minimum number of 40 steps

set_max(max: float)
Sets the maximum quantity value of the calculation axis.

There is no default value set, it always needs to be defined.

Parameters max – The maximum quantity value of the axis [unit according to the axis quantity]

Returns This CalculationAxis object

set_min(min: float)
Sets the minimum quantity value of the calculation axis.

There is no default value set, it always needs to be defined.

Parameters min – The minimum quantity value of the axis [unit according to the axis quantity]

Returns This CalculationAxis object

set_start_at(at: float)
Sets the starting point of the calculation on the axis.

Default: The default starting point is the center between the minimum and maximum quantity value

Parameters at – The starting point on the axis [unit according to the axis quantity]

Returns This CalculationAxis object

with_axis_type(axis_type: tc_python.step_or_map_diagrams.AxisType)
Sets the type of the axis.

Default: A Linear axis with a minimum number of 40 steps

Parameters axis_type – The axis type (linear or logarithmic)

Returns This CalculationAxis object

class tc_python.step_or_map_diagrams.Direction(value)
Bases: enum.Enum

An enumeration.

DECREASE_FIRST_AXIS = 3
DECREASE_SECOND_AXIS = 4
INCREASE_FIRST_AXIS = 0
INCREASE_SECOND_AXIS = 1

```python
class tc_python.step_or_map_diagrams.InitialEquilibrium(first_axis: float, second_axis: float):
    
    Bases: object
    
    add_equilibria_at_all_phase_changes()
    This generates one start point for each set of phase change in the chosen direction of the specified axis.
    This ensures finding all possible phase boundary lines (not just the first one) along such an axis direction.
    Default behavior is to only generate one start point at the first phase change.
    
    Returns This InitialEquilibrium object

    add_equilibria_at_first_phase_change()
    This generates one start point at the first phase change.
    This is the default behavior.
    
    Returns This InitialEquilibrium object

    set_direction(direction_enum: tc_python.step_or_map_diagrams.Direction)
    Specifies along which axes the initial equilibria should be added.
    The default direction is INCREASE_FIRST_AXIS.
    
    Parameters direction_enum –
    
    Returns This InitialEquilibrium object
```

```python
class tc_python.step_or_map_diagrams.Linear:
    Bases: tc_python.step_or_map_diagrams.AxisType
    
    Represents a linear axis.

    get_type() → str
    Convenience method for getting axis type.
    
    Returns The type

    set_max_step_size(max_step_size: float)
    Sets the axis to use the maximum step size configuration.
    
    Default: This is not the default which is minimum number of steps
    
    Parameters max_step_size – The maximum step size [unit according to the axis quantity]
    
    Returns This Linear object

    set_min_nr_of_steps(min_nr_of_steps: float = 40)
    Sets the axis to use the minimum number of steps configuration.
    
    Default: This is the default option (with a minimum number of steps of 40)
    
    Parameters min_nr_of_steps – The minimum number of steps
    
    Returns This Linear object
```

5.1. Calculations
class tc_python.step_or_map_diagrams.Logarithmic(scale_factor: float = 1.1)

Bases: tc_python.step_or_map_diagrams.AxisType

Represents a logarithmic axis.

Note: A logarithmic axis is useful for low fractions like in a gas phase where 1E-7 to 1E-2 might be an interesting range. For the pressure a logarithmic axis is often also useful.

get_type() → str
Convenience method for getting axis type.

Returns The type

set_scale_factor(scale_factor: float = 1.1)
Sets the scale factor.

Default: 1.1

Parameters scale_factor – The scale factor setting the maximum factor between two calculated values, must be larger than 1.0

Returns This Logarithmic object

class tc_python.step_or_map_diagrams.PhaseDiagramCalculation(calculator)

Bases: tc_python.step_or_map_diagrams.AbstractPhaseDiagramCalculation

Configuration for a phase diagram calculation.

Note: Specify the conditions, the calculation is performed with calculate().

add_initial_equilibrium(initial_equilibrium: tc_python.step_or_map_diagrams.InitialEquilibrium)
Add initial equilibrium start points from which a phase diagram is calculated.

Scans along the axis variables and generates start points when the scan procedure crosses a phase boundary.

It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the core remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria.

Parameters initial_equilibrium – The initial equilibrium

Returns This PhaseDiagramCalculation object

calculate(keep_previous_results: bool = False) → tc_python.step_or_map_diagrams.PhaseDiagramResult
Performs the phase diagram calculation.

Warning: If you use keep_previous_results=True, you must not use another calculator or even get results in between the calculations using calculate(). Then the previous results will actually be lost.

Parameters keep_previous_results – If True, results from any previous call to this method are appended. This can be used to combine calculations with multiple start points if the mapping fails at a certain condition.

Returns A new PhaseDiagramResult object which later can be used to get specific values from the calculated result.
disable_global_minimization()
Disables global minimization.

Default: Enabled

Returns This PhaseDiagramCalculation object
dont_keep_default_equilibria()
Do not keep the initial equilibria added by default.
This is only relevant in combination with add_initial_equilibrium().
This is the default behavior.

Returns This PhaseDiagramCalculation object
enable_global_minimization()
Enables global minimization.

Default: Enabled

Returns This PhaseDiagramCalculation object
get_components() \rightarrow \text{List}[\text{str}]
Returns the names of the components in the system (including all components auto-selected by the
database(s)).

Returns The component names
get_gibbs_energy_addition_for (phase: \text{str}) \rightarrow \text{float}
Used to get the additional energy term (always being a constant) of a given phase. The value given is added
to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface
tension, elastic energy, etc.
It is not composition-, temperature- or pressure-dependent.

Parameters phase – Specify the name of the (stoichiometric or solution) phase with the addition

Returns Gibbs energy addition to G per mole formula unit.
get_system_data() \rightarrow \text{tc_python.abstract_base.SystemData}
Returns the content of the database for the currently loaded system. This can be used to modify the param-
eters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data
keep_default_equilibria()
Keep the initial equilibria added by default. This is only relevant in combination with
add_initial_equilibrium().
Default behavior is to not keep default equilibria.

Returns This PhaseDiagramCalculation object
remove_all_conditions()
Removes all set conditions.

Returns This PhaseDiagramCalculation object
remove_all_initial_equilibria()
Removes all previously added initial equilibria.

Returns This PhaseDiagramCalculation object

remove_condition(quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str])
Removes the specified condition.

Parameters quantity – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example X(Cr))

Returns This ThermodynamicCalculation object

run_poly_command(command: str)
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

Parameters command – The Thermo-Calc Console Mode command

Returns This PhaseDiagramCalculation object

Note: It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

Warning: As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

set_condition(quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], value: float)
Sets the specified condition.

Parameters

• quantity – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example X(Cr))

• value – The value of the condition

Returns This PhaseDiagramCalculation object

set_gibbs_energy_addition_for(phase: str, gibbs_energy: float)
Used to specify the additional energy term (always being a constant) of a given phase. The value (gibbs_energy) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

Parameters

• phase – Specify the name of the (stoichiometric or solution) phase with the addition

• gibbs_energy – Addition to G per mole formula unit

Returns This PhaseDiagramCalculation object

set_phase_to_dormant(phase: str)
Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

Parameters phase – The phase name or ALL_PHASES for all phases

Returns This PhaseDiagramCalculation object
**set_phase_to_entered** *(phase: str, amount: float = 1.0)*

Sets the phase to the status ENTERED, that is the default state.

**Parameters**

- **phase** – The phase name or `ALL_PHASES` for all phases
- **amount** – The phase fraction (between 0.0 and 1.0)

**Returns** This `PhaseDiagramCalculation` object

**set_phase_to_fixed** *(phase: str, amount: float)*

Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

**Parameters**

- **phase** – The phase name
- **amount** – The fixed phase fraction (between 0.0 and 1.0)

**Returns** This `PhaseDiagramCalculation` object

**set_phase_to_suspended** *(phase: str)*

Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters** **phase** – The phase name or `ALL_PHASES` for all phases

**Returns** This `PhaseDiagramCalculation` object

**with_first_axis** *(axis: tc_python.step_or_map_diagrams.CalculationAxis)*

Sets the first calculation axis.

**Parameters** **axis** – The axis

**Returns** This `PhaseDiagramCalculation` object

**with_options** *(options: tc_python.step_or_map_diagrams.PhaseDiagramOptions)*

Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This `PhaseDiagramCalculation` object

**with_reference_state** *(component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)*

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.
Parameters

- **component** – The name of the element must be given.
- **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
- **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
- **pressure** – The Pressure (in Pa) for the reference state.

Returns This PhaseDiagramCalculation object

**with_second_axis** *(axis: tc_python.step_or_map_diagrams.CalculationAxis)*

Sets the second calculation axis.

Parameters **axis** – The axis

Returns This PhaseDiagramCalculation object

**with_system_modifications** *(system_modifications: tc_python.abstract_base.SystemModifications)*

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Note: This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb*-file.

Parameters **system_modifications** – The system modification to be performed

Returns This PhaseDiagramCalculation object

```python
class tc_python.step_or_map_diagrams.PhaseDiagramOptions
    Bases: object

    Simulation options for phase diagram calculations.

    disable_approximate_driving_force_for_metastable_phases()
        Disables the approximation of the driving force for metastable phases.
        Default: Enabled

        Note: When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

        If it is important that these driving forces are correct, use disable_approximate_driving_force_for_metastable_phases() to force the calculation to converge for the metastable phases.

        Returns This PhaseDiagramOptions object

    disable_control_step_size_during_minimization()
        Disables stepsize control during minimization (non-global).
        Default: Enabled

        Returns This PhaseDiagramOptions object
```

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disable_force_positive_definite_phase_hessian()

Disables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

**Default:** Enabled

**Returns** This `PhaseDiagramOptions` object

dont_use_auto_start_points()

Switches the usage of automatic starting points for the mapping off.

**Default:** Switched on

**Returns** This `PhaseDiagramOptions` object

dont_use_inside_mesh_points()

Switches the usage of inside meshing points for the mapping off.

**Default:** Switched off

**Returns** This `PhaseDiagramOptions` object

enable_approximate_driving_force_for_metastable_phases()

Enables the approximation of the driving force for metastable phases.

**Default:** Enabled

**Note:** When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, use `disable_approximate_driving_force_for_metastable_phases()` to force the calculation to converge for the metastable phases.

**Returns** This `PhaseDiagramOptions` object

enable_control_step_size_during_minimization()

Enables stepsize control during normal minimization (non-global).

**Default:** Enabled

**Returns** This `PhaseDiagramOptions` object

enable_force_positive_definite_phase_hessian()

Enables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

**Default:** Enabled

**Returns** This `PhaseDiagramOptions` object

set_global_minimization_max_grid_points(max_grid_points: int = 2000)

Sets the maximum number of grid points in global minimization. ** Only applicable if global minimization is actually used**.

**Default:** 2000 points

**Parameters** `max_grid_points` – The maximum number of grid points

**Returns** This `PhaseDiagramOptions` object
**set_global_minimization_test_interval** *(global_test_interval: int = 0)*

Sets the interval for the global test.

Default: 0

Parameters **global_test_interval** – The global test interval

Returns This `PhaseDiagramOptions` object

**set_max_no_of_iterations** *(max_no_of_iterations: int = 500)*

Set the maximum number of iterations.

Default: max. 500 iterations

Note: As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Parameters **max_no_of_iterations** – The max. number of iterations

Returns This `PhaseDiagramOptions` object

**set_no_of_mesh_along_axis** *(no_of_mesh_along_axis: int = 3)*

Sets the number of meshes along an axis for the mapping.

Default: 3

Parameters **no_of_mesh_along_axis** – The number of meshes

Returns This `PhaseDiagramOptions` object

**set_required_accuracy** *(accuracy: float = 1e-06)*

Sets the required relative accuracy.

Default: 1.0E-6

Note: This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Parameters **accuracy** – The required relative accuracy

Returns This `PhaseDiagramOptions` object

**set_smallest_fraction** *(smallest_fraction: float = 1e-12)*

Sets the smallest fraction for constituents that are unstable.

It is normally only in the gas phase that you can find such low fractions.

The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.

Parameters **smallest_fraction** – The smallest fraction for constituents that are unstable

Returns This `PhaseDiagramOptions` object
use_auto_start_points()
Switches the usage of automatic starting points for the mapping on.
Default: Switched on
Returns This PhaseDiagramOptions object

use_inside_mesh_points()
Switches the usage of inside meshing points for the mapping off.
Default: Switched off
Returns This PhaseDiagramOptions object

class tc_python.step_or_map_diagrams.PhaseDiagramResult(result)
Bases: tc_python.abstract_base.AbstractResult
Result of a phase diagram calculation, it can be evaluated using quantities or Console Mode syntax.

add_coordinate_for_phase_label (x: float, y: float)
Sets a coordinate in the result plot for which the stable phases will be evaluated and provided in the result data object. This can be used to plot the phases of a region into the phase diagram or just to programmatically evaluate the phases in certain regions.

Warning: This method takes coordinates of the plot axes and not of the calculation axis.

Parameters

• x – The coordinate of the first plot axis (“x-axis”) [unit of the plot axis]
• y – The coordinate of the second plot axis (“y-axis”) [unit of the plot axis]

Returns This PhaseDiagramResult object

get_values_grouped_by_quantity_of (x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) → tc_python.step_or_map_diagrams.PhaseDiagramResultValues

Returns x-y-line data grouped by the multiple datasets of the specified quantities (for example in dependency of components). The available quantities can be found in the documentation of the factory class ThermodynamicQuantity. Usually the result data represents the phase diagram.

Note: The different datasets will contain NaN-values between different subsections and are not sorted (because they are unsortable due to their nature).

Note: Its possible to use functions as axis variables, either by using ThermodynamicQuantity.user_defined_function, or by using an expression that contains ‘=’.

Example get_values_grouped_by_quantity_of(T, ThermodynamicQuantity.user_defined_function('HM.T'))

Example get_values_grouped_by_quantity_of(T, 'CP=HM.T')

Parameters

• x_quantity – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), or even a function (for example ‘f=T*1.01’)

5.1. Calculations
• **y_quantity** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), or even a function (for example ‘CP=HM.T’)

**Returns** The phase diagram data

```
get_values_grouped_by_stable_phases_of(x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) → tc_python.step_or_map_diagrams.PhaseDiagramResultValues
```

Returns x-y-line data grouped by the sets of “stable phases” (for example “LIQUID” or “LIQUID + FCC_A1”). The available quantities can be found in the documentation of the factory class ThermodynamicQuantity. Usually the result data represents the phase diagram.

**Note:** The different datasets will contain NaN-values between different subsections and are not sorted (because they are unsortable due to their nature).

**Note:** It’s possible to use functions as axis variables, either by using ThermodynamicQuantity.user_defined_function, or by using an expression that contains ‘=’.

**Example**
```
get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))
```

**Example**
```
get_values_grouped_by_quantity_of('T', 'CP=HM.T')
```

**Parameters**

• **x_quantity** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), or even a function (for example ‘f=T*1.01’)

• **y_quantity** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), or even a function (for example ‘CP=HM.T’)

**Returns** The phase diagram data

**remove_phase_labels()**
Erases all added coordinates for phase labels.

**Returns** This PhaseDiagramResult object

**save_to_disk(path: str)**
Saves the result to disc. Note that a result is a folder, containing potentially many files. The result can later be loaded with load_result_from_disk()

**Parameters**

• **path** – the path to the folder you want the result to be saved in. It can be relative or absolute.

**Returns** this PhaseDiagramResult object

**set_phase_name_style(phase_name_style_enum: tc_python.step_or_map_diagrams.PhaseNameStyle = <PhaseNameStyle.NONE: 0>)**
Sets the style of the phase name labels that will be used in the result data object (constitution description, ordering description, ...).

**Default:** PhaseNameStyle.NONE

**Parameters**

• **phase_name_style_enum** – The phase name style

**Returns** This PhaseDiagramResult object
class tc_python.step_or_map_diagrams.PhaseDiagramResultValues(phase_diagram_values_java)
    Bases: object
    Represents the data of a phase diagram.

    get_invariants() → tc_python.utils.ResultSetValueGroup
    Returns the x- and y-datasets of all invariants in the phase diagram.

    Note: The datasets will normally contain different sections separated by NaN-values.

    Returns  The invariants dataset object

get_lines() → Dict[str, tc_python.utils.ResultSetValueGroup]
    Returns the x- and y-datasets of all phase boundaries in the phase diagram.

    Note: The datasets will normally contain different sections separated by NaN-values.

    Returns  Containing the phase boundary datasets with the quantities or stable phases as keys
              (depending on the used method to get the values)

get_phase_labels() → List[tc_python.step_or_map_diagrams.PhaseLabel]
    Returns the phase labels added for certain coordinates using PhaseDiagramResult.
    add_coordinate_for_phase_label().

    Returns  The list with the phase label data (that contains plot coordinates and stable phases)

get_tie_lines() → tc_python.utils.ResultSetValueGroup
    Returns the x- and y-datasets of all tie-lines in the phase diagram.

    Note: The datasets will normally contain different sections separated by NaN-values.

    Returns  The tie-line dataset object

class tc_python.step_or_map_diagrams.PhaseLabel(phase_label_java)
    Bases: object
    Represents a phase label at a plot coordinate, i.e. the stable phases that are present at that plot coordinate.

    get_text() → str
        Accessor for the phase label :return: the phase label

    get_x() → List[float]
        Accessor for the x-value :return: the x value

    get_y() → List[float]
        Accessor for the y-value :return: the y value

class tc_python.step_or_map_diagrams.PhaseNameStyle(value)
    Bases: enum.Enum
    The style of the phase names used in the labels.

    ALL = 1
        Adding ordering and constitution description.
CONSTITUTION_DESCRIPTION = 3
Adding only constitution description.

NONE = 0
Only the phase names.

ORDERING_DESCRIPTION = 4
Adding only ordering description.

class tc_python.step_or_map_diagrams.PropertyDiagramCalculation (calculator)
Bases: tc_python.step_or_map_diagrams.AbstractPropertyDiagramCalculation

calculate (keep_previous_results: bool = False) \rightarrow tc_python.step_or_map_diagrams.PropertyDiagramResult
Performs the property diagram calculation.

**Warning:** If you use `keep_previous_results=True`, you must not use another calculator or even get results in between the calculations using `calculate()`. Then the previous results will actually be lost.

Parameters **keep_previous_results** – If `True`, results from any previous call to this method are appended. This can be used to combine calculations with multiple start points if the stepping fails at a certain condition.

Returns A new `PropertyDiagramResult` object which later can be used to get specific values from the calculated result

disable_global_minimization ()
Disables global minimization.

Default: Enabled

Returns This `PropertyDiagramCalculation` object

disable_step_separate_phases ()
Disables `step separate phases`. This is the default setting.

Returns This `PropertyDiagramCalculation` object

enable_global_minimization ()
Enables global minimization.

Default: Enabled

Returns This `PropertyDiagramCalculation` object

enable_step_separate_phases ()
Enables `step separate phases`.

Default: By default separate phase stepping is disabled

**Note:** This is an advanced option, it is used mostly to calculate how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIGMA-phase, G-phase, MU-phase, etc.).

Returns This `PropertyDiagramCalculation` object
get_components() \rightarrow \text{List}[\text{str}]
Returns the names of the components in the system (including all components auto-selected by the database(s)).

Returns The component names

get_gibbs_energy_addition_for(phase: \text{str}) \rightarrow \text{float}
Used to get the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.
It is not composition-, temperature- or pressure-dependent.

Parameters phase – Specify the name of the (stoichiometric or solution) phase with the addition

Returns Gibbs energy addition to G per mole formula unit.

get_system_data() \rightarrow \text{tc_python.abstract_base.SystemData}
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

remove_all_conditions()
Removes all set conditions.

Returns This \text{PropertyDiagramCalculation} object

remove_condition(quantity: \text{Union[tc_python.quantity_factory.ThermodynamicQuantity, str]})
Removes the specified condition.

Parameters quantity – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example $X(Cr)$)

Returns This \text{PropertyDiagramCalculation} object

run_poly_command(command: \text{str})
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

Parameters command – The Thermo-Calc Console Mode command

Returns This \text{PropertyDiagramCalculation} object

Note: It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

Warning: As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

set_condition(quantity: \text{Union[tc_python.quantity_factory.ThermodynamicQuantity, str]}, value: \text{float})
Sets the specified condition.

Parameters
• **quantity** – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example $X(Cr)$)

• **value** – The value of the condition

**Returns**
This `PropertyDiagramCalculation` object

**set_gibbs_energy_addition_for**(phase: `str`, gibbs_energy: `float`)

Used to specify the additional energy term (always being a constant) of a given phase. The value (gibbs_energy) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

**Parameters**

• **phase** – Specify the name of the (stoichiometric or solution) phase with the addition

• **gibbs_energy** – Addition to $G$ per mole formula unit

**Returns**
This `PropertyDiagramCalculation` object

**set_phase_to_dormant**(phase: `str`)

Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

**Parameters**

• **phase** – The phase name or `ALL_PHASES` for all phases

**Returns**
This `PropertyDiagramCalculation` object

**set_phase_to_entered**(phase: `str`, amount: `float = 1.0`)

Sets the phase to the status ENTERED, that is the default state.

**Parameters**

• **phase** – The phase name or `ALL_PHASES` for all phases

• **amount** – The phase fraction (between 0.0 and 1.0)

**Returns**
This `PropertyDiagramCalculation` object

**set_phase_to_fixed**(phase: `str`, amount: `float`)

Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

**Parameters**

• **phase** – The phase name

• **amount** – The fixed phase fraction (between 0.0 and 1.0)

**Returns**
This `PropertyDiagramCalculation` object

**set_phase_to_suspended**(phase: `str`)

Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters**

• **phase** – The phase name or `ALL_PHASES` for all phases

**Returns**
This `PropertyDiagramCalculation` object

**with_axis**(axis: `tc_python.step_or_map_diagrams.CalculationAxis`)

Sets the calculation axis.

**Parameters**

• **axis** – The axis

**Returns**
This `PropertyDiagramCalculation` object
with_options(options: tc_python.step_or_map_diagrams.PropertyDiagramOptions)
    "Sets the simulation options."

    Parameters options -- The simulation options

    Returns This PropertyDiagramCalculation object

with_reference_state(component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)
    "The reference state for a component is important when calculating activities, chemical potentials and
    enthalpies and is determined by the database being used. For each component the data must be referred to
    a selected phase, temperature and pressure, i.e. the reference state.

    All data in all phases where this component dissolves must use the same reference state. However, different
    databases can use different reference states for the same element/component. It is important to be careful
    when combining data obtained from different databases.

    By default, activities, chemical potentials and so forth are computed relative to the reference state used by
    the database. If the reference state in the database is not suitable for your purposes, use this command to
    set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set
    as default for a major component in alloys dominated by the component). In such cases, the temperature
    and pressure for the reference state is not needed.

    For a phase to be usable as a reference for a component, the component needs to have the same composition
    as an end member of the phase. The reference state is an end member of a phase. The selection of the end
    member associated with the reference state is only performed once this command is executed.

    If a component has the same composition as several end members of the chosen reference phase, then the
    end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

    Parameters

    • component -- The name of the element must be given.

    • phase -- Name of a phase used as the new reference state. Or SER for the Stable Element Reference.

    • temperature -- The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.

    • pressure -- The Pressure (in Pa) for the reference state.

    Returns This PropertyDiagramCalculation object

with_system_modifications(system_modifications: tc_python.abstract_base.SystemModifications)
    "Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions)."

    Note: This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb-file.

    Parameters system_modifications -- The system modification to be performed

    Returns This PropertyDiagramCalculation object

class tc_python.step_or_map_diagrams.PropertyDiagramOptions
    Bases: object

    Simulation options for the property diagram calculations.

5.1. Calculations
disable_approximate_driving_force_for_metastable_phases()
Disables the approximation of the driving force for metastable phases.

**Default:** Enabled

**Note:** When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, use `disable_approximate_driving_force_for_metastable_phases()` to force the calculation to converge for the metastable phases.

**Returns** This `PropertyDiagramOptions` object

disable_control_step_size_during_minimization()
Disables stepsize control during minimization (non-global).

**Default:** Enabled

**Returns** This `PropertyDiagramOptions` object

disable_force_positive_definite_phase_hessian()
Disables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

**Default:** Enabled

**Returns** This `PropertyDiagramOptions` object

enable_approximate_driving_force_for_metastable_phases()
Enables the approximation of the driving force for metastable phases.

**Default:** Enabled

**Note:** When enabled, the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, use `disable_approximate_driving_force_for_metastable_phases()` to force the calculation to converge for the metastable phases.

**Returns** This `PropertyDiagramOptions` object

enable_control_step_size_during_minimization()
Enables stepsize control during normal minimization (non-global).

**Default:** Enabled

**Returns** This `PropertyDiagramOptions` object

enable_force_positive_definite_phase_hessian()
Enables forcing of positive definite phase Hessian. This determines how the minimum of an equilibrium state in a normal minimization procedure (non-global) is reached. For details, search the Thermo-Calc documentation for “Hessian minimization”.

**Default:** Enabled
Returns This \texttt{PropertyDiagramOptions} object

\texttt{set\_global\_minimization\_max\_grid\_points} \hspace{1em} (max\_grid\_points: \texttt{int} = 2000)

Sets the maximum number of grid points in global minimization. \textit{Only applicable if global minimization is actually used.}

Default: 2000 points

Parameters \texttt{max\_grid\_points} – The maximum number of grid points

Returns This \texttt{PropertyDiagramOptions} object

\texttt{set\_global\_minimization\_test\_interval} \hspace{1em} (global\_test\_interval: \texttt{int} = 0)

Sets the interval for the global test.

Default: 0

Parameters \texttt{global\_test\_interval} – The global test interval

Returns This \texttt{PropertyDiagramOptions} object

\texttt{set\_max\_no\_of\_iterations} \hspace{1em} (max\_no\_of\_iterations: \texttt{int} = 500)

Set the maximum number of iterations.

Default: max. 500 iterations

\underline{Note:} As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Parameters \texttt{max\_no\_of\_iterations} – The max. number of iterations

Returns This \texttt{PropertyDiagramOptions} object

\texttt{set\_required\_accuracy} \hspace{1em} (accuracy: \texttt{float} = 1e-06)

Sets the required relative accuracy.

Default: 1.0E-6

\underline{Note:} This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Parameters \texttt{accuracy} – The required relative accuracy

Returns This \texttt{PropertyDiagramOptions} object

\texttt{set\_smallest\_fraction} \hspace{1em} (smallest\_fraction: \texttt{float} = 1e-12)

Sets the smallest fraction for constituents that are unstable.

It is normally only in the gas phase that you can find such low fractions.

The \texttt{default value} for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.

Parameters \texttt{smallest\_fraction} – The smallest fraction for constituents that are unstable

Returns This \texttt{PropertyDiagramOptions} object
class tc_python.step_or_map_diagrams.PropertyDiagramResult (result)
Bases: tc_python.abstract_base.AbstractResult

Result of a property diagram. This can be used to query for specific values.

get_values_grouped_by_quantity_of (x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], sort_and_merge: bool = True) → Dict[str, tc_python.utils.ResultValueGroup]

Returns x-y-line data grouped by the multiple datasets of the specified quantities (typically the phases). The available quantities can be found in the documentation of the factory class ThermodynamicQuantity.

Note: The different datasets might contain NaN-values between different subsections and might not be sorted even if the flag `sort_and_merge` has been set (because they might be unsortable due to their nature).

Note: It is possible to use functions as axis variables, either by using ThermodynamicQuantity.user_defined_function, or by using an expression that contains ‘=’.

Example get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))

Example get_values_grouped_by_quantity_of('T', 'CP=HM.T')

Parameters

• x_quantity – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), or even a function (for example ‘f=T*1.01’)

• y_quantity – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), or even a function (for example ‘CP=HM.T’)

• sort_and_merge – If True, the data is sorted and merged into as few subsections as possible (divided by NaN)

Returns Containing the datasets with the quantities as their keys

get_values_grouped_by_stable_phases_of (x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], sort_and_merge: bool = True) → Dict[str, tc_python.utils.ResultValueGroup]

Returns x-y-line data grouped by the sets of “stable phases” (for example “LIQUID” or “LIQUID + FCC_A1”). The available quantities can be found in the documentation of the factory class ThermodynamicQuantity.

Note: The different datasets might contain NaN-values between different subsections and different lines of an ambiguous dataset. They might not be sorted even if the flag `sort_and_merge` has been set (because they might be unsortable due to their nature).

Note: It is possible to use functions as axis variables, either by using ThermodynamicQuantity.user_defined_function, or by using an expression that contains ‘=’.
**Example**  
`get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))`

**Example**  
`get_values_grouped_by_quantity_of('T', 'CP=HM.T')`

**Parameters**

- **x_quantity** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), or even a function (for example ‘f=T*1.01’)

- **y_quantity** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), or even a function (for example ‘CP=HM.T’)

- **sort_and_merge** – If True, the data will be sorted and merged into as few subsections as possible (divided by NaN)

**Returns**  
Containing the datasets with the quantities as their keys

**get_values_of**

```python
get_values_of(x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str],
              y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) →  
[typing.List[float], typing.List[float]]
```

Returns sorted x-y-line data without any separation. Use `get_values_grouped_by_quantity_of()` or `get_values_grouped_by_stable_phases_of()` instead if you need such a separation. The available quantities can be found in the documentation of the factory class `ThermodynamicQuantity`.

**Note:** This method will always return sorted data without any NaN-values. If it is unsortable that might give data that is hard to interpret. In such a case you need to choose the quantity in another way or use one of the other methods. One example of this is to use quantities with All-markers, for example `MassFractionOfAComponent("All")`.

**Note:**  
It’s possible to use functions as axis variables, either by using `ThermodynamicQuantity.user_defined_function`, or by using an expression that contains ‘=’.

**Example**  
`get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))`

**Example**  
`get_values_grouped_by_quantity_of('T', 'CP=HM.T')`

**Parameters**

- **x_quantity** – The first Thermodynamic quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’) or even a function (for example ‘f=T*1.01’)

- **y_quantity** – The second Thermodynamic quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), or even a function (for example ‘CP=HM.T’)

**Returns**  
A tuple containing the x- and y-data in lists

**save_to_disk**(path: str)

Saves the result to disc. Note that a result is a folder, containing potentially many files. The result can later be loaded with `load_result_from_disk()`

**Parameters**

- **path** – the path to the folder you want the result to be saved in. It can be relative or absolute.

5.1. Calculations
Returns this `PropertyDiagramResult` object

```python
set_phase_name_style(phrase_name_style_enum: tc_python.step_or_map_diagrams.PhaseNameStyle = <PhaseNameStyle.NONE: 0>)
```

Sets the style of the phase name labels that will be used in the result data object (constitution description, ordering description, ...).

**Default:** PhaseNameStyle.NONE

**Parameters**

- `phrase_name_style_enum` – The phase name style

**Returns** This `PropertyDiagramResult` object

### 5.1.6 Module “diffusion”

**class** `tc_python.diffusion.AbstractBoundaryCondition`

**Bases:** object

The abstract base class for all boundary conditions.

**class** `tc_python.diffusion.AbstractCalculatedGrid`

**Bases:** `tc_python.diffusion.AbstractGrid`

The abstract base class for calculated grids.

**class** `tc_python.diffusion.AbstractElementProfile`

**Bases:** object

The abstract base class for all initial composition profile types.

**class** `tc_python.diffusion.AbstractGrid`

**Bases:** object

The abstract base class for all grids.

**class** `tc_python.diffusion.AbstractSolver`

**Bases:** object

Abstract base class for the solvers (Classic, Homogenization and Automatic).

**class** `tc_python.diffusion.ActivityFluxFunction`

**Bases:** `tc_python.diffusion.BoundaryCondition`

**get_type** () → str

The type of the boundary condition.

**Returns** The type

```python
set_flux_function(element_name: str, f: str = '0', g: str = '1', n: float = 1.0, to_time: float = 1.7976931348623157e+308)
```

The flux for the independent components must be given in the format:

\[ J = f(T,P,TIME) \times (ACTIVITY^N - g(T,P,TIME)) \]

where f and g may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer.

f and g must be expressed in DICTRA Console Mode syntax.

**Parameters**

- `element_name` – The name of the element
- `f` – the function f in the formula above
- `g` – the function g in the formula above
- n – the constant N in the formula above
- to_time – The max-time for which the flux function is used.

```python
class tc_python.diffusion.AutomaticSolver
    Bases: tc_python.diffusion.Solver

    Solver using the homogenization model if any region has more than one phase, otherwise using the classic model.
```

**Note:** This is the default solver and recommended for most applications.

```python
def get_type() -> str:
    return 'AutomaticSolver'
```

```python
def set_flux_balance_equation_accuracy(accuracy: float = 1e-16):
    Sets the required accuracy during the solution of the flux balance equations. Default: 1.0e-16

    Parameters
    ----------
    accuracy : float
        The required accuracy

    Returns
    -------
    A new AutomaticSolver object
```

```python
def set_tieline_search_variable_to_activity() -> str:
    Configures the solver to use the activity of a component to find the correct tie-line at the phase interface. Either activity or chemical potential are applied to reduce the degrees of freedom at the local equilibrium. Default: This is the default setting

    Returns
    -------
    A new AutomaticSolver object
```

```python
def set_tieline_search_variable_to_potential() -> str:
    Configures the solver to use the chemical potential of a component to find the correct tie-line at the phase interface. Either activity or chemical potential are applied to reduce the degrees of freedom at the local equilibrium. Default: To use the activity

    Returns
    -------
    A new AutomaticSolver object
```

```python
class tc_python.diffusion.BoundaryCondition
    Bases: tc_python.diffusion.AbstractBoundaryCondition

    Contains factory methods for the different boundary conditions available.
```

```python
def activity_flux_function() -> str:
    Factory method that creates a new activity-flux-function boundary condition.

    This type of boundary condition is used to take into account the finite rate of a surface reaction.
    The flux for the independent components must be given in the format:
    \[ J = f(T,P,TIME) * (ACTIVITY^N - g(T,P,TIME)) \]
    where f and g may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer.
    f and g must be expressed in DICTRA Console Mode syntax.
```

5.1. Calculations
Note: The activities are those with user-defined reference states. The function mass transfer coefficient is the mass transfer coefficient, activity of the corresponding species in the gas is the activity of the corresponding species in the gas and N is a stoichiometric coefficient.


Returns A new ActivityFluxFunction object

classmethod closed_system()  
Factory method that creates a new closed-system boundary condition.

Returns A new ClosedSystem object

classmethod fix_flux_value()  
Factory method that creates a new fix-flux-value boundary condition.

This type of boundary condition makes it possible to enter functions that yield the flux times the molar volume for the independent components. May be a function of time, temperature and pressure: \( J(T,P,TIME) \).

Returns A new FixFluxValue object

classmethod fixed_compositions(unit_enum: tc_python.diffusion.Unit = <Unit.MASS_PERCENT: 3>)  
Factory method that creates a new fixed-composition boundary condition.

Parameters unit_enum – The composition unit

Returns A new FixedCompositions object

classmethod mixed_zero_flux_and_activity()  
Factory method that creates a new mixed zero-flux and activity boundary condition

Returns A new MixedZero FluxAndActivity object

class tc_python.diffusion.CalculatedGrid  
Bases: tc_python.diffusion.AbstractCalculatedGrid

Factory class for grids generated by a mathematical series (linear, geometric, ...). Use tc_python.diffusion.PointByPointGrid instead if you want to use an existing grid from experimental data or a previous calculation.

Note: A region must contain a number of grid points. The composition is only known at these grid points and the software assumes that the composition varies linearly between them. The amount and composition of all the phases present at a single grid point in a certain region are those given by thermodynamic equilibrium keeping the over-all composition at the grid point fixed.

classmethod double_geometric(no_of_points: int = 50, lower_geometrical_factor: float = 1.1, upper_geometrical_factor: float = 0.9)  
Factory method that creates a new double geometric grid.

Note: Double geometric grids have a high number of grid points in the middle or at both ends of a region. One geometrical factor for the lower (left) and upper (right) half of the region need to specified. In both
cases a geometrical factor of larger than one yields a higher density of grid points at the lower end of the half and vice versa for a factor smaller than one.

Parameters
- **no_of_points** – The number of points
- **lower_geometrical_factor** – The geometrical factor for the left half
- **upper_geometrical_factor** – The geometrical factor for the right half

Returns A new `DoubleGeometricGrid` object

```python
classmethod geometric(no_of_points: int = 50, geometrical_factor: float = 1.1)
```
Factory method that creates a new geometric grid.

Note: A grid that yields a varying density of grid points in the region. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.

Parameters
- **no_of_points** – The number of points
- **geometrical_factor** – The geometrical factor

Returns A new `GeometricGrid` object

```python
classmethod linear(no_of_points: int = 50)
```
Factory method that creates a new equally spaced grid.

Parameters **no_of_points** – The number of points

Returns A new `LinearGrid` object

```python
class tc_python.diffusion.ClassicSolver
Bases: tc_python.diffusion.Solver
```
Solver using the Classic model.

Note: This solver never switches to the homogenization model even if it fails to converge. Use the `tc_python.diffusion.AutomaticSolver` if necessary instead.

```python
def get_type() -> str
    Convenience method for getting the type of the solver.
```

Returns The type of the solver

```python
def set_flux_balance_equation_accuracy(accuracy: float = 1e-16)
```
Sets the required accuracy during the solution of the flux balance equations. Default: 1.0e-16

Parameters **accuracy** – The required accuracy

Returns A new `ClassicSolver` object

```python
def set_tieline_search_variable_to_activity()
```
Configures the solver to use the activity of a component to find the correct tie-line at the phase interface.

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Either activity or chemical potential are applied to reduce the degrees of freedom at the local equilibrium. 

**Default**: This is the default setting

```python
set_tieline_search_variable_to_potential()
```

Configures the solver to use the chemical potential of a component to find the correct tie-line at the phase interface. Either activity or chemical potential are applied to reduce the degrees of freedom at the local equilibrium. **Default**: To use the activity

**Returns**: A new `ClassicSolver` object

```python
class tc_python.diffusion.ClosedSystem
    Bases: tc_python.diffusion.BoundaryCondition
```

Represents a boundary for a closed system.

```python
get_type() ➞ str
```

Convenience method for getting the type of the boundary condition.

**Returns**: The type of the boundary condition

```python
class tc_python.diffusion.CompositionProfile
    Bases: object
```

Contains initial concentration profiles for the elements.

```python
add(element_name: str, profile: tc_python.diffusion.ElementProfile)
```

Adds a concentration profile for the specified element.

**Parameters**

- `element_name` – The name of the element
- `profile` – The initial concentration profile

**Returns**: A `CompositionProfile` object

```python
class tc_python.diffusion.ConstantProfile
    Bases: tc_python.diffusion.ElementProfile
```

Represents a constant initial concentration profile.

```python
get_type() ➞ str
```

The type of the element profile.

**Returns**: The type

```python
class tc_python.diffusion.ContinuedDiffusionCalculation
    Bases: tc_python.abstract_base.AbstractCalculation
```

Configuration for a diffusion calculation that is a continuation of a previous isothermal or non-isothermal diffusion calculation. It contains a subset of the settings possible in the original calculation.

Use `set_simulation_time()` to set a simulation time that is higher than the original calculation.

```python
calculate() ➞ tc_python.diffusion.DiffusionCalculationResult
```

Runs the diffusion calculation.

**Returns**: A `DiffusionCalculationResult` which later can be used to get specific values from the calculated result

```python
set_simulation_time(simulation_time: float)
```

Sets the simulation time.

**Parameters**: `simulation_time` – The simulation time [s]

**Returns**: This `DiffusionIsoThermalCalculation` object
**with_left_boundary_condition** *(boundary_condition: tc_python.diffusion.BoundaryCondition, to: float = 1.7976931348623157e+308)*

Defines the boundary condition on the left edge of the system.

**Default:** A closed-system boundary condition.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

---

**Note:** You can specify time-dependent boundary conditions by calling `with_left_boundary_condition()` many times, with different values of the “to” parameter.

Examples:

- `with_left_boundary_condition(BoundaryCondition.closed_system(), to=100)`
- `with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)`
- `with_left_boundary_condition(BoundaryCondition.closed_system())`

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

**Parameters**

- `boundary_condition` – The boundary condition
- `to` – The upper time-limit for `boundary_condition`.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_options** *(options: tc_python.diffusion.Options, to: float = 1.7976931348623157e+308)*

Sets the general simulation conditions.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

**Parameters**

- `options` – The general simulation conditions
- `to` – The upper time-limit for `options`.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_right_boundary_condition** *(boundary_condition: tc_python.diffusion.BoundaryCondition, to: float = 1.7976931348623157e+308)*

Defines the boundary condition on the right edge of the system.

**Default:** A closed-system boundary condition

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

---

**Note:** You can specify time-dependent boundary conditions by calling `with_right_boundary_condition()` many times, with different values of the “to” parameter.
Examples:

• `with_right_boundary_condition(BoundaryCondition.closed_system(), to=100)`
• `with_right_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)`
• `with_right_boundary_condition(BoundaryCondition.closed_system())`

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

**Parameters**

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_solver** *(solver: tc_python.diffusion.Solver, to: float = 1.7976931348623157e+308)*

Sets the solver to use (Classic, Homogenization or Automatic). **Default is Automatic.**

**Default:** The end of the simulation.

**Parameters**

- **solver** – The solver to use
- **to** – The upper time-limit for solver.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_timestep_control** *(timestep_control: tc_python.diffusion.TimestepControl, to: float = 1.7976931348623157e+308)*

Sets the timestep control options.

**Default:** The end of the simulation.

**Parameters**

- **timestep_control** – The new timestep control options
- **to** – The upper time-limit for timestep_control.

**Returns** This `DiffusionIsoThermalCalculation` object

**class** `tc_python.diffusion.DiffusionCalculationResult` *(result)*

**Bases:** `tc_python.abstract_base.AbstractResult`

Result of a diffusion calculation. This can be used to query for specific values. For details of the axis variables, search the Thermo-Calc help.

**get_mass_fraction_at_lower_interface** *(region: str, component: str) → [typing.List[float], typing.List[float]]*

Returns the mass fraction of the specified component at the lower boundary of the specified region, in dependency of time.

**Parameters**

- **region** – The name of the region
- **component** – The name of the component
Returns A tuple of two lists of floats (time [s], mass fraction of the specified component)

\texttt{get\_mass\_fraction\_at\_upper\_interface (region: str, component: str) \rightarrow [typing.List[float], typing.List[float]]}

Returns the mass fraction of the specified component at the upper boundary of the specified region, in dependency of time.

Parameters

- **region** – The name of the region
- **component** – The name of the component

Returns A tuple of two lists of floats (time [s], mass fraction of the specified component)

\texttt{get\_mass\_fraction\_of\_component\_at\_time (component: str, time: Union[tc\_python\_diffusion\_SimulationTime, float]) \rightarrow [typing.List[float], typing.List[float]]}

Returns the mass fraction of the specified component at the specified time.

Note: Use the enum \texttt{tc\_python\_diffusion\_SimulationTime} to choose the first or the last timepoint of the simulation. A timepoint close to the last one should never be specified manually because the actual end of the simulation can slightly deviate.

Parameters

- **component** – The name of the component
- **time** – The time [s]

Returns A tuple of two lists of floats (distance [m], mass fraction of component at the specified time)

\texttt{get\_mass\_fraction\_of\_phase\_at\_time (phase: str, time: Union[tc\_python\_diffusion\_SimulationTime, float]) \rightarrow [typing.List[float], typing.List[float]]}

Returns the mass fraction of the specified phase.

Note: Use the enum \texttt{tc\_python\_diffusion\_SimulationTime} to choose the first or the last timepoint of the simulation. A timepoint close to the last one should never be specified manually because the actual end of the simulation can slightly deviate.

Parameters

- **phase** – The name of the phase
- **time** – The time [s]

Returns A tuple of two lists of floats (distance [m], mass fraction of the phase at the specified time)

\texttt{get\_mole\_fraction\_at\_lower\_interface (region: str, component: str) \rightarrow [typing.List[float], typing.List[float]]}

Returns the mole fraction of the specified component at the lower boundary of the specified region, in dependency of time.

Parameters
• **region** – The name of the region

• **component** – The name of the component

**Returns** A tuple of two lists of floats (time [s], mole fraction of the specified component)

```python
def get_mole_fraction_at_upper_interface(region: str, component: str) -> [typing.List[float], typing.List[float]]
```

Returns the mole fraction of the specified component at the upper boundary of the specified region, in dependency of time.

**Parameters**

• **region** – The name of the region

• **component** – The name of the component

**Returns** A tuple of two lists of floats (time [s], mole fraction of the specified component)

```python
def get_mole_fraction_of_component_at_time(component: str, time: Union[tc_python.diffusion.SimulationTime, float]) -> [typing.List[float], typing.List[float]]
```

Returns the mole fraction of the specified component at the specified time.

**Note:** Use the enum `tc_python.diffusion.SimulationTime` to choose the first or the last timepoint of the simulation. A timepoint close to the last one should never be specified manually because the actual end of the simulation can slightly deviate.

**Parameters**

• **component** – The name of the component

• **time** – The time [s]

**Returns** A tuple of two lists of floats (distance [m], mole fraction of component at the specified time)

```python
def get_mole_fraction_of_phase_at_time(phase: str, time: Union[tc_python.diffusion.SimulationTime, float]) -> [typing.List[float], typing.List[float]]
```

Returns the mole fraction of the specified phase.

**Note:** Use the enum `tc_python.diffusion.SimulationTime` to choose the first or the last timepoint of the simulation. A timepoint close to the last one should never be specified manually because the actual end of the simulation can slightly deviate.

**Parameters**

• **phase** – The name of the phase

• **time** – The time [s]

**Returns** A tuple of two lists of floats (distance [m], mole fraction of the phase at the specified time)

```python
def get_position_of_lower_boundary_of_region(region: str) -> [typing.List[float], typing.List[float]]
```

Returns the position of the lower boundary of the specified region in dependency of time.
Parameters `region` – The name of the region

Returns A tuple of two lists of floats (time [s], position of lower boundary of region [m])

```python
def get_position_of_upper_boundary_of_region(region: str) -> [typing.List[float], typing.List[float]]
```

Returns the position of the upper boundary of the specified region in dependency of time.

Parameters `region` – The name of the region

Returns A tuple of two lists of floats (time [s], position of upper boundary of region [m])

```python
def get_regions() -> List[str]
```

Returns the regions of the diffusion simulation.

Note: Automatically generated regions (R_###) are included in the list.

Returns The region names

```python
def get_time_steps() -> List[float]
```

Returns the timesteps of the diffusion simulation.

Returns The timesteps [s]

```python
def get_total_mass_fraction_of_component(component: str) -> [typing.List[float], typing.List[float]]
```

Returns the total mass fraction of the specified component in dependency of time.

Parameters `component` – The name of the component

Returns A tuple of two lists of floats (time [s], total mass fraction of the component)

```python
def get_total_mass_fraction_of_component_in_phase(component: str, phase: str) -> [typing.List[float], typing.List[float]]
```

Returns the total mass fraction of the specified component in the specified phase in dependency of time.

Parameters

- `component` – The name of the component
- `phase` – The name of the phase

Returns A tuple of two lists of floats (time [s], total mass fraction of the component in the phase)

```python
def get_total_mass_fraction_of_phase(phase: str) -> [typing.List[float], typing.List[float]]
```

Returns the total mass fraction of the specified phase in dependency of the time.

Parameters `phase` – The name of the phase

Returns A tuple of two lists of floats (time [s], total mass fraction of the phase)

```python
def get_total_mole_fraction_of_component(component: str) -> [typing.List[float], typing.List[float]]
```

Returns the total mole fraction of the specified component in dependency of time.

Parameters `component` – The name of the component

Returns A tuple of two lists of floats (time [s], total mole fraction of the component)

```python
def get_total_mole_fraction_of_component_in_phase(component: str, phase: str) -> [typing.List[float], typing.List[float]]
```

Returns the total mole fraction of the specified component in the specified phase in dependency of time.

Parameters
- **component** – The name of the component
- **phase** – The name of the phase

Returns A tuple of two lists of floats (time [s], total mole fraction of the component in the phase)

```python
get_total_mole_fraction_of_phase(phase: str) \rightarrow \text{[typing.List[float], typing.List[float]]}
```

Returns the total mole fraction of the specified phase in dependency of time.

Parameters **phase** – The name of the phase

Returns A tuple of two lists of floats (time [s], total mole fraction of the phase)

```python
get_total_volume_fraction_of_phase(phase: str) \rightarrow \text{[typing.List[float], typing.List[float]]}
```

Returns the total volume fraction of the specified phase in dependency of the time.

Parameters **phase** – The name of the phase

Returns A tuple of two lists of floats (time [s], total volume fraction of the phase)

```python
get_values_of(x_axis: \text{Union[tc_python.quantity_factory.DiffusionQuantity, str]}, y_axis: \text{Union[tc_python.quantity_factory.DiffusionQuantity, str]}, plot_condition: \text{Union[tc_python.quantity_factory.PlotCondition, str]} = '', independent_variable: \text{Union[tc_python.quantity_factory.IndependentVariable, str]} = '') \rightarrow \text{[typing.List[float], typing.List[float]]}
```

Returns the specified result from the simulation, allows all possible settings.

**Note:** As an alternative, DICTRA Console Mode syntax can be used as well for each quantity and condition.

**Warning:** This is an advanced mode that is equivalent to the possibilities in the DICTRA Console Mode. Not every combination of settings will return a result.

Parameters
- **x_axis** – The first result quantity
- **y_axis** – The second result quantity
- **plot_condition** – The plot conditions
- **independent_variable** – The independent variable

Returns A tuple of two lists of floats (the x_axis quantity result, the y_axis quantity result) [units according to the quantities]

```python
get_velocity_of_lower_boundary_of_region(region: str) \rightarrow \text{[typing.List[float], typing.List[float]]}
```

Returns the velocity of the lower boundary of the specified region in dependency of time.

Parameters **region** – The name of the region

Returns A tuple of two lists of floats (time [s], velocity of lower boundary of region [m/s])

```python
get_velocity_of_upper_boundary_of_region(region: str) \rightarrow \text{[typing.List[float], typing.List[float]]}
```

Returns the velocity of the upper boundary of the specified region in dependency of time.

Parameters **region** – The name of the region

Returns A tuple of two lists of floats (time [s], velocity of upper boundary of region [m/s])
**get_width_of_region** *(region: str) → [typing.List[float], typing.List[float]]*

Returns the width of region, in dependency of time.

**Parameters**
- **region** – The name of the region

**Returns**
A tuple of two lists of floats (time [s], width of the specified region [m])

**save_to_disk** *(path: str)*

Saves the result to disk. The result can later be loaded using `tc_python.server.SetUp.load_result_from_disk()`.

**Note:** The result data is represented by a whole folder containing multiple files.

**Parameters**
- **path** – The path to the result folder, can be relative or absolute.

**Returns**
This `DiffusionCalculationResult` object

**with_continued_calculation()**

Returns a `ContinuedDiffusionCalculation` that is used for continuing a diffusion calculation with altered settings.

**Returns**
A `ContinuedDiffusionCalculation`

**class tc_python.diffusion.DiffusionIsoThermalCalculation**(calculation)

**Bases:** `tc_python.abstract_base.AbstractCalculation`

Configuration for an isothermal diffusion calculation.

**add_console_command** *(console_command: str)*

Registers a DICTRA Console Mode command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands are stored and used until explicitly deleted using `tc_python.diffusion.DiffusionIsoThermoCalculation.remove_all_console_commands()`.

**Parameters**
- **console_command** – The DICTRA Console Mode command

**Returns**
This `DiffusionIsoThermalCalculation` object

**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw DICTRA-commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten parenthesis, ...).

**add_region** *(region: tc_python.diffusion.Region)*

Adds a region to the calculation. Regions are always added in the simulation domain from left to right.

If you want to replace an already added region, call `remove_all_regions()`, and add the regions that you want to keep.

**Warning:** Regions must have unique names.

**Parameters**
- **region** – The region to be added
**Returns** This `DiffusionIsoThermalCalculation` object

`calculate()` → `tc_python.diffusion.DiffusionCalculationResult`
Runs the diffusion calculation.

**Returns** A `DiffusionCalculationResult` which later can be used to get specific values from the calculated result

`get_system_data()` → `tc_python.abstract_base.SystemData`
Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

**Note:** Parameters can only be read from unencrypted (i.e. `user`) databases loaded as *.tdb*-file.

**Returns** The system data

`remove_all_console_commands()`
Removes all previously added Console Mode commands.

**Returns** This `DiffusionIsoThermalCalculation` object

`remove_all_regions()`
Removes all previously added regions.

`set_simulation_time`(*simulation_time*: float)
Sets the simulation time.

**Parameters** `simulation_time` – The simulation time [s]

**Returns** This `DiffusionIsoThermalCalculation` object

`set_temperature`(*temperature*: float)
Sets the temperature for the isothermal simulation.

**Parameters** `temperature` – The temperature [K]

**Returns** This `DiffusionIsoThermalCalculation` object

`with_cylindrical_geometry`(*first_interface_position*: float = 0.0)
Sets geometry to cylindrical, corresponds to an infinitely long cylinder of a certain radius.

**Default:** A planar geometry

**Note:** With a cylindrical or spherical geometry, the system’s zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the `first_interface_position`, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

**Parameters** `first_interface_position` – The position of the left-most coordinate along the axis, only necessary for modeling a tube geometry [m]

**Returns** This `DiffusionIsoThermalCalculation` object

`with_left_boundary_condition`(*boundary_condition*: `tc_python.diffusion.BoundaryCondition`, *to*: float = 1.7976931348623157e+308)
Defines the boundary condition on the left edge of the system.
**Default:** A closed-system boundary condition.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

---

**Note:** You can specify time-dependent boundary conditions by calling `with_left_boundary_condition()` many times, with different values of the “to” parameter.

Examples:

- `with_left_boundary_condition(BoundaryCondition.closed_system(), to=100)`
- `with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)`
- `with_left_boundary_condition(BoundaryCondition.closed_system())`

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

**Parameters**

- `boundary_condition` – The boundary condition
- `to` – The upper time-limit for boundary_condition.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_options (options: tc_python.diffusion.Options, to: float = 1.7976931348623157e+308)**

Sets the general simulation conditions.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

**Parameters**

- `options` – The general simulation conditions
- `to` – The upper time-limit for options.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_planar_geometry ()**

Sets geometry to planar.

This is default.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_reference_state (element: str, phase: str = 'SER', temperature: float = - 1.0, pressure: float = 100000.0)**

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to...
set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

**Parameters**

- `element` – The name of the element
- `phase` – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
- `temperature` – The Temperature (in K) for the reference state. Or `CURRENT_TEMPERATURE` which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
- `pressure` – The pressure (in Pa) for the reference state

**Returns** This `DiffusionIsoThermalCalculation` object

```python
with_right_boundary_condition(boundary_condition: tc_python.diffusion.BoundaryCondition, to: float = 1.7976931348623157e+308)
```

Defines the boundary condition on the right edge of the system.

**Default:** A closed-system boundary condition

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

**Note:** You can specify time-dependent boundary conditions by calling `with_right_boundary_condition()` many times, with different values of the “to” parameter.

**Examples:**

- `with_right_boundary_condition(BoundaryCondition.closed_system(), to=100)`
- `with_right_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)`
- `with_right_boundary_condition(BoundaryCondition.closed_system())`

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

**Parameters**

- `boundary_condition` – The boundary condition
- `to` – The upper time-limit for boundary_condition.

**Returns** This `DiffusionIsoThermalCalculation` object

```python
with_solver(solver: tc_python.diffusion.Solver, to: float = 1.7976931348623157e+308)
```

Sets the solver to use (Classic, Homogenization or Automatic). **Default is Automatic.**
It is possible to specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

**Parameters**

- **solver** – The solver to use
- **to** – The upper time-limit for solver.

**Returns** This `DiffusionIsoThermalCalculation` object

with spherical geometry (first_interface_position: float = 0.0)

Sets geometry to `spherical`, corresponds to a sphere with a certain radius.

**Default:** A spherical geometry

**Note:** With a cylindrical or spherical geometry, the system’s zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the `first_interface_position`, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

**Parameters** `first_interface_position` – The position of the left-most coordinate along the axis, only necessary for modeling a hollow sphere geometry [m]

**Returns** This `DiffusionIsoThermalCalculation` object

with system modifications (system_modifications: tc_python.abstract_base.SystemModifications)

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

**Note:** This is only possible if the system has been read from unencrypted (i.e. `user`) databases loaded as a *.tdb*-file.

**Parameters** `system_modifications` – The system modification to be performed

**Returns** This `DiffusionIsoThermalCalculation` object

with timestep control (timestep_control: tc_python.diffusion.TimestepControl, to: float = 1.7976931348623157e+308)

Sets the timestep control options.

It is possible to specify the upper time-point for which this setting is valid using the parameter “to”.

**Default:** The end of the simulation.

**Parameters**

- **timestep_control** – The new timestep control options
- **to** – The upper time-limit for timestep_control.

**Returns** This `DiffusionIsoThermalCalculation` object

class tc_python.diffusion.DiffusionNonIsoThermalCalculation (calculation)

**Bases:** tc_python.abstract_base.AbstractCalculation

Configuration for a non-isothermal diffusion calculation.
add_console_command (console_command: str)
Registers a DICTRA Console Mode command for execution. These commands are executed after all
other configuration directly before the calculation starts to run. All commands are stored and used until
explicitly deleted using tc_python.diffusion.DiffusionNonIsoThermalCalculation.
remove_all_console_commands.

Parameters console_command – The DICTRA Console Mode command

Returns This DiffusionNonIsoThermalCalculation object

Note: It should not be necessary for most users to use this method, try to use the corresponding method
implemented in the API instead.

Warning: As this method runs raw DICTRA-commands directly in the engine, it may hang the
program in case of spelling mistakes (e.g. forgotten parenthesis, ...).

add_region (region: tc_python.diffusion.Region)
Adds a region to the calculation. Regions are always added in the simulation domain from left to right.
If you want to replace an already added region, call remove_all_regions(), and add the regions
that you want to keep.

Warning: Regions must have unique names.

Parameters region – The region to be added

Returns This DiffusionNonIsoThermalCalculation object

calculate () \rightarrow tc_python.diffusion.DiffusionCalculationResult
Runs the diffusion calculation.

Returns A DiffusionCalculationResult which later can be used to get specific values
from the calculated result

get_system_data () \rightarrow tc_python.abstract_base.SystemData
Returns the content of the database for the currently loaded system. This can be used to modify the param-
eters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

remove_all_console_commands ()
Removes all previously added Console Mode commands.

Returns This DiffusionNonIsoThermalCalculation object

remove_all_regions ()
Removes all previously added regions.

Returns This DiffusionNonIsoThermalCalculation object
**set_simulation_time** *(simulation_time: float)*
Sets the simulation time.

**Parameters**
- **simulation_time** – The simulation time [s]

**Returns**
This **DiffusionNonIsoThermalCalculation** object

**with_cylindrical_geometry** *(first_interface_position: float = 0.0)*
Sets geometry to **cylindrical**, corresponds to an infinitely long cylinder of a certain radius.

**Default**
A planar geometry

**Note:** With a cylindrical or spherical geometry, the system’s zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the **first_interface_position**, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

**Parameters**
- **first_interface_position** – The position of the left-most coordinate along the axis, only necessary for modeling a tube geometry [m]

**Returns**
This **DiffusionNonIsoThermalCalculation** object

**with_left_boundary_condition** *(boundary_condition: tc_python.diffusion.BoundaryCondition, to: float = 1.7976931348623157e+308)*
Defines the boundary condition on the left edge of the system.

**Default**
A closed-system boundary condition.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

**Default**
The end of the simulation.

**Note:** You can specify time-dependent boundary conditions by calling **with_left_boundary_condition()** many times, with different values of the “to” parameter.

**Examples:**
- **with_left_boundary_condition(BoundaryCondition.closed_system(), to=100)**
- **with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)**
- **with_left_boundary_condition(BoundaryCondition.closed_system())**

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

**Parameters**
- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns**
This **DiffusionNonIsoThermalCalculation** object

**with_options** *(options: tc_python.diffusion.Options, to: float = 1.7976931348623157e+308)*
Sets the general simulation conditions.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

---

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---
Default: The end of the simulation.

Parameters

• **options** – The general simulation conditions
• **to** – The upper time-limit for options.

Returns This `DiffusionNonIsoThermalCalculation` object

**with_planar_geometry()**
Sets geometry to planar.

This is default.

Returns This `DiffusionNonIsoThermalCalculation` object

**with_reference_state**

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

Parameters

• **element** – The name of the element
• **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
• **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
• **pressure** – The pressure (in Pa) for the reference state

Returns This `DiffusionNonIsoThermalCalculation` object

**with_right_boundary_condition**

Defines the boundary condition on the right edge of the system.

Default: A closed-system boundary condition

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

Default: The end of the simulation.
Note: You can specify time-dependent boundary conditions by calling `with_right_boundary_condition()` many times, with different values of the “to” parameter.

Examples:

- `with_right_boundary_condition(BoundaryCondition.closed_system(), to=100)`
- `with_right_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)`
- `with_right_boundary_condition(BoundaryCondition.closed_system())`

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

Parameters

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

Returns This `DiffusionNonIsoThermalCalculation` object

**with_solver** *(solver: tc_python.diffusion.Solver, to: float = 1.7976931348623157e+308)*

Sets the solver to use (Classic, Homogenization or Automatic). **Default is Automatic.**

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

Default: The end of the simulation.

Parameters

- **solver** – The solver to use
- **to** – The upper time-limit for solver.

Returns This `DiffusionNonIsoThermalCalculation` object

**with_spherical_geometry** *(first_interface_position: float = 0.0)*

Sets geometry to spherical, corresponds to a sphere with a certain radius.

Default: A spherical geometry

Note: With a cylindrical or spherical geometry, the system’s zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the `first_interface_position`, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

Parameters **first_interface_position** – The position of the left-most coordinate along the axis, only necessary for modeling a hollow sphere geometry [m]

Returns This `DiffusionNonIsoThermalCalculation` object

**with_system_modifications** *(system_modifications: tc_python.abstract_base.SystemModifications)*

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).
Note: This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb-file.

Parameters **system_modifications** – The system modification to be performed

Returns This **DiffusionNonIsoThermalCalculation** object

**with_temperature_profile** *(temperature_profile: tc_python.utils.TemperatureProfile)*

Sets the temperature profile to use with this calculation.

Parameters **temperature_profile** – The temperature profile object (specifying time / temperature points)

Returns This **DiffusionNonIsoThermalCalculation** object

**with_timestep_control** *(timestep_control: tc_python.diffusion.TimestepControl, to: float = 1.7976931348623157e+308)*

Sets the timestep control options.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

Default: The end of the simulation.

Parameters

• **timestep_control** – The new timestep control options
• **to** – The upper time-limit for timestep_control.

Returns This **DiffusionNonIsoThermalCalculation** object

**class tc_python.diffusion.DoubleGeometricGrid**(no_of_points: int = 50, lower_geometrical_factor: float = 1.1, upper_geometrical_factor: float = 0.9)

Bases: **tc_python.diffusion.CalculatedGrid**

Represents a double geometric grid.

**get_lower_geometrical_factor** () ➔ float

Returns the lower geometrical factor (for the left half).

Returns The lower geometrical factor

**get_no_of_points** () ➔ int

Returns number of grid points.

Returns The number of grid points

**get_type** () ➔ str

Type of the grid.

Returns The type of the grid

**get_upper_geometrical_factor** ()

Returns the upper geometrical factor (for the right half).

Returns The upper geometrical factor

**set_lower_geometrical_factor** *(geometrical_factor: float = 1.1)*

Sets the lower (left half) geometrical factor.
Note: A geometrical factor of larger than one yields a higher density of grid points at the lower end of the half and vice versa for a factor smaller than one.

**Parameters** `geometrical_factor` – The geometrical factor for the left half

**Returns** This `DoubleGeometricGrid` object

### `set_no_of_points(no_of_points: int = 50)`
Sets the number of grid points.

**Parameters** `no_of_points` – The number of points

**Returns** This `DoubleGeometricGrid` object

### `set_upper_geometrical_factor(geometrical_factor: float = 0.9)`
Sets the upper (right half) geometrical factor.

Note: A geometrical factor of larger than one yields a higher density of grid points at the lower end of the half and vice versa for a factor smaller than one.

**Parameters** `geometrical_factor` – The geometrical factor for the right half

**Returns** This `DoubleGeometricGrid` object

class `tc_python.diffusion.ElementProfile`
Bases: `tc_python.diffusion.AbstractElementProfile`

Factory class providing objects for configuring a step, function or linear initial concentration profile.

**classmethod constant(value: float)**
Factory method that creates a new constant initial concentration profile.

**Parameters** `value` – The constant composition in the region. [unit as defined in `CompositionProfile`].

**Returns** A new `ConstantProfile` object

**classmethod funct(dictra_console_mode_function: str)**
Factory method that creates a new initial concentration profile defined by a function in DICTRA Console Mode syntax.

**Parameters** `dictra_console_mode_function` – The function, expressed in DICTRA Console Mode syntax.

**Returns** A new `FunctionProfile` object

Note: This is an advanced feature, preferably a complex concentration profile should be generated using third party libraries and added to the simulation using `tc_python.diffusion.PointByPointGrid`.

**classmethod linear(start_value: float, end_value: float)**
Factory method that creates a new linear initial concentration profile.

Parameters
• **start_value** – Composition at the left side of the region [unit as defined in \( \text{CompositionProfile} \)].

• **end_value** – Composition at the right side of the region [unit as defined in \( \text{CompositionProfile} \)].

**Returns** A new \( \text{LinearProfile} \) object

#### classmethod step(lower_bound: float, upper_bound: float, step_at: float)
Factory method that creates a new initial concentration profile with a step at the specified distance, otherwise the composition is constant at the specified values.

**Parameters**

• **lower_bound** – Composition before the step [unit as defined in \( \text{CompositionProfile} \)].

• **upper_bound** – Composition after the step [unit as defined in \( \text{CompositionProfile} \)].

• **step_at** – The distance where the step should be [m].

**Returns** A new \( \text{StepProfile} \) object

```python
class tc_python.diffusion.FixFluxValue
    Bases: tc_python.diffusion.BoundaryCondition

    def get_type(self) -> str
        return self._type

    def set_flux(self, element_name: str, J: str = '0', to_time: float = 1.7976931348623157e+308)
        # Enter functions that yield the flux times the molar volume for the specified element. May be a function of
time, temperature and pressure: \( J(T,P,\text{TIME}) \).

    Parameters

    • **element_name** – The name of the element

    • **J** – the function \( J(T,P,\text{TIME}) \)

    • **to_time** – The max-time for which the flux function is used.

class tc_python.diffusion.FixedCompositions
    Bases: tc_python.diffusion.BoundaryCondition

    Represents a boundary having fixed composition values.

    def get_type(self) -> str
        return self._type

    def set_composition(self, element_name: str, value: float)
        # Sets the composition for the specified element.

    Parameters

    • **element_name** – The name of the element
```

---

**Note:** The boundary composition needs to be specified for each element.

---

**Parameters**

• **element_name** – The name of the element
• **value** – The composition value [unit according to the constructor parameter]

```python
class tc_python.diffusion.FunctionProfile(dictra_console_mode_function: str)
Bases: tc_python.diffusion.ElementProfile

Creates an initial concentration profile defined by a function in DICTRA Console Mode syntax.
```

**Note:** This is an advanced feature, preferably a complex concentration profile should be generated using third party libraries and added to the simulation using `tc_python.diffusion.PointByPointGrid`.

```python
def get_type() -> str
    """The type of the element profile."

    Returns
    The type
```

```python
class tc_python.diffusion.GeneralLowerHashinShtrikman
Bases: tc_python.diffusion.HomogenizationFunctions

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.
Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.
```

```python
class tc_python.diffusion.GeneralLowerHashinShtrikmanExcludedPhase(excluded_phases: List[str] = [])
Bases: tc_python.diffusion.HomogenizationFunctions

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.
Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.
The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.
```

```python
class tc_python.diffusion.GeneralUpperHashinShtrikman
Bases: tc_python.diffusion.HomogenizationFunctions

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.
Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.
```

```python
class tc_python.diffusion.GeneralUpperHashinShtrikmanExcludedPhase(excluded_phases: List[str] = [])
Bases: tc_python.diffusion.HomogenizationFunctions

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.
Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.
The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.
```

```python
class tc_python.diffusion.GeometricGrid(no_of_points: int = 50, geometrical_factor: float = 1.1)
Bases: tc_python.diffusion.CalculatedGrid
```

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Represents a geometric grid.

**get_geometrical_factor() → float**

Returns the geometrical factor.

**get_no_of_points() → int**

Returns the number of grid points.

**get_type() → str**

Returns the type of grid.

**set_geometrical_factor(geometrical_factor: float = 1.1)**

Sets the geometrical factor.

**set_no_of_points(no_of_points: int = 50)**

Sets the number of grid points.

---

**Note:** A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.

**Parameters**
- **geometrical_factor** – The geometrical factor
- **no_of_points** – The number of points

**Returns**
- This GeometricGrid object

---

**class tc_python.diffusion.GridPoint(distance: float)**

Bases: object

Represents a grid point, this is used in combination with grids of the type `tc_python.diffusion.PointByPointGrid`.

**add_composition(element: str, value: float)**

Adds a composition for the specified element to the grid point.

**Parameters**
- **element** – The element
- **value** – The composition value [unit as defined for the grid]

**Returns**
- This GridPoint object

**class tc_python.diffusion.HashinShtrikmanBoundMajority**

Bases: `tc_python.diffusion.HomogenizationFunctions`

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.
class tc_python.diffusion.HashinShtrikmanBoundMajorityExcludedPhase(excluded_phases: List[str] = [])

Bases: tc_python.diffusion.HomogenizationFunctions

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

class tc_python.diffusion.HashinShtrikmanBoundPrescribed(matrix_phase: str)
Bases: tc_python.diffusion.HomogenizationFunctions

Hashin-Shtrikman bounds with prescribed phase as matrix phase: the outermost shell consists of the prescribed phase.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

Bases: tc_python.diffusion.HomogenizationFunctions

class tc_python.diffusion.HomogenizationFunction(value)
Bases: enum.Enum

Homogenization function used for the homogenization solver. Many homogenization functions are based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. Default: RULE_OF_MIXTURES (i.e. upper Wiener bounds)

GENERAL_LOWER_HASHIN_SHTRIKMAN = 0
General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

GENERAL_UPPER_HASHIN_SHTRIKMAN = 1
General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

HASHIN_SHTRIKMAN_BOUND_MAJORITY = 2
Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

INVERSE_RULE_OF_MIXTURES = 4
Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion

RULE_OF_MIXTURES = 3
Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion

class tc_python.diffusion.HomogenizationFunctions
Bases: object

classmethod general_lower_hashin_shtrikman()
Factory method that creates a new homogenization function of the type

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**GeneralLowerHashinShtrikman.**

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

**Returns** A new `GeneralLowerHashinShtrikman` object

**classmethod general_lower_hashin_shtrikman_excluded_phase**(excluded_phases:
`List[str] = []`)

Factory method that creates a new homogenization function of the type `GeneralLowerHashinShtrikmanExcludedPhase`.

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

**Parameters** `excluded_phases` – The excluded phases

**Returns** A new `GeneralLowerHashinShtrikmanExcludedPhase` object

**classmethod general_upper_hashin_shtrikman()**

Factory method that creates a new homogenization function of the type `GeneralUpperHashinShtrikman`.

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

**Returns** A new `GeneralUpperHashinShtrikman` object

**classmethod general_upper_hashin_shtrikman_excluded_phase**(excluded_phases:
`List[str] = []`)

Factory method that creates a new homogenization function of the type `GeneralUpperHashinShtrikmanExcludedPhase`.

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

**Parameters** `excluded_phases` – The excluded phases

**Returns** A new `GeneralUpperHashinShtrikmanExcludedPhase` object

**classmethod hashin_shtrikman_bound_majority()**

Factory method that creates a new homogenization function of the type `HashinShtrikmanBoundMajority`.

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

**Returns** A new `HashinShtrikmanBoundMajority` object
classmethod hashin_shtrikman_bound_majority_excluded_phase(excluded_phases: List[str] = [])

Factory method that creates a new homogenization function of the type HashinShtrikmanBoundMajorityExcludedPhase.

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction. Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Parameters excluded_phases – The excluded phases

Returns A new HashinShtrikmanBoundMajorityExcludedPhase object

classmethod hashin_shtrikman_bound_prescribed(matrix_phase: str)

Factory method that creates a new homogenization function of the type HashinShtrikmanBoundPrescribed.

Hashin-Shtrikman bounds with prescribed phase as matrix phase: the outermost shell consists of the prescribed phase.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

Parameters matrix_phase – The matrix phase

Returns A new HashinShtrikmanBoundPrescribed object

classmethod hashin_shtrikman_bound_prescribed_excluded_phase(matrix_phase: str, excluded_phases: List[str] = [])

Factory method that creates a new homogenization function of the type HashinShtrikmanBoundPrescribedExcludedPhase.

Hashin-Shtrikman bounds with prescribed phase as matrix phase: the outermost shell consists of the prescribed phase.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Parameters

- matrix_phase – The matrix phase
- excluded_phases – The excluded phases

Returns A new HashinShtrikmanBoundPrescribedExcludedPhase object

classmethod inverse_rule_of_mixtures()

Factory method that creates a new homogenization function of the type InverseRuleOfMixtures.

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion.

Returns A new InverseRuleOfMixtures object

classmethod inverse_rule_of_mixtures_excluded_phase(excluded_phases: List[str] = [])

Factory method that creates a new homogenization function of the type InverseRuleOfMixturesExcludedPhase.
Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion. Excluded phases are not considered in the diffusion calculations.

**Parameters**

- `excluded_phases` — The excluded phases

**Returns**

A new `InverseRuleOfMixturesExcludedPhase` object

classmethod **labyrinth_factor_f** *(matrix_phase: str)*

Factory method that creates a new homogenization function of the type `LabyrinthFactorF`.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase.

**Parameters**

- `matrix_phase` — The matrix phase

**Returns**

A new `LabyrinthFactorF` object

classmethod **labyrinth_factor_f2** *(matrix_phase: str)*

Factory method that creates a new homogenization function of the type `LabyrinthFactorF2`.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase squared.

**Parameters**

- `matrix_phase` — The matrix phase

**Returns**

A new `LabyrinthFactorF2` object

classmethod **rule_of_mixtures**()

Factory method that creates a new homogenization function of the type `RuleOfMixtures`.

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion.

**Returns**

A new `RuleOfMixtures` object

classmethod **rule_of_mixtures_excluded_phase** *(excluded_phases: List[str] = [])*

Factory method that creates a new homogenization function of the type `RuleOfMixturesExcludedPhase`.

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion. Excluded phases are not considered in the diffusion calculations.

**Parameters**

- `excluded_phases` — The excluded phases

**Returns**

A new `RuleOfMixturesExcludedPhase` object

class **tc_python.diffusion.HomogenizationSolver**

Bases: `tc_python.diffusion.Solver`

Solver using the *Homogenization model*.

**Note:** This solver always uses the homogenization model, even if all regions have only one phase. The solver is significantly slower than the *Classic model*. Use the `tc_python.diffusion.AutomaticSolver` instead if you do not need that behavior.

**disable_global_minimization()**

Disables global minimization to be used in equilibrium calculations. **Default:** Disabled
Note: In general, using global minimization significantly increases the simulation time, but there is also a significantly reduced risk for non-converged equilibrium calculations.

Returns A new HomogenizationSolver object

disable_interpolation_scheme()
Configures the simulation not use any interpolation scheme. Default: To use the logarithmic interpolation scheme with 10000 discretization steps

Note: The homogenization scheme can be switched on by using with_linear_interpolation_scheme or with_logarithmic_interpolation_scheme.

enable_global_minimization()
Enables global minimization to be used in equilibrium calculations. Default: Disabled

Note: In general, using global minimization significantly increases the simulation time, but there is also a significantly reduced risk for non-converged equilibrium calculations.

Returns A new HomogenizationSolver object

get_type() -> str
The type of solver.

Returns The type

set_fraction_of_free_memory_to_use(fraction: float)
Sets the maximum fraction of free physical memory to be used by the interpolation scheme. Default: 1 / 10 of the free physical memory

Parameters fraction – The maximum free physical memory fraction to be used

Returns A new HomogenizationSolver object

set_homogenization_function(homogenization_function_enum: tc_python.diffusion.HomogenizationFunction = <HomogenizationFunction.RULE_OF_MIXTURES: 3>)
Sets the homogenization function used by the homogenization model.

Note: Deprecated in version 2021b: Use with_function() instead. This method will be removed in release 2022b.

Default is RULE_OF_MIXTURES.

Parameters homogenization_function_enum – The homogenization function used by the homogenization model

Returns A new HomogenizationSolver object

set_memory_to_use(memory_in_megabytes: float)
Sets the maximum physical memory in megabytes to be used by the interpolation scheme. Default: 1000 MBytes of the free physical memory

Parameters memory_in_megabytes – The maximum physical memory to be used
Returns A new `HomogenizationSolver` object

**with_function** *(homogenization_function: tc_python.diffusion.HomogenizationFunctions)*

Sets the homogenization function used by the homogenization model.

**Parameters** homogenization_function – The homogenization function used by the homogenization model

**Returns** A new `HomogenizationSolver` object

**with_linear_interpolation_scheme** *(steps: int = 10000)*

Configures the simulation to use the linear interpolation scheme. Default: To use the logarithmic interpolation scheme with 10000 discretization steps.

**Parameters** steps – The number of discretization steps in each dimension

**Returns** A new `HomogenizationSolver` object

**with_logarithmic_interpolation_scheme** *(steps: int = 10000)*

Configures the simulation to use the logarithmic interpolation scheme.

**Parameters** steps – The number of discretization steps in each dimension

**Returns** A new `HomogenizationSolver` object

**class** tc_python.diffusion.InverseRuleOfMixtures

**Bases:** tc_python.diffusion.HomogenizationFunctions

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion.

**class** tc_python.diffusion.InverseRuleOfMixturesExcludedPhase *(excluded_phases: List[ str ] = [])*

**Bases:** tc_python.diffusion.HomogenizationFunctions

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion.

Excluded phases are not considered in the diffusion calculations.

**class** tc_python.diffusion.LabyrinthFactorF *(matrix_phase: str)*

**Bases:** tc_python.diffusion.HomogenizationFunctions

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase.

**class** tc_python.diffusion.LabyrinthFactorF2 *(matrix_phase: str)*

**Bases:** tc_python.diffusion.HomogenizationFunctions

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase squared.

**class** tc_python.diffusion.LinearGrid *(no_of_points: int = 50)*

**Bases:** tc_python.diffusion.CalculatedGrid

Represents an equally spaced grid.

**get_no_of_points** () → int

Returns the number of grid points.

**Returns** The number of grid points
get_type() → str
Type of the grid.

Returns The type

set_no_of_points (no_of_points: int = 50)
Sets the number of grid points.

Parameters no_of_points – The number of points

Returns This LinearGrid object

class tc_python.diffusion.LinearProfile (start_value: float, end_value: float)
Bases: tc_python.diffusion.ElementProfile

Represents a linear initial concentration profile.

get_type() → str
The type of the element profile.

Returns The type

class tc_python.diffusion.MixedZeroFluxAndActivity
Bases: tc_python.diffusion.BoundaryCondition

Represents a boundary having zero-flux as well as fixed-activity conditions.

Default: On that boundary for every element without an explicitly defined condition, a zero-flux boundary condition is used.

get_type() → str
The type of the boundary condition.

Returns The type

set_activity_for_element (element_name: str, activity: str, to_time: float = 1.7976931348623157e+308)
Sets an activity expression for an element at the boundary. Enter a formula that the software evaluates during the calculation.

The formula can be:
• a function of the variable TIME
• a constant

The formula must be written with these rules:
• a number must begin with a number (not a .)
• a number must have a dot or an exponent (E)

The operators +, -, *, /, ** (exponentiation) can be used and with any level of parenthesis. As shown, the following operators must be followed by open and closed parentheses ()
• SQRT(X) is the square root
• EXP(X) is the exponential
• LOG(X) is the natural logarithm
• LOG10(X) is the base 10 logarithm
• SIN(X), COS(X), TAN(X), ASIN(X), ACOS(X), ATAN(X)
• SINH(X), COSH(X), TANH(X), ASINH(X), ACOSH(X), ATANH(X)
• SIGN(X)
• \( ERF(X) \) is the error function

**Default:** the expression entered is used for the entire simulation.

**Parameters**
- **element_name** – The name of the element
- **activity** – The activity
- **to_time** – The max-time for which the activity is used.

### set_zero_flux_for_element(element_name: str)
Sets a zero-flux condition for an element at the boundary. **Default** for all elements at the boundary without an explicitly defined condition

**Parameters**
- **element_name** – The name of the element

---

```python
class tc_python.diffusion.Options
    Bases: object

    General simulation conditions for the diffusion calculations.

    disable_forced_starting_values_in_equilibrium_calculations()
        Disables forced starting values for the equilibrium calculations. The default is ‘enable_automatic_forced_starting_values_in_equilibrium_calculations’.
        Returns This Options object

disable_save_results_to_file()
    Disables the saving of results to file during the simulation. Default: Saving of the results at every timestep
    Returns This Options object

enable_automatic_forced_starting_values_in_eq_calculations()
    Lets calculation engine decide if forced start values for the equilibrium calculations should be used. This is the default setting.
    Returns This Options object

enable_forced_starting_values_in_equilibrium_calculations()
    Enables forced start values for the equilibrium calculations. The default is ‘enable_automatic_forced_starting_values_in_equilibrium_calculations’.
    Returns This Options object

enable_save_results_to_file(every_nth_step: int = -1)
    Enables and configures saving of results to file during the simulation. They can be saved for every n-th or optionally for every timestep (-1). Default: Saving of the results at every timestep
    Parameters every_nth_step = -1 or a value ranging from 0 to 99
    Returns This Options object

enable_time_integration_method_automatic()
    Enables automatic selection of integration method. This is the default method.
    Returns This Options object

enable_time_integration_method_euler_backwards()
    Enables \( Euler \) \( backwards \) integration. The default method is enable_time_integration_method_automatic.
```
Note: This method is more stable but less accurate and may be necessary if large fluctuations occur in the profiles.

**Returns** This `Options` object

`enable_time_integration_method_trapezoidal()` Enables *trapezoidal* integration.

**Note:** If large fluctuations occur in the profiles, it may be necessary to use the more stable but less accurate *Euler backwards method.*

**Returns** This `Options` object

`set_default_driving_force_for_phases_allowed_to_form_at_interf(driving_force: float = 1e-05)` Sets the default required driving force for phases allowed to form at the interfaces. **Default:** 1.0e-5

**Note:** The required driving force (evaluated as $DGM(ph)$) is used for determining whether an inactive phase is stable, i.e. actually formed. $DGM$ represents the driving force normalized by $RT$ and is dimensionless.

**Parameters** `driving_force` – The driving force ($DGM(ph)$) [-]

**Returns** This `Options` object

```python
class tc_python.diffusion.PointByPointGrid(unit_enum: tc_python.diffusion.Unit = \<Unit.MASS_PERCENT: 3>)
    Bases: tc_python.diffusion.AbstractGrid

    Represents a point-by-point grid. This is setting the grid and the compositions at once, it is typically used to enter a measured composition profile or the result from a previous calculation.

    **Note:** If a point-by-point grid is used, it is not necessary to specify the grid and composition profile separately.
```

**add_point(grid_point: tc_python.diffusion.GridPoint)**

Adds a grid point to the grid.

**Parameters** `grid_point` – The grid point

**Returns** This `PointByPointGrid` object

```python
def get_type() \rightarrow str
    Type of the grid.

    **Returns** The type
```

```python
class tc_python.diffusion.Region(name: str)
    Bases: object

    Represents a region of the simulation domain that can contain more than one phase.
```
Note: The first added phase represents the matrix phase, while all later added phases are *spheriod phases*, i.e. precipitate phases.

**add_phase** *(phase_name: str, is_matrix_phase: bool = False)*

Adds a phase to the region, each region must contain at least one phase.

Note: Normally the *matrix phase* and the *precipitate phases* are automatically chosen based on the presence of all profile elements in the phase and if it has diffusion data. If multiple phases have equal properties, the phase that was added first is chosen. The matrix phase can be explicitly set by using `is_matrix_phase=True`.

Note: If multiple phases are added to a region, the *homogenization model* is applied. That means that average properties of the local phase mixture are used.

**Parameters**

- **phase_name** – The phase name
- **is_matrix_phase** – If set to True this phase is explicitly set as matrix phase for the region, if no phase is set to True, the matrix phase is chosen automatically

**Returns** This *Region* object

**add_phase_allowed_to_form_at_left_interface** *(phase_name: str, driving_force: float = 1e-05)*

Adds a phase allowed to form at the left boundary of the region (an *inactive phase*). The phase will only appear at the interface as a new automatic region if the driving force to form it is sufficiently high.

**Parameters**

- **phase_name** – The phase name
- **driving_force** – The driving force for the phase to form *(DGM(ph))*

**Returns** This *Region* object

**add_phase_allowed_to_form_at_right_interface** *(phase_name: str, driving_force: float = 1e-05)*

Adds a phase allowed to form at the right boundary of the region (an *inactive phase*). The phase will only appear at the interface as a new automatic region if the driving force to form it is sufficiently high.

**Parameters**

- **phase_name** – The phase name
- **driving_force** – The driving force for the phase to form *(DGM(ph))*

**Returns** This *Region* object

**remove_all_phases** *

Removes all previously added phases from the region.

**Returns** This *Region* object

**set_width** *(width: float)*

Defined the width of the region.
Note: This method needs only to be used if a calculated grid has been defined (using `with_grid()`).

**Parameters** `width` – The width [m]

**Returns** This `Region` object

### `with_composition_profile` (initial_compositions: tc_python.diffusion.CompositionProfile)

Defines the initial composition profiles for all elements in the region.

Note: This method needs only to be used if a calculated grid has been defined (using `with_grid()`).

**Parameters** `initial_compositions` – The initial composition profiles for all elements

**Returns** This `Region` object

### `with_grid` (grid: tc_python.diffusion.CalculatedGrid)

Defines a calculated grid in the region. If measured composition profiles or the result from a previous calculation should be used, instead `with_point_by_point_grid_containing_compositions()` needs to be applied.

Note: The composition profiles need to be defined separately using `with_composition_profile()`, additionally the region width needs to be specified using `set_width()`.

**Parameters** `grid` – The grid

**Returns** This `Region` object

### `with_point_by_point_grid_containing_compositions` (grid: tc_python.diffusion.PointByPointGrid)

Defines a point-by-point grid in the region. This is setting the grid and the compositions at once, it is typically used to enter a measured composition profile or the result from a previous calculation. If the composition profile should be calculated (linear, geometric,...) `with_grid()` should be used instead.

Note: If a point-by-point grid is used, `with_grid()`, `with_composition_profile()` and `set_width()` are unnecessary and must not be used.

**Parameters** `grid` – The point-by-point grid

**Returns** This `Region` object

---

### `RuleOfMixtures`

**Bases:** `tc_python.diffusion.HomogenizationFunctions`

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion.

### `RuleOfMixturesExcludedPhase`

**Bases:** `tc_python.diffusion.HomogenizationFunctions`

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Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion.

Excluded phases are not considered in the diffusion calculations.

class tc_python.diffusion.SimulationTime(value)
Bases: enum.Enum

Specifying special time steps for the evaluation of diffusion results.

Note: These placeholders should be used because especially the actual last timestep will slightly differ from the specified end time of the simulation.

FIRST = 0
Represents the first timestep of the simulation

LAST = 1
Represents the last timestep of the simulation

class tc_python.diffusion.Solver
Bases: tc_python.diffusion.AbstractSolver

Factory class providing objects representing a solver.

classmethod automatic()
Factory method that creates a new automatic solver. This is the default solver and recommended for most applications.

Note: This solver uses the homogenization model if any region has more than one phase, otherwise it uses the classic model.

Returns A new AutomaticSolver object

classmethod classic()
Factory method that creates a new classic solver.

Note: This solver never switches to the homogenization model even if the solver fails to converge. Use the tc_python.diffusion.AutomaticSolver if necessary instead.

Returns A new ClassicSolver object

classmethod homogenization()
Factory method that creates a new homogenization solver.

Note: This solver always uses the homogenization model, even if all regions have only one phase. The solver is significantly slower than the Classic model. Use the tc_python.diffusion.AutomaticSolver instead if you do not need that behavior.

Returns A new HomogenizationSolver object
class tc_python.diffusion.StepProfile(lower_boundary: float, upper_boundary: float, step_at: float)

Bases: tc_python.diffusion.ElementProfile

Represents an initial constant concentration profile with a step at the specified position.

get_type() -> str

The type of the element profile.

class tc_python.diffusion.TimestepControl

Bases: object

Settings that control the time steps in the simulation.

disable_check_interface_position()

Disables checking of the interface position, i.e. the timesteps are not controlled by the phase interface displacement during the simulation. The default setting is :func:`enable_automatic_check_interface_position`.

Returns This TimestepControl object

enable_automatic_check_interface_position()

Lets calculation engine decide if checking of the interface position should be used. This is the default setting.

Returns This TimestepControl object

enable_check_interface_position()

Enables checking of the interface position, i.e. the timesteps are controlled by the phase interface displacement during the simulation. The default setting is :func:`enable_automatic_check_interface_position`.

Returns This TimestepControl object

set_initial_time_step(initial_time_step: float = 1e-07)

Sets the initial timestep. Default: 1.0e-7 s

Parameters initial_time_step – The initial timestep [s]

Returns This TimestepControl object

set_max_absolute_error(absolute_error: float = 1e-05)

Sets the maximum absolute error. Default: 1.0e-5

Parameters absolute_error – The maximum absolute error

Returns This TimestepControl object

set_max_relative_error(relative_error: float = 0.05)

Sets the maximum relative error. Default: 0.05

Parameters relative_error – The maximum relative error

Returns This TimestepControl object

set_max_timestep_allowed_as_percent_of_simulation_time(max_timestep_allowed_as_percent_of_simulation_time: float = 10.0)

The maximum timestep allowed during the simulation, specified in percent of the simulation time. Default: 10.0%

Parameters max_timestep_allowed_as_percent_of_simulation_time – The maximum timestep allowed [%]

Returns This TimestepControl object
set_max_timestep_increase_factor(max_timestep_increase_factor: float = 2.0)
Sets the maximum timestep increase factor. Default: 2

Note: For example, if 2 is entered the maximum time step is twice as long as the previous time step taken.

Parameters max_timestep_increase_factor – The maximum timestep increase factor

Returns This TimestepControl object

set_smallest_time_step_allowed(smallest_time_step_allowed: float = 1e-07)
Sets the smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step. Default: 1.0e-7 s

Parameters smallest_time_step_allowed – The smallest timestep allowed [s]

Returns This TimestepControl object

class tc_python.diffusion.Unit(value)
Bases: enum.Enum
Represents a composition unit.

MASS_FRACTION = 2
Mass fraction.

MASS_PERCENT = 3
Mass percent.

MOLE_FRACTION = 0
Mole fraction.

MOLE_PERCENT = 1
Mole percent.

U_FRACTION = 4
U fraction

5.1.7 Module “propertymodel”

class tc_python.propertymodel.PropertyModelCalculation(calculator)
Bases: tc_python.abstract_base.AbstractCalculation
Configuration for a Property Model calculation.

Note: Specify the settings, the calculation is performed with calculate().

add_poly_command(poly_command: str)
Registers a POLY Console Mode command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands are stored and used until explicitly deleted using remove_all_poly_commands.

Parameters poly_command – The POLY Console Mode command

Returns This PropertyModelCalculation object
**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw POLY-commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten parenthesis, ...).

```python
calculate() → tc_python.propertymodel.PropertyModelResult
```

Runs the Property Model calculation.

**Returns** A `PropertyModelResult` which later can be used to get specific values from the simulation.

```python
def get_argument_default(argument_id: str) → object
```

Returns the default value for the specified argument. The argument id can be obtained with `get_arguments()`.

**Parameters**
- `argument_id` - The argument id

**Returns** The default value (the type depends on the argument)

```python
def get_argument_description(argument_id: str) → str
```

Returns the detailed description of the argument. The id can be obtained with `get_arguments()`.

**Parameters**
- `argument_id` - The argument id

**Returns** The detailed description

```python
def get_arguments() → Set[str]
```

Returns a list of the arguments of the Property Model.

**Returns** The ids of the available arguments

```python
def get_dynamic_arguments() → Set[str]
```

Returns a list of the dynamic arguments of the Property Model.

**Note:** Dynamic arguments are “extra” arguments created by pressing the “plus” button that can occur next to the UI-panel for some models, when running the Property Model from within Thermo-Calc. You can use them also from the API by `invoke_dynamic_argument()`.

**Returns** The ids of the available dynamic arguments

```python
def get_model_description() → str
```

Returns the description text of the current model.

**Returns** the description

```python
def get_model_parameter_value(model_parameter_id: str) → float
```

Returns the current value of an optimizable model parameter. The id can be obtained with `get_model_parameters()`.

**Returns**

---

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Parameters **model_parameter_id** – The model parameter id

**Returns** The current value [unit according to the parameter meaning]

```python
def get_model_parameters() -> Set[str]
```

Returns a list of the optimizable model parameters.

---

**Note:** The model parameters are an optional set of variables that can be used within the Property Model. Typically they are used to provide the possibility to inject parameter values during an optimization into the model. This allows the dynamic development of Property Models that need to be fitted to experimental data. The model parameters are controlled with the Property Model interface methods `provide_model_parameters` and `set_model_parameter`.

**Returns** The ids of the optimizable model parameters

```python
def get_system_data() -> tc_python.abstract_base.SystemData
```

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

---

**Note:** Parameters can only be read from unencrypted (i.e. *user*) databases loaded as *.tdb*-file.

**Returns** The system data

```python
def invoke_dynamic_argument(argument_id: str)
```

Increases the number of instances of this dynamic argument by one, the argument will have an id such as `argument_1, argument_2, ...` if the dynamic argument is called `argument`.

---

**Note:** You can obtain all available dynamic arguments by using `get_dynamic_arguments()`.

**Parameters** **argument_id** – argument_id: The argument id

**Returns** This `PropertyModelCalculation` object

```python
def remove_all_conditions()
```

Removes all classic POLY conditions.

---

**Note:** This does not affect the compositions set by `set_composition()`.

**Returns** This `PropertyModelCalculation` object

```python
def remove_all_poly_commands()
```

Removes all previously added POLY Console Mode commands.

**Returns** This `PropertyModelCalculation` object

```python
def remove_dependent_element()
```

Removes a manually set dependent element. This method does not affect the automatic choice of the dependent element if `set_composition()` is used.

**Returns** This `PropertyModelCalculation` object
set_argument (argument: str, value: str)
Sets the specified model argument to the specified value. The id can be obtained with get_arguments().

Parameters
- argument – The argument id
- value – The value [unit according to the argument meaning]

Returns This PropertyModelCalculation object

set_composition (element_name: str, value: float)
Sets the composition of an element. The unit for the composition can be changed using set_composition_unit().

Default: Mole percent (CompositionUnit.MOLE_PERCENT)

Parameters
- element_name – The element
- value – The composition value [composition unit defined for the calculation]

Returns This PropertyModelCalculation object

set_composition_unit (unit_enum: tc_python.utils.CompositionUnit = CompositionUnit.MOLE_PERCENT)
Sets the composition unit.

Default: Mole percent (CompositionUnit.MOLE_PERCENT).

Parameters unit_enum – The new composition unit

Returns This PropertyModelCalculation object

set_condition (classic_condition: str, value: float)
Adds a classic POLY condition. If that method is used, all conditions need to be specified in such a way. If this method is used, it is necessary to set the dependent element manually using set_dependent_element().

Default if not specified: pressure P = 1e5 Pa, system size N = 1, Temperature T = 1000 K

Warning: It is not possible to mix POLY-commands and compositions using set_composition().

Note: It should not be necessary for most users to use this method, try to use set_composition() instead.

Warning: As this method runs raw POLY-commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten parenthesis, ...).

Parameters
- classic_condition – The classic POLY condition (for example: X(CR))
- value – The value of the condition

Returns This PropertyModelCalculation object
**set_dependent_element** *(dependent_element_name: str)*
Sets the dependent element manually.

**Note:** It should not be necessary for most users to use this method. Setting the dependent element manually is only necessary and allowed if *set_condition()* is used.

**Parameters**
- **dependent_element_name** – The name of the dependent element

**Returns**
This *PropertyModelCalculation* object

**set_model_parameter** *(model_parameter_id: str, value)*
Resets an optimizable model parameter. The id can be obtained with *get_model_parameters()*.

**Parameters**
- **model_parameter_id** – The model parameter id
- **value** – The new value of the parameter

**Returns**
This *PropertyModelCalculation* object

**set_temperature** *(temperature: float = 1000)*
Sets the temperature.

**Default:** 1000 K

**Parameters**
- **temperature** – The temperature [K]

**Returns**
This *PropertyModelCalculation* object

**with_system_modifications** *(system_modifications: tc_python.abstract_base.SystemModifications)*
Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

**Note:** This is only possible if the system has been read from unencrypted (i.e. *user*) databases loaded as a *.tdb*-file.

**Parameters**
- **system_modifications** – The system modification to be performed

**Returns**
This *PropertyModelCalculation* object

---

**class** *tc_python.propertymodel.PropertyModelResult*(result)*

**Bases:** *tc_python.abstract_base.AbstractResult*

The result of a Property Model calculation.

**get_result_quantities** () → Set[str]

Returns a list of the available result quantities defined in the Property Model.

**Returns**
The ids of the defined result quantities

**get_result_quantity_description** *(result_quantity_id) → str*

Returns the detailed description of the result quantity. The id can be obtained by *get_result_quantities()*.

**Parameters**
- **result_quantity_id** – The result quantity id

**Returns**
The detailed description
**get_single_equilibrium_result** *(result_quantity_id: str = '') → tc_python.single_equilibrium.SingleEquilibriumResult*

Returns a result quantity value. The available result quantities can be obtained by `get_result_quantities()`.

**Parameters**
- **result_quantity_id** – The id of the result quantity.

**Returns**
- The requested value [unit depending on the quantity], if the result is a SingleEquilibriumResult, is returned.

**get_value_of** *(result_quantity_id: str) → Union[float, Dict[str, float]]*

Returns a result quantity value. The available result quantities can be obtained by `get_result_quantities()`.

**Parameters**
- **result_quantity_id** – The id of the result quantity

**Returns**
- The requested value [unit depending on the quantity]. If the result is parameterized, parameter-value pairs are returned.

**save_to_disk** *(path: str)*

Saves the result to disk. The result can later be loaded using `tc_python.server.SetUp.load_result_from_disk()`.

**Parameters**
- **path** – The path to the result folder, can be relative or absolute.

**Returns**
- This `PropertyModelResult` object

---

**Note:** The result data is represented by a whole folder possibly containing multiple files.

---

### 5.1.8 Module “material_to_material”

**class** `tc_python.material_to_material.AbstractConstantCondition`

**Bases:** object

The abstract base class for all constant conditions.

**class** `tc_python.material_to_material.AbstractMaterialToMaterialCalculationAxis`

**Bases:** object

The abstract base class of all calculation axis.

**class** `tc_python.material_to_material.ConstantCondition`

**Bases:** `tc_python.material_to_material.AbstractConstantCondition`

A constant condition.

**classmethod** `fraction_of_material_b` *(fraction_of_material_b: float = 0.5)*

Creates a constant fraction of material B condition object.

**Note:** The unit depends on the composition unit setting in the calculator object.
classmethod temperature (temperature: float = 1000)
Creates a constant temperature condition object.

Parameters temperature – The temperature [K]

Returns The condition object

class tc_python.material_to_material.FractionOfMaterialBAxis (from_fraction: float = 0.0, 
to_fraction: float = 1.0, start_fraction: float = 0.5)
Bases: tc_python.material_to_material.MaterialToMaterialCalculationAxis
A fraction of material B axis.

class tc_python.material_to_material.FractionOfMaterialBCondition (fraction_of_material_b: float = 0.5)
Bases: tc_python.material_to_material.ConstantCondition
A constant fraction of material B condition.

class tc_python.material_to_material.MaterialToMaterialCalculationAxis
Bases: tc_python.material_to_material.AbstractMaterialToMaterialCalculationAxis
A calculation axis.

classmethod fraction_of_material_b (from_fraction: float = 0.0, to_fraction: float = 1.0, 
start_fraction: float = 0.5)
Creates a fraction of material B axis object.

Note: The unit depends on the composition unit setting in the calculator.

Parameters
• from_fraction – The left axis limit [weight-fraction or mole-fraction]
• to_fraction – The right axis limit [weight-fraction or mole-fraction]
• start_fraction – The start fraction of the calculation [weight-fraction or mole-fraction]

Returns A new FractionOfMaterialBAxis axis object

classmethod temperature (from_temperature: float = 1000, to_temperature: float = 3000, 
start_temperature: float = 2000)
Creates a temperature calculation axis object.

Parameters
• from_temperature – The left axis limit [K]
• to_temperature – The right axis limit [K]
• start_temperature – The start temperature of the calculation [K]

Returns A new TemperatureAxis condition object

class tc_python.material_to_material.MaterialToMaterialCalculationContainer (instance)
Bases: object
Provides access to the calculation objects for all Material to Material calculations.
These are specialised calculations for mixtures of two materials A and B. Otherwise they behave identical to the corresponding regular single equilibrium, property diagram and phase diagram calculations.

```python
with_phase_diagram_calculation (default_conditions: bool = True, components: List[str] = []) →
tc_python.material_to_material.MaterialToMaterialPhaseDiagramCalculation
```

Creates a Material to Material phase diagram (map) calculation.

**Parameters**

- **default_conditions** – If True, automatically sets the conditions $N=1$ and $P=100000$

- **components** – Specify here the components of the system (for example: [AL2O3, ...]), only necessary if they differ from the elements. If this option is used, all elements of the system need to be replaced by a component.

**Returns** A new `MaterialToMaterialPhaseDiagramCalculation` object

```python
with_property_diagram_calculation (default_conditions: bool = True, components: List[str] = []) →
tc_python.material_to_material.MaterialToMaterialPropertyDiagramCalculation
```

Creates a Material to Material property diagram (step) calculation.

**Parameters**

- **default_conditions** – If True, automatically sets the conditions $N=1$ and $P=100000$

- **components** – Specify here the components of the system (for example: [AL2O3, ...]), only necessary if they differ from the elements. If this option is used, all elements of the system need to be replaced by a component.

**Returns** A new `MaterialToMaterialPropertyDiagramCalculation` object

```python
with_single_equilibrium_calculation (default_conditions: bool = True, components: List[str] = []) →
tc_python.material_to_material.MaterialToMaterialSingleEquilibriumCalculation
```

Creates a Material to Material single equilibrium calculation.

**Parameters**

- **default_conditions** – If True, automatically sets the conditions $N=1$ and $P=100000$

- **components** – Specify here the components of the system (for example: [AL2O3, ...]), only necessary if they differ from the elements. If this option is used, all elements of the system need to be replaced by a component.

**Returns** A new `MaterialToMaterialSingleEquilibriumCalculation` object

```python
class tc_python.material_to_material.MaterialToMaterialPhaseDiagramCalculation (calculator)
Bases: tc_python.step_or_map_diagrams.AbstractPhaseDiagramCalculation
```

Configuration for a Material to Material phase diagram calculation.

**Note:** Specify the conditions, the calculation is performed with `calculate()`.

```python
add_initial_equilibrium (initial_equilibrium: tc_python.step_or_map_diagrams.InitialEquilibrium)
```

Add initial equilibrium start points from which a phase diagram is calculated.

Scans along the axis variables and generates start points when the scan procedure crosses a phase boundary.
It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the core remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria.

Parameters

- initial_equilibrium – The initial equilibrium

Returns

This `MaterialToMaterialPhaseDiagramCalculation` object

`calculate(keep_previous_results: bool = False) → tc_python.material_to_material.MaterialToMaterialPhaseDiagramResult`

Performs the phase diagram calculation.

**Warning:** If you use `keep_previous_results=True`, you must not use another calculator or even get results in between the calculations using `calculate()`. Then the previous results will actually be lost.

Parameters

- keep_previous_results – If True, results from any previous call to this method are appended. This can be used to combine calculations with multiple start points if the mapping fails at a certain condition.

Returns

A new `MaterialToMaterialPhaseDiagramResult` object which later can be used to get specific values from the calculated result.

disable_global_minimization()  
Disables global minimization.

Default: Enabled

Returns

This `MaterialToMaterialPhaseDiagramCalculation` object
dont_keep_default_equilibria()  
Do not keep the initial equilibria added by default.

This is only relevant in combination with `add_initial_equilibrium()`.

This is the default behavior.

Returns

This `MaterialToMaterialPhaseDiagramCalculation` object

enable_global_minimization()  
Enables global minimization.

Default: Enabled

Returns

This `MaterialToMaterialPhaseDiagramCalculation` object

get_components() → List[str]

Returns the names of the components in the system (including all components auto-selected by the database(s)).

Returns

The component names

get_gibbs_energy_addition_for(phase: str) → float

Used to get the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

Parameters

- phase – Specify the name of the (stoichiometric or solution) phase with the addition
Returns Gibbs energy addition to G per mole formula unit.

get_system_data() \rightarrow tc_python.abstract_base.SystemData

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

keep_default_equilibria()

Keep the initial equilibria added by default. This is only relevant in combination with add_initial_equilibrium().

Default behavior is to not keep default equilibria.

Returns This MaterialToMaterialPhaseDiagramCalculation object

remove_all_initial_equilibria()

Removes all previously added initial equilibria.

Returns This MaterialToMaterialPhaseDiagramCalculation object

run_poly_command(command: str)

Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

Parameters command – The Thermo-Calc Console Mode command

Returns This MaterialToMaterialPhaseDiagramCalculation object

Note: It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

Warning: As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

set_activities(activities: Dict[str, float])

Sets the constant activity conditions.

Note: The activity conditions are identical for both materials.

Parameters activities – The constant activities

Returns This MaterialToMaterialPhaseDiagramCalculation object

set_composition_unit(unit: tc_python.utils.CompositionUnit = <CompositionUnit.MASS_PERCENT: 3>)

Sets the composition unit of both materials A and B.

Default: Weight percent

Parameters unit – The composition unit of both materials A and B

Returns This MaterialToMaterialPhaseDiagramCalculation object
set_gibbs_energy_addition_for (phase: str, gibbs_energy: float)

Used to specify the additional energy term (always being a constant) of a given phase. The value (gibbs_energy) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

Parameters

• phase – Specify the name of the (stoichiometric or solution) phase with the addition

• gibbs_energy – Addition to G per mole formula unit

Returns This MaterialToMaterialPhaseDiagramCalculation object

set_material_a (composition: Dict[str, float], dependent_component: str = None)

Sets the composition of the material A.

The unit is set with set_composition_unit().

Tip: The material can also have constant activity conditions, they are set in set_activities().

Parameters

• composition – The composition of the material A

• dependent_component – The dependent component of the material A

Returns This MaterialToMaterialPhaseDiagramCalculation object

set_material_b (composition: Dict[str, float], dependent_component: str = None)

Sets the composition of the material B.

The unit is set with set_composition_unit().

Tip: The material can also have constant activity conditions, they are set in set_activities().

Parameters

• composition – The composition of the material B

• dependent_component – The dependent component of the material B

Returns This MaterialToMaterialPhaseDiagramCalculation object

set_phase_to_dormant (phase: str)

Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

Parameters phase – The phase name or ALL_PHASES for all phases

Returns This MaterialToMaterialPhaseDiagramCalculation object

set_phase_to_entered (phase: str, amount: float = 1.0)

Sets the phase to the status ENTERED, that is the default state.

Parameters

• phase – The phase name or ALL_PHASES for all phases

• amount – The phase fraction (between 0.0 and 1.0)
Returns This MaterialToMaterialPhaseDiagramCalculation object

**set_phase_to_fixed**(phase: str, amount: float)
Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

**Parameters**
- **phase** – The phase name
- **amount** – The fixed phase fraction (between 0.0 and 1.0)

**Returns** This MaterialToMaterialPhaseDiagramCalculation object

**set_phase_to_suspended**(phase: str)
Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters**
- **phase** – The phase name or ALL_PHASES for all phases

**Returns** This MaterialToMaterialPhaseDiagramCalculation object

**set_pressure**(pressure: float)
Sets the pressure (i.e. the condition $P$).

**Note:** If the flag default_conditions=True has been set during the creation of the calculator, the pressure is set to 1000 hPa by default.

**Parameters**
- **pressure** – The pressure [Pa]

**Returns** This MaterialToMaterialPhaseDiagramCalculation object

**set_system_size**(system_size: float)
Sets the system size (i.e. the condition ‘N’, the number of moles).

**Note:** If the flag default_conditions=True has been set during the creation of the calculator, the system size is set to 1.0 moles by default.

**Parameters**
- **system_size** – The system size [mole]

**Returns** This MaterialToMaterialPhaseDiagramCalculation object

**with_first_axis**(axis: tc_python.material_to_material.MaterialToMaterialCalculationAxis)
Sets the first axis (either temperature of fraction of material B). This calculation type requires that both temperature and fraction of material B axis are set.

**Parameters**
- **axis** – The axis

**Returns** This MaterialToMaterialPhaseDiagramCalculation object

**with_options**(options: tc_python.step_or_map_diagrams.PhaseDiagramOptions)
Sets the simulation options.

**Parameters**
- **options** – The simulation options

**Returns** This PhaseDiagramCalculation object

**with_reference_state**(component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)
The reference state for a component is important when calculating activities, chemical potentials and
enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

Parameters

- **component** – The name of the element must be given.
- **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
- **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
- **pressure** – The Pressure (in Pa) for the reference state.

Returns This `MaterialToMaterialPhaseDiagramCalculation` object

`with_second_axis` *(axis: tc_python.material_to_material.MaterialToMaterialCalculationAxis)*

Sets the second axis (either temperature or fraction of material B). This calculation type requires that both temperature and fraction of material B axis are set.

Parameters **axis** – The axis

Returns This `MaterialToMaterialPhaseDiagramCalculation` object

`with_system_modifications` *(system_modifications: tc_python.abstract_base.SystemModifications)*

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Note: This is only possible if the system has been read from unencrypted (i.e. *user*) databases loaded as a *.tdb*-file.

Parameters **system_modifications** – The system modification to be performed

Returns This `MaterialToMaterialPhaseDiagramCalculation` object

**class** `tc_python.material_to_material.MaterialToMaterialPhaseDiagramResult` *(result)*

**Bases:** `tc_python.step_or_map_diagrams.PhaseDiagramResult`

Result of a Material to Material phase diagram calculation, it can be evaluated using quantities or Console Mode syntax.
add_coordinates_for_phase_label (x: float, y: float)

Sets a coordinate in the result plot for which the stable phases will be evaluated and provided in the result data object. This can be used to plot the phases of a region into the phase diagram or just to programmatically evaluate the phases in certain regions.

**Warning:** This method takes coordinates of the plot axes and not of the calculation axis.

**Parameters**
- **x** – The coordinate of the first plot axis (“x-axis”) [unit of the plot axis]
- **y** – The coordinate of the second plot axis (“y-axis”) [unit of the plot axis]

**Returns** This MaterialToMaterialPhaseDiagramResult object

get_values_grouped_by_quantity_of (x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) → tc_python.step_or_map_diagrams.PhaseDiagramResultValues

Returns x-y-line data grouped by the multiple datasets of the specified quantities (for example in dependency of components). The available quantities can be found in the documentation of the factory class ThermodynamicQuantity. Usually the result data represents the phase diagram.

**Note:** The different datasets will contain NaN-values between different subsections and are not sorted (because they are unsortable due to their nature).

**Note:** It's possible to use functions as axis variables, either by using ThermodynamicQuantity, user_defined_function, or by using an expression that contains ‘=’.

**Example**

get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))

**Example**

get_values_grouped_by_quantity_of('T', 'CP=HM.T')

**Parameters**
- **x_quantity** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), MATERIAL_B_FRACTION, or even a function (for example ‘f=T+1.01’)
- **y_quantity** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), MATERIAL_B_FRACTION, or even a function (for example ‘CP=HM.T’)

**Returns** The phase diagram data

get_values_grouped_by_stable_phases_of (x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) → tc_python.step_or_map_diagrams.PhaseDiagramResultValues

Returns x-y-line data grouped by the sets of “stable phases” (for example “LIQUID” or “LIQUID + FCC_A1”). The available quantities can be found in the documentation of the factory class ThermodynamicQuantity. Usually the result data represents the phase diagram.
Note: The different datasets will contain NaN-values between different subsections and are not sorted (because they are unsortable due to their nature).

Note: It's possible to use functions as axis variables, either by using `ThermodynamicQuantity.user_defined_function`, or by using an expression that contains `='.`

Example

```python
get_values_grouped_by_quantity_of('T', 'ThermodynamicQuantity.user_defined_function('HM.T'))
```

Example

```python
get_values_grouped_by_quantity_of('T', 'CP=HM.T')
```

Parameters

- **x_quantity** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), `MATERIAL_B_FRACTION`, or even a function (for example ‘f=T*1.01’)

- **y_quantity** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), `MATERIAL_B_FRACTION`, or even a function (for example ‘CP=HM.T’)

Returns The phase diagram data

```python
remove_phase_labels()
```

Erases all added coordinates for phase labels.

Returns This `MaterialToMaterialPhaseDiagramResult` object

```python
save_to_disk(path: str)
```

Saves the result to disc. Note that a result is a folder, containing potentially many files. The result can later be loaded with `load_result_from_disk()`

Parameters `path` – the path to the folder you want the result to be saved in. It can be relative or absolute.

Returns this `MaterialToMaterialPhaseDiagramResult` object

```python
set_phase_name_style(phase_name_style_enum: tc_python.step_or_map_diagrams.PhaseNameStyle = <PhaseNameStyle.NONE: 0>)
```

Sets the style of the phase name labels that will be used in the result data object (constitution description, ordering description, …).

Default: PhaseNameStyle.NONE

Parameters `phase_name_style_enum` – The phase name style

Returns This `MaterialToMaterialPhaseDiagramResult` object

```python
class tc_python.material_to_material.MaterialToMaterialPropertyDiagramCalculation(calculator)
```

Bases: `tc_python.step_or_map_diagrams.AbstractPropertyDiagramCalculation`

Configuration for a Material to Material property diagram calculation.

Note: Specify the conditions and possibly other settings, the calculation is performed with `calculate()`.

```python
calculate(keep_previous_results: bool = False) -> tc_python.material_to_material.MaterialToMaterialPropertyDiagramResult
```

Performs the Material to Material property diagram calculation.
**Warning:** If you use `keep_previous_results=True`, you must not use another calculator or even get results in between the calculations using `calculate()`. Then the previous results will actually be lost.

**Parameters** `keep_previous_results` – If `True`, results from any previous call to this method are appended. This can be used to combine calculations with multiple start points if the stepping fails at a certain condition.

**Returns** A new `MaterialToMaterialPropertyDiagramResult` object which later can be used to get specific values from the calculated result

`disable_global_minimization()`  
Disables global minimization.  
**Default:** Enabled  
**Returns** This `MaterialToMaterialPropertyDiagramCalculation` object

`disable_step_separate_phases()`  
Disables step separate phases. This is the `default` setting.  
**Returns** This `MaterialToMaterialPropertyDiagramCalculation` object

`enable_global_minimization()`  
Enables global minimization.  
**Default:** Enabled  
**Returns** This `MaterialToMaterialPropertyDiagramCalculation` object

`enable_step_separate_phases()`  
Enables step separate phases.  
**Default:** By default separate phase stepping is `disabled`  
**Note:** This is an advanced option, it is used mostly to calculate how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIGMA-phase, G-phase, MU-phase, etc.).  
**Returns** This `MaterialToMaterialPropertyDiagramCalculation` object

`get_components()` → List[str]  
Returns the names of the components in the system (including all components auto-selected by the database(s)).  
**Returns** The component names

`get_gibbs_energy_addition_for(phase: str)` → float  
Used to get the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.  
It is not composition-, temperature- or pressure-dependent.  
**Parameters** `phase` – Specify the name of the (stoichiometric or solution) phase with the addition  
**Returns** Gibbs energy addition to G per mole formula unit.
get_system_data() \rightarrow tc_python.abstract_base.SystemData

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

**Note:** Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

Returns The system data

run_poly_command(command: str)

Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

**Parameters** command – The Thermo-Calc Console Mode command

**Returns** This MaterialToMaterialPropertyDiagramCalculation object

**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

set_activities(activities: Dict[str, float])

Sets the constant activity conditions.

**Note:** The activity conditions are identical for both materials.

**Parameters** activities – The constant activities

**Returns** This MaterialToMaterialPropertyDiagramCalculation object

set_composition_unit(unit: tc_python.utils.CompositionUnit = <CompositionUnit.MASS_PERCENT: 3>)

Sets the composition unit of both materials A and B.

Default: Weight percent

**Parameters** unit – The composition unit of both materials A and B

**Returns** This MaterialToMaterialPropertyDiagramCalculation object

set_gibbs_energy_addition_for(phase: str, gibbs_energy: float)

Used to specify the additional energy term (always being a constant) of a given phase. The value (gibbs_energy) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

**Parameters**

• phase – Specify the name of the (stoichiometric or solution) phase with the addition

• gibbs_energy – Addition to G per mole formula unit

**Returns** This MaterialToMaterialPropertyDiagramCalculation object
set_material_a (composition: Dict[str, float], dependent_component: str = None)
Sets the composition of the material A.
The unit is set with set_composition_unit().

**Tip:** The material can also have constant activity conditions, they are set in set_activities().

**Parameters**
- **composition** – The composition of the material A
- **dependent_component** – The dependent component of the material A

**Returns** This MaterialToMaterialPropertyDiagramCalculation object

set_material_b (composition: Dict[str, float], dependent_component: str = None)
Sets the composition of the material B.
The unit is set with set_composition_unit().

**Tip:** The material can also have constant activity conditions, they are set in set_activities().

**Parameters**
- **composition** – The composition of the material B
- **dependent_component** – The dependent component of the material B

**Returns** This MaterialToMaterialPropertyDiagramCalculation object

set_phase_to_dormant (phase: str)
Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

**Parameters** **phase** – The phase name or ALL_PHASES for all phases

**Returns** This MaterialToMaterialPropertyDiagramCalculation object

set_phase_to_entered (phase: str, amount: float = 1.0)
Sets the phase to the status ENTERED, that is the default state.

**Parameters**
- **phase** – The phase name or ALL_PHASES for all phases
- **amount** – The phase fraction (between 0.0 and 1.0)

**Returns** This MaterialToMaterialPropertyDiagramCalculation object

set_phase_to_fixed (phase: str, amount: float)
Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

**Parameters**
- **phase** – The phase name
- **amount** – The fixed phase fraction (between 0.0 and 1.0)

**Returns** This MaterialToMaterialPropertyDiagramCalculation object
set_phase_to_suspended (phase: str)
Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.

Parameters phase – The phase name or ALL_PHASES for all phases

Returns This `MaterialToMaterialPropertyDiagramCalculation` object

set_pressure (pressure: float)
Sets the pressure (i.e. the condition \( P \)).

Note: If the flag default_conditions=True has been set during the creation of the calculator, the pressure is set to 1000 hPa by default.

Parameters pressure – The pressure [Pa]

Returns This `MaterialToMaterialPropertyDiagramCalculation` object

set_system_size (system_size: float)
Sets the system size (i.e. the condition ‘N’, the number of moles).

Note: If the flag default_conditions=True has been set during the creation of the calculator, the system size is set to 1.0 moles by default.

Parameters system_size – The system size [mole]

Returns This `MaterialToMaterialPropertyDiagramCalculation` object

with_axis (axis: `tc_python.material_to_material.MaterialToMaterialCalculationAxis`)
Sets the axis (either temperature of fraction of material B). This calculation type requires that either temperature or fraction of material B is set as a constant condition - the other one is set as an axis.

Parameters axis – The axis

Returns This `MaterialToMaterialPropertyDiagramCalculation` object

with_constant_condition (condition: `tc_python.material_to_material.ConstantCondition`)
Sets the constant condition (either temperature of fraction of material B). This calculation type requires that either temperature or fraction of material B is set as a constant condition - the other one is set as an axis.

Parameters condition – The condition

Returns This `MaterialToMaterialPropertyDiagramCalculation` object

with_options (options: `tc_python.step_or_map_diagrams.PropertyDiagramOptions`)
Sets the simulation options.

Parameters options – The simulation options

Returns This `MaterialToMaterialPropertyDiagramCalculation` object

with_reference_state (component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)
The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.
All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

Parameters

- **component** – The name of the element must be given.
- **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
- **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
- **pressure** – The Pressure (in Pa) for the reference state.

Returns

This `MaterialToMaterialPropertyDiagramCalculation` object

with_system_modifications (system_modifications: tc_python.abstract_base.SystemModifications)

Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Note: This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb*-file.

5.1. Calculations

Note: The different datasets might contain NaN-values between different subsections and might not be sorted even if the flag `sort_and_merge` has been set (because they might be unsortable due to their nature).
Note: It’s possible to use functions as axis variables, either by using `ThermodynamicQuantity.user_defined_function`, or by using an expression that contains ‘='.  

Example
```python
get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))
```

Example
```python
get_values_grouped_by_quantity_of('T', 'CP=HM.T')
```

Parameters

- **x_quantity** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), `MATERIAL_B_FRACTION`, or even a function (for example ‘f=T*1.01’)

- **y_quantity** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), `MATERIAL_B_FRACTION`, or even a function (for example ‘CP=HM.T’)

- **sort_and_merge** – If True, the data is sorted and merged into as few subsections as possible (divided by NaN)

Returns

Containing the datasets with the quantities as their keys

```python
def get_values_grouped_by_stable_phases_of(x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], sort_and_merge: bool = True) -> Dict[str, tc_python.utils.ResultValueGroup]
```

Returns x-y-line data grouped by the sets of “stable phases” (for example “LIQUID” or “LIQUID + FCC_A1”). The available quantities can be found in the documentation of the factory class `ThermodynamicQuantity`.

Note: The different datasets might contain NaN-values between different subsections and different lines of an ambiguous dataset. They might not be sorted even if the flag `sort_and_merge` has been set (because they might be unsortable due to their nature).

Parameters

- **x_quantity** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’), `MATERIAL_B_FRACTION`, or even a function (for example ‘f=T*1.01’)

- **y_quantity** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’), `MATERIAL_B_FRACTION`, or even a function (for example ‘CP=HM.T’)

Returns

Containing the datasets with the quantities as their keys

```python
def get_values_grouped_by_quantity_of(x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], sort_and_merge: bool = True) -> Dict[str, tc_python.utils.ResultValueGroup]
```
• **sort_and_merge** – If True, the data will be sorted and merged into as few subsections as possible (divided by NaN)

**Returns** Containing the datasets with the quantities as their keys

```python
get_values_of(x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], y_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]) → [typing.List[float], typing.List[float]]
```

Returns sorted x-y-line data without any separation. Use `get_values_grouped_by_quantity_of()` or `get_values_grouped_by_stable_phases_of()` instead if you need such a separation. The available quantities can be found in the documentation of the factory class `ThermodynamicQuantity`.

**Note:** This method will always return sorted data without any NaN-values. If it is unsortable that might give data that is hard to interpret. In such a case you need to choose the quantity in another way or use one of the other methods. One example of this is to use quantities with All-markers, for example `MassFractionOfAComponent("All")`.

**Note:** It’s possible to use functions as axis variables, either by using `ThermodynamicQuantity.user_defined_function()`, or by using an expression that contains ‘=’.

**Example**

```python
get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))
```

**Example**

```python
get_values_grouped_by_quantity_of('T', 'CP=HM.T')
```

**Parameters**

• **x_quantity** – The first thermodynamic quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example ‘T’, `MATERIAL_B_FRACTION`, or even a function (for example ‘f=T*1.01’)).

• **y_quantity** – The second thermodynamic quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example ‘NV’, `MATERIAL_B_FRACTION`, or even a function (for example ‘CP=HM.T’))

**Returns** A tuple containing the x- and y-data in lists

```python
save_to_disk(path: str)
```

Saves the result to disc. Note that a result is a folder, containing potentially many files. The result can later be loaded with `load_result_from_disk()`

**Parameters** **path** – the path to the folder you want the result to be saved in. It can be relative or absolute.

**Returns** this `MaterialToMaterialPropertyDiagramResult` object

```python
set_phase_name_style(phase_name_style_enum: tc_python.step_or_map_diagrams.PhaseNameStyle = <PhaseNameStyle.NONE: 0>)
```

Sets the style of the phase name labels that will be used in the result data object (constitution description, ordering description, ...).

**Default:** PhaseNameStyle.NONETYPE

**Parameters** **phase_name_style_enum** – The phase name style

**Returns** This `MaterialToMaterialPropertyDiagramResult` object

## 5.1. Calculations
class tc_python.material_to_material.MaterialToMaterialSingleEquilibriumCalculation(calculator):
    Bases: tc_python.single_equilibrium.AbstractSingleEquilibriumCalculation

    Configuration for a Material to Material single fraction of B calculation.

    **Note:** Specify the conditions and possibly other settings, the calculation is performed with `calculate()`.

    `calculate()` → `tc_python.material_to_material.MaterialToMaterialSingleEquilibriumResult`

    Performs the material to material calculation.

    **Note:** The calculation result is **no** temporary result object.

    Returns A new `MaterialToMaterialSingleEquilibriumResult` object which can be used to get specific values from the calculated result. It is undefined behavior to use that object after the state of the calculation has been changed.

disable_global_minimization()
    Turns the global minimization completely off.

    Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

enable_global_minimization()
    Turns the global minimization on (using the default settings).

    Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

get_components() → List[str]
    Returns a list of components in the system (including all components auto-selected by the database(s)).

    Returns The components

get_gibbs_energy_addition_for(phase: str) → float
    Used to get the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

    It is not composition-, temperature- or pressure-dependent.

    **Parameters** phase – Specify the name of the (stoichiometric or solution) phase with the addition

    Returns Gibbs energy addition to G per mole formula unit.

get_system_data() → tc_python.abstract_base.SystemData
    Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

    **Note:** Parameters can only be read from unencrypted (i.e. `user`) databases loaded as `*.tdb-file`.

    Returns The system data

run_poly_command(command: str)
    Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

    **Parameters** command – The Thermo-Calc Console Mode command
Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

```python
set_activities(activities: Dict[str, float])
```
Sets the constant activity conditions.

**Note:** The activity conditions are identical for both materials.

**Parameters**
- **activities** – The constant activities

**Returns** This `MaterialToMaterialSingleEquilibriumCalculation` object

```python
set_component_to_entered(component: str)
```
Sets the specified component to the status ENTERED, that is the default state.

**Parameters**
- **component** – The component name or `ALL_COMPONENTS`

**Returns** This `MaterialToMaterialSingleEquilibriumCalculation` object

```python
set_component_to_suspended(component: str, reset_conditions: bool = False)
```
Sets the specified component to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters**
- **reset_conditions** – if ‘True’ also remove composition conditions for the component if they are defined
- **component** – The component name or `ALL_COMPONENTS`

**Returns** This `MaterialToMaterialSingleEquilibriumCalculation` object

```python
set_composition_unit(unit: tc_python.utils.CompositionUnit = <CompositionUnit.MASS_PERCENT: 3>)
```
Sets the composition unit of both materials A and B.

**Default:** Weight percent

**Parameters**
- **unit** – The composition unit of both materials A and B

**Returns** This `MaterialToMaterialSingleEquilibriumCalculation` object

```python
set_gibbs_energy_addition_for(phase: str, gibbs_energy: float)
```
Used to specify the additional energy term (always being a constant) of a given phase. The value given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature- or pressure-dependent.

**Parameters**
- **phase** – Specify the name of the (stoichiometric or solution) phase with the addition
- **gibbs_energy** – Addition to G per mole formula unit
Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_material_a** (composition: Dict[str, float], dependent_component: str = None)
Sets the composition of the material A.
The unit is set with `set_composition_unit()`.

Tip: The material can also have constant activity conditions, they are set in `set_activities()`.

Parameters

- composition – The composition of the material A
- dependent_component – The dependent component of the material A

Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_material_b** (composition: Dict[str, float], dependent_component: str = None)
Sets the composition of the material B.
The unit is set with `set_composition_unit()`.

Tip: The material can also have constant activity conditions, they are set in `set_activities()`.

Parameters

- composition – The composition of the material B
- dependent_component – The dependent component of the material B

Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_phase_to_dormant** (phase: str)
Sets the phase to the status DORMANT, necessary for calculating the driving force to form the specified phase.

Parameters phase – The phase name or `ALL_PHASES` for all phases

Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_phase_to_entered** (phase: str, amount: float = 1.0)
Sets the phase to the status ENTERED, that is the default state.

Parameters

- phase – The phase name or `ALL_PHASES` for all phases
- amount – The phase fraction (between 0.0 and 1.0)

Returns This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_phase_to_fixed** (phase: str, amount: float)
Sets the phase to the status FIXED, i.e. it is guaranteed to have the specified phase fraction after the calculation.

Parameters

- phase – The phase name
- amount – The fixed phase fraction (between 0.0 and 1.0)
**Returns**  This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_phase_to_suspended**(phase: str)  
Sets the phase to the status SUSPENDED, i.e. it is ignored in the calculation.  

**Parameters**  phase – The phase name or `ALL_PHASES` for all phases  

**Returns**  This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_pressure**(pressure: float)  
Sets the pressure (i.e. the condition $P$).

**Note:** If the flag `default_conditions=True` has been set during the creation of the calculator, the pressure is set to 1000 hPa by default.

**Parameters**  pressure – The pressure [Pa]  

**Returns**  This `MaterialToMaterialSingleEquilibriumCalculation` object

**set_system_size**(system_size: float)  
Sets the system size (i.e. the condition ‘N’, the number of moles).

**Note:** If the flag `default_conditions=True` has been set during the creation of the calculator, the system size is set to 1.0 moles by default.

**Parameters**  system_size – The system size [mole]  

**Returns**  This `MaterialToMaterialSingleEquilibriumCalculation` object

**with_first_constant_condition**(condition: `tc_python.material_to_material.ConstantCondition`)  
Sets the first constant condition (either temperature or fraction of material B).

**Parameters**  condition – The condition  

**Returns**  This `MaterialToMaterialSingleEquilibriumCalculation` object

**with_options**(options: `tc_python.single_equilibrium.SingleEquilibriumOptions`)  
Sets the simulation options.

**Parameters**  options – The simulation options  

**Returns**  This `SingleEquilibriumCalculation` object

**with_reference_state**(component: str, phase: str = 'SER', temperature: float = -1.0, pressure: float = 100000.0)  
The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using SER, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.
For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

Parameters

- **component** – The name of the element must be given.
- **phase** – Name of a phase used as the new reference state. Or SER for the Stable Element Reference.
- **temperature** – The Temperature (in K) for the reference state. Or CURRENT_TEMPERATURE which means that the current temperature is used at the time of evaluation of the reference energy for the calculation.
- **pressure** – The Pressure (in Pa) for the reference state.

Returns

This `MaterialToMaterialSingleEquilibriumCalculation` object

```python
with_second_constant_condition(condition: tc_python.material_to_material.ConstantCondition)
```
Sets the second constant condition (either temperature of fraction of material B).

Parameters condition – The condition

Returns

This `MaterialToMaterialSingleEquilibriumCalculation` object

```python
with_system_modifications(system_modifications: tc_python.abstract_base.SystemModifications)
```
Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

Parameters system_modifications – The system modification to be performed

Returns

This `MaterialToMaterialSingleEquilibriumCalculation` object

```python
class tc_python.material_to_material.MaterialToMaterialSingleEquilibriumResult(result)
Bases: tc_python.single_equilibrium.SingleEquilibriumResult
```
Result of a Material To Material calculation for a single fraction of material B, it can be evaluated using a quantity or Console Mode syntax.

```python
change_pressure(pressure: float)
```
Change the pressure and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with higher performance. The properties are calculated at the new pressure using the phase amount, temperature and composition of phases from the initial equilibrium. Use `get_value_of()` to obtain them.

Parameters pressure – The pressure [Pa]

Returns

This `MaterialToMaterialSingleEquilibriumResult` object

```python
change_temperature(temperature: float)
```
Change the temperature and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with high performance. The properties are calculated at the new temperature using the phase amount, pressure and composition of phases from the initial equilibrium. Use `get_value_of()` to obtain them.
**Note:** This is typically used when calculating room temperature properties (e.g. density) for a material when it is assumed that the equilibrium phase amount and composition freeze-in at a higher temperature during cooling.

**Parameters** `temperature` – The temperature [K]

**Returns** This `MaterialToMaterialSingleEquilibriumResult` object

`get_components()` → List[str]

Returns the names of the components selected in the system (including any components auto-selected by the database(s)).

**Returns** The names of the selected components

`get_conditions()` → List[str]

Returns the conditions.

**Returns** The selected conditions

`get_phases()` → List[str]

Returns the phases present in the system due to its configuration. It also contains all phases that have been automatically added during the calculation, this is the difference to the method `System.get_phases_in_system()`.

**Returns** The names of the phases in the system including automatically added phases

`get_stable_phases()` → List[str]

Returns the stable phases (i.e. the phases present in the current equilibrium).

**Returns** The names of the stable phases

`get_value_of(quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str])` → float

Returns a value from a single equilibrium calculation.

**Parameters** `quantity` – The thermodynamic quantity to get the value of; a Console Mode syntax strings can be used as an alternative (for example “NPM(FCC_A1)”)  

**Returns** The requested value

`run_poly_command(command: str)`  

Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine. This affects only the state of the result object.

**Parameters** `command` – The Thermo-Calc Console Mode command

**Returns** This `MaterialToMaterialSingleEquilibriumResult` object

**Note:** It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

**Warning:** As this method runs raw Thermo-Calc commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten equals sign).

`save_to_disk(path: str)`  

Saves the result to disk. Note that the result is a folder, containing potentially many files. The result can later be loaded with `load_result_from_disk()`
Parameters **path** – the path to the folder you want the result to be saved in. It can be relative or absolute.

**Returns** this `MaterialToMaterialSingleEquilibriumResult` object

class `tc_python.material_to_material.TemperatureAxis` *(from_temperature: float = 1000, to_temperature: float = 3000, start_temperature: float = 2000)*

Bases: `tc_python.material_to_material.MaterialToMaterialCalculationAxis`

A temperature calculation axis.

class `tc_python.material_to_material.TemperatureCondition` *(temperature: float = 1000.0)*

Bases: `tc_python.material_to_material.ConstantCondition`

A constant temperature condition.

### 5.2 Module “system”

class `tc_python.system.MultiDatabaseSystemBuilder` *(multi_database_system_builder)*

Bases: object

Used to select databases, elements, phases etc. and create a System object. The difference to the class SystemBuilder is that the operations are performed on all the previously selected databases. The system is then used to create calculations.

*create_and_select_species* *(stoichiometry: str)*

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. The created species will also be automatically selected.

**Note:** The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis “()” nor an underscore “_” is allowed in the chemical formula, while the special combination “/-” or “/+” can be used. Consult the Thermo-Calc database documentation for details about the syntax.

Parameters **stoichiometry** – The stoichiometry of the species

**Returns** This `MultiDatabaseSystemBuilder` object

deselect_constituent_on_sublattice *(phase_name: str, sublattice_no: int, constituent_name_to_deselect: str)*

Rejects a constituent on a sublattice in a phase in both the thermodynamic and the kinetic database.

Parameters

- **phase_name** – The name of the phase
- **sublattice_no** – The number of the sublattice (starting with 1)
- **constituent_name_to_deselect** – The name of the constituent to deselect

**Returns** This `MultiDatabaseSystemBuilder` object

deselect_phase *(phase_name_to_deselect: str)*

Rejects a phase for both the thermodynamic and the kinetic database.

Parameters **phase_name_to_deselect** – The phase name

**Returns** This `MultiDatabaseSystemBuilder` object
deselect_species(species_name: str)
Removes the species from the system.

Parameters
species_name – The species

Returns This MultiDatabaseSystemBuilder object

get_system() → tc_python.system.System
Creates a new System object that is the basis for all calculation types. Several calculation types can be defined later from the object; these are independent.

Returns A new System object

select_constituent_on_sublattice(phase_name: str, sublattice_no: int, constituent_name_to_select: str)
Selects a constituent on a sublattice in a phase in both the thermodynamic and the kinetic database.

Note: Previously the third parameter constituent_name_to_select had a wrong name, it has been corrected in version 2021b.

Parameters
• phase_name – The name of the phase
• sublattice_no – The number of the sublattice (starting with 1)
• constituent_name_to_select – The name of the constituent to select

Returns This MultiDatabaseSystemBuilder object

select_phase(phase_name_to_select: str)
Selects a phase for both the thermodynamic and the kinetic database.

Parameters
phase_name_to_select – The phase name

Returns This MultiDatabaseSystemBuilder object

select_species(species_name: str)
Adds the species to the system. Up to 1000 species can be defined in a single system.

Parameters
species_name – The species

Returns This MultiDatabaseSystemBuilder object

with_new_composition_set(composition_set: tc_python.entities.CompositionSet)
Used to enter two or more composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.

The databases often create the typical composition sets for phases automatically when data are retrieved. The equilibrium calculations (using the default settings with global minimization) will usually add new composition sets if needed.

Note: Precipitation and diffusion calculations can require the user to define additional composition sets. E.g. in the case where the new composition set is needed in the configuration of the calculation.

Parameters
composition_set – the composition set

Returns This MultiDatabaseSystemBuilder object
without_default_phases()
Rejects all the default phases from both the thermodynamic and the kinetic database, any phase now needs to be selected manually for the databases.

Returns This MultiDatabaseSystemBuilder object

class tc_python.system.System (system_instance)
Bases: object
A system containing selections for databases, elements, phases etc.

Note: For the defined system, different calculations can be configured and run. Instances of this class should always be created from a SystemBuilder.

Note: The system object is immutable, i.e. it cannot be changed after it has been created. If you want to change the system, you must instead create a new one.

convert_composition (input_composition: Dict[str, float],
                          input_unit: tc_python.utils.ConversionUnit,
                          output_unit: tc_python.utils.ConversionUnit,
                          dependent_component: str = '') ➞ Dict[str, float]
Provides conversion between composition units for any combination of chemical compounds. It is fast because no thermodynamic equilibrium calculation is involved.


Note: It is not required that the chemical compounds are components of the database. The only requirement is that all elements are present in the database.

Parameters

• input_composition – Composition (for example: {“Al2O3”: 25.0, “FeO”: 75.0})
• input_unit – Unit of the input composition
• output_unit – Requested output unit
• dependent_component – The dependent component (optional), for example: “Fe”.
  If no dependent component is specified the sum of the input composition needs to match 100% / 1

Returns The composition in the requested output unit

get_all_elements_in_databases () ➞ List[str]
Returns the names of all elements present in the selected databases, regardless of the actual selection of elements.

Returns A list of element names

get_all_phases_in_databases () ➞ List[str]
Returns all phase names present in the selected databases, regardless of selected elements, phases etc.

Returns A list of phase names

get_all_species_in_databases () ➞ List[str]
Returns all species names present in the selected databases, regardless of the actual selection of elements, phases, ….
Returns A list of species names

\texttt{get\_element\_object}(element\_name: str) \rightarrow tc\_python.entities.Element

Returns the \texttt{Element} object of an element. This can be used to obtain detailed information about the element.

\textbf{Parameters} element\_name – The element name

\textbf{Returns} A \texttt{Element}: object

\texttt{get\_elements\_in\_system}() \rightarrow List[str]

Returns the names of all elements present in the selected system.

\textbf{Note:} The list does not contain any elements or components that have been auto-selected by the database(s) in a calculator. Use the \texttt{get\_components()} of the calculator object instead to get the complete information.

\textbf{Returns} A list of element names

\texttt{get\_phase\_object}(phase\_name: str) \rightarrow tc\_python.entities.Phase

Returns the \texttt{Phase} object of a phase. This can be used to obtain detailed information about the phase.

\textbf{Parameters} phase\_name – The phase name

\textbf{Returns} A \texttt{Phase}: object

\texttt{get\_phases\_in\_system}() \rightarrow List[str]

Returns all phase names present in the system due to its configuration (selected elements, phases, etc.).

\textbf{Returns} A list of phase names

\texttt{get\_references}() \rightarrow Dict[str, List[str]]

Provides a dictionary with database references per database in the selected system.

\textbf{Returns} The database references

\texttt{get\_species\_in\_system}() \rightarrow List[str]

Returns the names of all species present in the selected system.

\textbf{Note:} The list does not contain any species or components that have been auto-selected by the database(s) in a calculator. Use the \texttt{get\_components()} of the calculator object instead to get the complete information.

\textbf{Returns} The list of species names

\texttt{get\_species\_object}(species\_name: str) \rightarrow tc\_python.entities.Species

Returns the \texttt{Species} object of an species. This can be used to obtain detailed information about the species.

\textbf{Parameters} species\_name – The species name

\textbf{Returns} A \texttt{Species}: object

\texttt{get\_system\_data}() \rightarrow tc\_python.abstract\_base.SystemData

Returns the content of the database. This can be used to modify the parameters and functions and to change the current system by using \texttt{with\_system\_modifications()}.  

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Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

**Returns** The system data

```python
with_batch_equilibrium_calculation(default_conditions: bool = True,
components: List[str] = []) → tc_python.batch_equilibrium.BatchEquilibriumCalculation
```

Creates a batch-equilibrium calculation (a vectorized equilibrium calculation).

**Note:** Use this instead of looping if you want to calculate equilibria for a larger number of compositions and know the conditions in advance. This calculation type has improved performance when calculating a large number of equilibria when each individual calculations is quick. E.g. when evaluating single phase properties for thousands of compositions.

**Parameters**

- **default_conditions** – If *True*, automatically sets the conditions $N=1$ and $P=100000$
- **components** – Specify here the components of the system (for example: `[AL2O3, ...]`), only necessary if they differ from the elements. If this option is used, all elements of the system need to be replaced by a component.

**Returns** A new `BatchEquilibriumCalculation` object

```python
with_cct_precipitation_calculation() → tc_python.precipitation.PrecipitationCCTCalculation
```

Creates a CCT diagram calculation.

**Returns** A new `PrecipitationCCTCalculation` object

```python
with_isothermal_diffusion_calculation() → tc_python.diffusion.DiffusionIsoThermalCalculation
```

Creates an isothermal diffusion calculation.

**Returns** A new `DiffusionIsoThermalCalculation` object

```python
with_isothermal_precipitation_calculation() → tc_python.precipitation.PrecipitationIsoThermalCalculation
```

Creates an isothermal precipitation calculation.

**Returns** A new `PrecipitationIsoThermalCalculation` object

```python
with_material_to_material() → tc_python.material_to_material.MaterialToMaterialCalculationContainer
```

Provides access to all Material to Material calculations. The actual calculation needs to be chosen in the returned object.

**Returns** A new `MaterialToMaterialCalculationContainer` object

```python
with_non_isothermal_diffusion_calculation() → tc_python.diffusion.DiffusionNonIsoThermalCalculation
```

Creates a non-isothermal precipitation calculation.

**Returns** A new `PrecipitationNonIsoThermalCalculation` object

```python
with_non_isothermal_precipitation_calculation() → tc_python.precipitation.PrecipitationNonIsoThermalCalculation
```

Creates a non-isothermal precipitation calculation.

**Returns** A new `PrecipitationNonIsoThermalCalculation` object
with_phase_diagram_calculation(default_conditions: bool = True,
components: List[str] = []) \rightarrow tc_python.step_or_map_diagrams.PhaseDiagramCalculation

Creates a phase diagram (map) calculation.

Parameters

• default_conditions – If True, automatically sets the conditions \( N=1 \) and \( P=100000 \)

• components – Specify here the components of the system (for example: [\( \text{AL}_2\text{O}_3, \ldots \)]), only necessary if they differ from the elements. If this option is used, all elements of the system need to be replaced by a component.

Returns A new PhaseDiagramCalculation object

with_property_diagram_calculation(default_conditions: bool = True,
components: List[str] = []) \rightarrow tc_python.step_or_map_diagrams.PropertyDiagramCalculation

Creates a property diagram (step) calculation.

Parameters

• default_conditions – If True, automatically sets the conditions \( N=1 \) and \( P=100000 \)

• components – Specify here the components of the system (for example: [\( \text{AL}_2\text{O}_3, \ldots \)]), only necessary if they differ from the elements. If this option is used, all elements of the system need to be replaced by a component.

Returns A new PropertyDiagramCalculation object

with_property_model_calculation(model: str, path_to_models: str = '',
default_conditions: bool = True,
components: List[str] = []) \rightarrow tc_python.propertymodel.PropertyModelCalculation

Creates a Property Model calculation.

The parameter debug_model is only used when debugging self-developed models.

Parameters

• model – The Property Model to be calculated.

• path_to_models – The path where the Property Models are installed. If no value is entered, the Property Models folder used by the normal Thermo-Calc application is used.

• debug_model – Used when debugging self-developed models.

Returns A new PropertyModelCalculation object

with_scheil_calculation() \rightarrow tc_python.scheil.ScheilCalculation

Creates a Scheil solidification calculation.

**Warning:** Scheil calculations do not support the GAS phase being selected, this means the "GAS" phase must always be deselected in the system if it is present in the database

Returns A new ScheilCalculation object

with_single_equilibrium_calculation(default_conditions: bool = True,
components: List[str] = []) \rightarrow tc_python.single_equilibrium.SingleEquilibriumCalculation

Creates a single equilibrium calculation.
Parameters

- **default_conditions** – If True, automatically sets the conditions \( N=1 \) and \( P=100000 \).

- **components** – Specify here the components of the system (for example: \([\text{AL}_2\text{O}_3, \ldots]\)), only necessary if they differ from the elements. If this option is used, all elements of the system need to be replaced by a component.

Returns A new `SingleEquilibriumCalculation` object

with_ttt_precipitation_calculation() \( \rightarrow \) `tc_python.precipitation.PrecipitationTTTCalculation`

Creates a TTT diagram calculation.

Returns A new `PrecipitationTTTCalculation` object

```python
class tc_python.system.SystemBuilder(system_builder)
Bases: object

Used to select databases, elements, phases etc. and create a System object. The system is then used to create calculations.

create_and_select_species(stoichiometry: str)

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. The created species will also be automatically selected.

Parameters

- **stoichiometry** – The stoichiometry of the species

Returns This `SystemBuilder` object

deselect_constituent_on_sublattice(phase_name: str, sublattice_no: int, constituent_name_to_deselect: str)

Rejects a constituent on a sublattice in a phase in the last specified database only.

Parameters

- **phase_name** – The name of the phase

- **sublattice_no** – The number of the sublattice (starting with 1)

- **constituent_name_to_deselect** – The name of the constituent to deselect

Returns This `SystemBuilder` object

deselect_phase(phase_name_to_deselect: str)

Rejects a phase in the last specified database only.

Parameters

- **phase_name_to_deselect** – The name of the phase

Returns This `SystemBuilder` object

deselect_species(stoichiometry: str)

Removes the species from the system.

Parameters

- **stoichiometry** – The species

Returns This `SystemBuilder` object
**get_system() → tc_python.system.System**

Creates a new System object that is the basis for all calculation types. Several calculation types can be defined later from the object; these are independent.

**Returns** A new System object

**get_system_for_scheil_calculations() → tc_python.system.System**

Creates a new System object without gas phases being selected, that is the basis for all calculation types, but its particularly useful for Scheil solidification calculations, where the model does not allow that a gas phase is selected in the system.

Several calculation types can be defined later from the object; these are independent.

**Returns** A new System object

**select_constituent_on_sublattice(phase_name: str, sublattice_no: int, constituent_name_to_select: str)**

Selects a constituent on a sublattice in a phase in the last specified database only.

**Note:** Previously the third parameter constituent_name_to_select had a wrong name, it has been corrected in version 2021b.

**Parameters**

- **phase_name** – The name of the phase
- **sublattice_no** – The number of the sublattice (starting with 1)
- **constituent_name_to_select** – The name of the constituent to select

**Returns** This SystemBuilder object

**select_database_and_elements(database_name: str, list_of_element_strings: List[str])**

Selects a thermodynamic or kinetic database and its selected elements (that will be appended). After that, phases can be selected or unselected.

**Parameters**

- **database_name** – The database name, for example “FEDEMO”
- **list_of_element_strings** – A list of one or more elements as strings, for example [“Fe”, “C”]

**Returns** This SystemBuilder object

**select_phase(phase_name_to_select: str)**

Selects a phase in the last specified database only.

**Parameters** **phase_name_to_select** – The name of the phase

**Returns** This SystemBuilder object

**select_species(stoichiometry: str)**

Adds the species to the system. Up to 1000 species can be defined in a single system.

**Parameters** **stoichiometry** – The species

**Returns** This SystemBuilder object

**select_user_database_and_elements(path_to_user_database: str, list_of_element_strings: List[str])**

Selects a thermodynamic database which is a user-defined database and select its elements (that will be appended).
Note: By using a r-literal, it is possible to use slashes on all platforms, also on Windows: `select_user_database_and_elements(r"my path/user_db.tdb", ["Fe", "Cr"])

Otherwise it is required to use **double** backslashes on Windows as separator.

Note: On Linux and Mac the path is case-sensitive, also the file ending.

Parameters

- **path_to_user_database** – The path to the database file ("database".TDB), defaults to the current working directory. Only the filename is required if the database is located in the same folder as the script.

- **list_of_element_strings** – A list of one or more elements as strings, for example ["Fe", "C"]

Returns This `SystemBuilder` object

**with_new_composition_set**(composition_set: `tc_python.entities.CompositionSet`)

Used to enter composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.

Parameters **composition_set** – The composition set

Returns This `SystemBuilder` object

**without_default_phases**()

Rejects all default phases in the last specified database only, any phase needs now to be selected manually for that database.

Returns This `SystemBuilder` object

### 5.3 Module “entities”

class `tc_python.entities.CompositionSet`(phase_name: str)

Bases: object

Used by the method `tc_python.system.SystemBuilder.with_new_composition_set()` to enter two or more composition sets for a phase.

Parameters **phase_name** – The name of the phase for which a new composition set is required

**set_major_constituents_for_sublattice**(sublattice_index: int, major_constituents: List[str])

Specify the new major constituent(s) for the sublattice.

Default: If not specified, a default is automatically chosen based on the specified composition set.

Note: This is useful in order to make calculations converge faster and more easily (because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set). **The databases often set major constituents for several phases automatically when the data is retrieved.**
Parameters

- `sublattice_index` – Index of the sublattice to set the major constituents for (starting with 1)
- `major_constituents` – Optional list of the major constituents, which must be selected from the phase constitution of the current system.

Returns This `CompositionSet` object

class `tc_python.entities.Element` (element)

Bases: `object`

Represents an element, making detailed information about the element accessible.

`get_enthalpy` () → float
Returns the enthalpy of the element at 298 K, part of the stable element reference state (SER).

Returns The enthalpy [J]

`get_entropy_diff_0_to_298k` () → float
Returns the entropy difference 0 - 298 K of the element, part of the stable element reference state (SER).

Returns The entropy difference 0 - 298 K [J/K]

`get_molar_mass` () → float
Returns the molar mass of the element.

Returns The molar mass [g/mol]

`get_name` () → str
Returns the name of the element.

Returns The element name

`get_stable_element_reference` () → str
Returns the stable element reference (i.e. the stable phase at 298.15 K and 1 bar, reference for all element thermodynamic data).

Returns The name of the stable element reference

`is_interstitial` () → bool
Returns if the element is interstitial.

Note: In the diffusion simulations (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes.

Returns If the element is interstitial

`is_special` () → bool
Returns if the element is special (i.e. vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase)).

Returns If the element is special

`is_valid` () → bool
Returns if the element is valid. Non-valid elements are represented by an empty name.

Returns If the element is valid

5.3. Module “entities”
class tc_python.entities.Phase(phase)
    Bases: object

Represents a phase, making detailed information about the phase accessible.

    get_name() \rightarrow \text{str}
        Returns the name of the phase.

        \textbf{Returns}: The phase name

    get_species() \rightarrow \text{Set[tc_python.entities.Species]}
        Returns the species of the phase.

        \textbf{Returns}: A set containing the species

    get_species_for_composition_profile() \rightarrow \text{Set[tc_python.entities.Species]}
        Returns all species that need to be defined in a composition profile of the phase for diffusion simulations - except for one species that needs to be the dependent species.

        \textbf{Note}: In a composition profile of a phase for diffusion simulations it is necessary to specify all non-stoichiometric and non-special species. In case of a DILUTE diffusion model, the database enforces the choice of a certain dependent species.

        \textbf{Returns}: Set with the species

    get_sublattices() \rightarrow \text{List[tc_python.entities.Sublattice]}
        Returns the sublattices of the phase in a well-defined contiguous order.

        \textbf{Returns}: A list containing the Sublattice objects

    get_type() \rightarrow \text{tc_python.entities.PhaseType}
        Returns the type of the phase (liquid, ionic liquid, solid, gas).

        \textbf{Returns}: The type of a phase

    has_diffusion_data() \rightarrow \text{bool}
        Returns if diffusion data exists for the phase.

        \textbf{Returns}: If diffusion data exists for the phase

    has_molar_volume_data() \rightarrow \text{bool}
        Returns if molar volume data exists for the phase.

        \textbf{Returns}: If molar volume data exists for the phase

    is_dilute_diffusion_model() \rightarrow \text{bool}
        Returns if diffusion is described using the DILUTE model for the phase. This will always return False if no diffusion data is available.

        \textbf{Returns}: If the DILUTE model is used

    is_gas() \rightarrow \text{bool}
        Returns if the phase is a gas phase.

        \textbf{Returns}: If the phase is a gas phase

    is_ionic_liquid() \rightarrow \text{bool}
        Returns if the phase is an ionic liquid phase.

        \textbf{Returns}: If the phase is an ionic liquid phase
is_liquid() \rightarrow \text{bool}

Returns if the phase is a liquid or ionic liquid phase.

**Returns** If the phase is a liquid phase

is_solid() \rightarrow \text{bool}

Returns if the phase is a solid phase.

**Returns** If the phase is a solid phase

class \text{tc\_python\_entities\_PhaseType}(\text{value})

Bases: \text{enum\_Enum}

The type of a phase.

\text{GAS} = 0

Gas phase.

\text{IONIC\_LIQUID} = 2

Ionic liquid phase.

\text{LIQUID} = 1

Liquid phase.

\text{SOLID} = 3

Solid phase.

class \text{tc\_python\_entities\_Species}(\text{species})

Bases: \text{object}

Represents a species, making detailed information about the species accessible.

get_all_elements() \rightarrow \text{List}[\text{Tuple}[\text{tc\_python\_entities\_Element}, \text{float}]]

Returns all the elements that the species is composed of.

**Returns** List of all elements of the species and their stoichiometry

get_charge() \rightarrow \text{int}

Returns the charge of the species.

**Returns** The charge of the species

get_name() \rightarrow \text{str}

Returns the name of the species.

**Returns** The species name

is_element() \rightarrow \text{bool}

Returns if the species actually represents an element.

**Returns** If the species represents an element

is_interstitial() \rightarrow \text{bool}

Returns if the species is interstitial.

**Note:** In the diffusion simulations (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes.

**Returns** If the species is interstitial
is_special() → bool
Returns if the species is special (i.e. vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase)).

Returns If the species is special

is_valid() → bool
Returns if the species is valid. Non-valid species are represented by an empty name.

Returns If the species is valid

to_element() → tc_python.entities.Element
Returns the Element representation of the species - if the species actually represents an element.

Returns The Element object

class tc_python.entities.Sublattice(sublattice)
Bases: object
Represents a sublattice of a phase.

get_constituents() → Set[tc_python.entities.Species]
Returns the constituents of the sublattice.

Returns A set containing the constituents

get_nr_of_sites() → float
Returns the number of sites in the sublattice.

Returns A float number

5.4 Module “server”

class tc_python.server.LoggingPolicy(value)
Bases: enum.Enum
Logging policy that determines how the TC-Python logs are presented to the user.

FILE = 1
Logging to a file.

NONE = 2
No logging at all.

SCREEN = 0
Logging to the screen.

class tc_python.server.ResultLoader(result_loader)
Bases: object
Contains methods for loading results from previously done calculations.

diffusion(path: str) → tc_python.diffusion.DiffusionCalculationResult
Loads a DiffusionCalculationResult from disc.

Parameters path – path to the folder where result was previously saved.

Returns A new DiffusionCalculationResult object which later can be used to get specific values from the calculated result

phase_diagram(path: str) → tc_python.step_or_map_diagrams.PhaseDiagramResult
Loads a PhaseDiagramResult from disc.
Parameters `path` – path to the folder where result was previously saved.

Returns A new `PhaseDiagramResult` object which later can be used to get specific values from the calculated result.

`precipitation_TTT_or_CCT(path: str) → tc_python.precipitation.PrecipitationCalculationTTTorCCTResult`

Loads a `PrecipitationCalculationTTTorCCTResult` from disc.

Parameters `path` – path to the folder where result was previously saved.

Returns A new `PrecipitationCalculationTTTorCCTResult` object which later can be used to get specific values from the calculated result.

`precipitation_single(path: str) → tc_python.precipitation.PrecipitationCalculationSingleResult`

Loads a `PrecipitationCalculationSingleResult` from disc.

Parameters `path` – path to the folder where result was previously saved.

Returns A new `PrecipitationCalculationSingleResult` object which later can be used to get specific values from the calculated result.

`property_diagram(path: str) → tc_python.step_or_map_diagrams.PropertyDiagramResult`

Loads a `PropertyDiagramResult` from disc.

Parameters `path` – path to the folder where result was previously saved.

Returns A new `PropertyDiagramResult` object which later can be used to get specific values from the calculated result.

`property_model(path: str) → tc_python.propertymodel.PropertyModelResult`

Loads a `PropertyModelResult` from disc.

Parameters `path` – path to the folder where result was previously saved.

Returns A new `PropertyModelResult` object which later can be used to get specific values from the calculated result.

`scheil(path: str) → tc_python.scheil.ScheilCalculationResult`

Loads a `ScheilCalculationResult` from disc.

Parameters `path` – path to the folder where result was previously saved.

Returns A new `ScheilCalculationResult` object which later can be used to get specific values from the calculated result.

`single_equilibrium(path: str) → tc_python.single_equilibrium.SingleEquilibriumResult`

Loads a `SingleEquilibriumResult` from disc.

Parameters `path` – path to the folder where result was previously saved.

Returns A new `SingleEquilibriumResult` object which later can be used to get specific values from the calculated result.

class `tc_python.server.SetUp(debug_logging=False)`

Bases: object

Starting point for all calculations.

**Note:** This class exposes methods that have no precondition, it is used for choosing databases and elements.

`disable_caching()`

A previously set cache folder is no longer used.
Note: Within the session, caching is activated and used through the default temporary directory.

Returns This SetUp object

get_database_info (database_short_name: str) \(\rightarrow\) str
Obtains the short information available for the specified database.

Parameters database_short_name – The name of the database (i.e. “FEDEMO”, …)

Returns The short information about the database

get_database_path_on_disk (database_short_name: str) \(\rightarrow\) str
Obtains the path to the database file on disk. TCPATH is a placeholder for the root path of the used Thermo-Calc installation.

Note: Encrypted databases (*.TDC) cannot be edited.

Parameters database_short_name – The name of the database (i.e. “FEDEMO”, …)

Returns The path to the database on disk

get_databases () \(\rightarrow\) List[str]
Obtains the short names of all databases available in the used Thermo-Calc installation.

Note: Only databases with a valid license are listed.

Returns List of the available databases

get_property_models (path_to_models: str = '') \(\rightarrow\) Set[str]
Lists the names of all Property Models in the specified directory.

If the directory is not specified, the Property Model folder used by the normal Thermo-Calc application is used.

Parameters path_to_models – The path where the Property Models are installed. If no value is entered, the Property Model folder used by the normal Thermo-Calc application is used.

Returns Set containing all Property Model names

load_result_from_disk () \(\rightarrow\) tc_python.server.ResultLoader
Loads a previously calculated result from disk.

Note: This only works for results created by calling one of the save_result () methods on a Result class created from a calculation.

Returns A new ResultLoader object

select_database_and_elements (database_name: str, list_of_elements: List[str]) \(\rightarrow\) tc_python.system.SystemBuilder
Selects a first thermodynamic or kinetic database and selects the elements in it.
Parameters

- **database_name** – The name of the database, for example “FEDEMO”
- **list_of_elements** – The list of the selected elements in that database, for example [“Fe”, “C”]

Returns A new SystemBuilder object

**select_thermodynamic_and_kinetic_databases_with_elements** *(thermodynamic_db_name: str, kinetic_db_name: str, list_of_elements: List[str]) → tc_python.system.MultiDatabaseSystemBuilder*

Selects the thermodynamic and kinetic database at once, guarantees that the databases are added in the correct order. Further rejection or selection of phases applies to both databases.

Parameters

- **thermodynamic_db_name** – The thermodynamic database name, for example “FEDEMO”
- **kinetic_db_name** – The kinetic database name, for example “MFEDMO”
- **list_of_elements** – The list of the selected elements in that database, for example [“Fe”, “C”]

Returns A new MultiDatabaseSystemBuilder object

**select_user_database_and_elements** *(path_to_user_database: str, list_of_elements: List[str]) → tc_python.system.SystemBuilder*

Selects a user-defined database and selects the elements in it.

**Note:** By using a r-literal, it is possible to use slashes on all platforms, also on Windows: *select_user_database_and_elements(r“my path/user_db.tdb”, [“Fe”, “Cr”])*

Otherwise it is required to use **double** back-slashes on Windows as separator.

**Note:** On Linux and Mac the path is case-sensitive, also the file ending.

Parameters

- **path_to_user_database** – The path to the database file (“database”.TDB), defaults to the current working directory. Only filename is required if the database is located in the same folder as the script.
- **list_of_elements** – The list of the selected elements in that database, for example [“Fe”, “C”]

Returns A new SystemBuilder object

**set_cache_folder** *(path: str = '', precision_for_floats: int = 12)*

Sets a folder where results from calculations and state of systems are saved. If at any time a calculation is run which has the exact same setting as a previous, the calculation is not re-run. The result is instead loaded from this folder.
Note: The same folder can be used in several scripts, and it can even be shared between different users. It can be a network folder.

Parameters

- **path** – path to the folder where results should be stored. It can be relative or absolute.
- **precision_for_floats** – The number of significant figures used when comparing if the calculation has the same setting as a previous.

Returns This SetUp object

```python
set_ges_version (version: int = 6)
```

Setting the version of the Gibbs Energy System (GES).

Parameters **version** – The GES-version (currently version 5 or 6)

Returns This SetUp object

```python
set_log_level_to_debug ()
```

Sets log level to DEBUG

Returns This SetUp object

```python
set_log_level_to_info ()
```

Sets log level to INFO

Returns This SetUp object

```python
class tc_python.server.TCPython (logging_policy=<LoggingPolicy.SCREEN: 0>, log_file=None, debug_mode=False, debug_logging=False, do_throw_on_backend_hard_crash=True, port_number=0)
```

Starting point of the API. Typical syntax:

```python
with TCPython() as session:
    session.select_database_and_elements(...)```

Note: Each usage of `with TCPython()` causes significant overhead (starting a new process, stopping the old one, cleaning up the temporary disk space). Usually it is recommendable to call `with TCPython()` only once for each process, even if working in a loop. Instead you should pass the session or calculator object into the loop and use them there.

If necessary, beginning from version 2019a it is however possible to call `with TCPython` safely multiple times.

```python
tc_python.server.start_api_server (logging_policy=<LoggingPolicy.SCREEN: 0>, log_file=None, debug_mode=False, is_unittest=False, do_throw_on_backend_hard_crash=True, port_number=0)
```

Starts a process of the API server and sets up the socket communication with it.

Parameters

- **logging_policy** – Determines if the TC-Python log output is sent to the screen (LoggingPolicy.SCREEN), to file (LoggingPolicy.FILE) or nothing is logged at all (LoggingPolicy.NONE) Default: LoggingPolicy.SCREEN. Note that the log-handlers can also be adapted through the `tc_python.LOGGER` object at any time.
- **log_file** – The log-file relative to the current path or absolute, only relevant if `logging_policy=LoggingPolicy.FILE`. Log-output will be appended.
- **debug_mode** – If True it is tried to open a connection to an already running API-server. This is only used for debugging the API itself.
- **is_unittest** – Should be True if called by a unit test, only to be used internally for development.
- **do_throw_on_backend_hard_crash** – If True an `UnrecoverableCalculationException` will be thrown if the Java-backend crashes hard, if False the application will simply crash with a FORTRAN-stacktrace. If True the exception can be caught outside of the ‘with’-clause and the application can continue, if False more information about the error is shown by the stacktrace.
- **port_number** – The port number for the communication with the Java-backend server. This is not required to be changed by normal users.

**Warning:** Most users should use **TCPython** using a with-statement for automatic management of the resources (network sockets and temporary files). If you anyway need to use that method, make sure to call `stop_api_server()` in any case using the try-finally-pattern.

```python
tc_python.server.start_matlab_server(logging_policy=<LoggingPolicy.SCREEN: 0>,
    log_file=None, debug_mode=False, is_unittest=False,
    do_throw_on_backend_hard_crash=True,
    port_number=0)
```

```python
tc_python.server.stop_api_server(gateway_id: str = None)
```

Cleans all resources used by the session (i.e. shuts down the API server and deletes all temporary files). The disk usage of temporary files might be significant.

**Warning:** Call this method only if you used `start_api_server()` initially. It should never be called when the API has been initialized in a with-statement using **TCPython**.

### 5.5 Module “quantity_factory”

class **tc_python.quantity_factory.DiffusionQuantity**  
**Bases:** tc_python.quantity.AbstractQuantity  

Factory class providing quantities used for defining diffusion simulations and their results.

**Note:** In this factory class only the most common quantities are defined, you can always use the Console Mode syntax strings in the respective methods as an alternative (for example: “NPM(*)”).

```python
classmethod activity_of_component(component: str, use_ser: bool = False) → tc_python.quantity.ActivityOfComponent
```

Creates a quantity representing the activity of a component.

**Parameters**

- **component** – The name of the component, use ALL_COMPONENTS to choose all components
• **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state is be
used if this setting is set to *False*.

**Returns** A new *ActivityOfComponent* object.

```python
classmethod chemical_diffusion_coefficient
tc_python.quantity.ChemicalDiffusionCoefficient
```

Creates a quantity representing the chemical diffusion coefficient of a phase \([m^2/s]\).

**Parameters**

- **phase** – The name of the phase
- **diffusing_element** – The diffusing element
- **gradient_element** – The gradient element
- **reference_element** – The reference element (for example “Fe” in a steel)

**Returns** A new *ChemicalDiffusionCoefficient* object.

```python
classmethod chemical_potential_of_component
    (component: str, use_ser: bool = False) →
tc_python.quantity.ChemicalPotentialOfComponent
```

Creates a quantity representing the chemical potential of a component \([J]\).

**Parameters**

- **component** – The name of the component, use *ALL_COMPONENTS* to choose all com-
  - **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state is used
  if this setting is set to *False*.

**Returns** A new *ChemicalPotentialOfComponent* object.

```python
classmethod distance
    (region: str = 'All') → tc_python.quantity.Distance
```

Creates a quantity representing the distance \([m]\).

**Parameters** **region** – The name of the region or *All* to choose global.

```python
classmethod intrinsic_diffusion_coefficient
tc_python.quantity.IntrinsicDiffusionCoefficient
```

Creates a quantity representing the intrinsic diffusion coefficient of a phase \([m^2/s]\).

**Parameters**

- **phase** – The name of the phase
- **diffusing_element** – The diffusing element
- **gradient_element** – The gradient element
- **reference_element** – The reference element (for example “Fe” in a steel)

**Returns** A new *IntrinsicDiffusionCoefficient* object.

```python
classmethod L_bis
tc_python.quantity.Lbis
```

Creates a quantity representing \(L^*\) of a phase \([m^2/s]\).

**Parameters**
• **phase** – The name of the phase
• **diffusing_element** – The diffusing element
• **gradient_element** – The gradient element
• **reference_element** – The reference element (for example “Fe” in a steel)

**Returns** A new \( Lbis \) object.

```python
classmethod mass_fraction_of_a_component(component: str) →
tc_python.quantity.MassFractionOfAComponent
```
Creates a quantity representing the mass fraction of a component.

**Parameters**
- **component** – The name of the component or **ALL_COMPONENTS** to choose all components

**Returns** A new MassFractionOfAComponent object.

```python
classmethod mass_fraction_of_a_phase(phase: str) →
tc_python.quantity.MassFractionOfAPhase
```
Creates a quantity representing the mass fraction of a phase.

**Parameters**
- **phase** – The name of the phase or **ALL_PHASES** to choose all phases.

**Returns** A new MassFractionOfAPhase object.

```python
classmethod mobility_of_component_in_phase(phase: str, component: str) →
tc_python.quantity.MobilityOfComponentInPhase
```
Creates a quantity representing the mobility of a component in a phase \([m^2/Js]\).

**Parameters**
- **phase** – The name of the phase
- **component** – The name of the component

**Returns** A new MobilityOfComponentInPhase object.

```python
classmethod mole_fraction_of_a_component(component: str) →
tc_python.quantity.MoleFractionOfAComponent
```
Creates a quantity representing the mole fraction of a component.

**Parameters**
- **component** – The name of the component or **ALL_COMPONENTS** to choose all components

**Returns** A new MoleFractionOfAComponent object.

```python
classmethod mole_fraction_of_a_phase(phase: str) →
tc_python.quantity.MoleFractionOfAPhase
```
Creates a quantity representing the mole fraction of a phase.

**Parameters**
- **phase** – The name of the phase or **ALL_PHASES** to choose all phases

**Returns** A new MoleFractionOfAPhase object.

```python
classmethod position_of_lower_boundary_of_region(region: str) →
tc_python.quantity.PositionOfLowerBoundaryOfRegion
```
Creates a quantity representing the position of lower boundary of a region \([m]\).

**Parameters**
- **region** – The name of the region

**Returns** A new PositionOfLowerBoundaryOfRegion object.

```python
classmethod position_of_upper_boundary_of_region(region: str) →
tc_python.quantity.PositionOfUpperBoundaryOfRegion
```
Creates a quantity representing the position of upper boundary of a region \([m]\).

---

5.5. Module “quantity_factory”
Parameters `region` – The name of the region


classmethod `temperature()` → `tc_python.quantity.Temperature`

Creates a quantity representing the temperature [K].

Returns A new `Temperature` object.


Creates a quantity representing thermodynamic factor of a phase.

Parameters

- `phase` – The name of the phase
- `diffusing_element` – The diffusing element
- `gradient_element` – The gradient element
- `reference_element` – The reference element (for example “Fe” in a steel)

Returns A new `ThermoDynamicFactor` object.

classmethod `time()` → `tc_python.quantity.Time`

Creates a quantity representing the time [s].


classmethod `total_mass_fraction_of_component(component: str)` → `tc_python.quantity.TotalMassFractionOfComponent`

Creates a quantity representing the total mass fraction of a component.

Parameters `component` – The name of the component

Returns A new `TotalMassFractionOfComponent` object.

classmethod `total_mass_fraction_of_component_in_phase(phase: str, component: str)` → `tc_python.quantity.TotalMassFractionOfComponentInPhase`

Creates a quantity representing the total mass fraction of a component in a phase.

Parameters

- `phase` – The name of the phase
- `component` – The name of the component

Returns A new `TotalMassFractionOfComponentInPhase` object.

classmethod `total_mass_fraction_of_phase(phase: str)` → `tc_python.quantity.TotalMassFractionOfPhase`

Creates a quantity representing the total mass fraction of a phase.

Parameters `phase` – The name of the phase.

Returns A new `TotalMassFractionOfPhase` object.

classmethod `total_mole_fraction_of_component(component: str)` → `tc_python.quantity.TotalMoleFractionOfComponent`

Creates a quantity representing the total mole fraction of a component.

Parameters `component` – The name of the component

Returns A new `TotalMoleFractionOfComponent` object.
classmethod total_mole_fraction_of_component_in_phase(phase: str, component: str) → tc_python.quantity.TotalMoleFractionOfComponentInPhase

Creates a quantity representing the total mole fraction of a component in a phase.

Parameters

• phase – The name of the phase
• component – The name of the component

Returns A new TotalMoleFractionOfComponentInPhase object.

classmethod total_volume_fraction_of_phase(phase: str) → tc_python.quantity.TotalVolumeFractionOfPhase

Creates a quantity representing the total volume fraction of a phase.

Parameters phase – The name of the phase.

Returns A new TotalVolumeFractionOfPhase object.

classmethod tracer_diffusion_coefficient(phase: str, diffusing_element: str) → tc_python.quantity.TracerDiffusionCoefficient

Creates a quantity representing tracer diffusion coefficient of a phase [m^2/s].

Parameters

• phase – The name of the phase
• diffusing_element – The diffusing element

Returns A new TracerDiffusionCoefficient object.

classmethod u_fraction_of_a_component(component: str) → tc_python.quantity.UFractionOfAComponent

Creates a quantity representing the u-fraction of a component.

Parameters component – The name of the component

Returns A new UFractionOfAComponent object.

classmethod user_defined_function(expression: str) → tc_python.quantity.Function

Creates a quantity representing a user-defined function.

Parameters expression – The function expression

Returns A new Function object

classmethod velocity_of_lower_boundary_of_region(region: str) → tc_python.quantity.VelocityOfLowerBoundaryOfRegion

Creates a quantity representing the velocity of lower boundary of a region [m/s].

Parameters region – The name of the region

Returns A new VelocityOfLowerBoundaryOfRegion object.

classmethod velocity_of_upper_boundary_of_region(region: str) → tc_python.quantity.VelocityOfUpperBoundaryOfRegion

Creates a quantity representing the velocity of upper boundary of a region [m/s].

Parameters region – The name of the region

Returns A new VelocityOfUpperBoundaryOfRegion object.

classmethod width_of_region(region: str) → tc_python.quantity.Function

Creates a quantity representing the width of a region [m].

Parameters region – The name of the region
Returns A new WidthOfRegion object.

class tc_python.quantity_factory.IndependentVariable
Bases: tc_python.quantity.AbstractQuantity

Factory class providing quantities used for defining the independent variable in general diffusion result querying.

classmethod distance(region: str = 'All') → tc_python.quantity.Distance

Creates an independent variable representing the distance [m].

Returns A new Distance object
classmethod time() → tc_python.quantity.Time

Creates an independent variable representing the time [s].

Returns A new Time object

class tc_python.quantity_factory.PlotCondition
Bases: tc_python.quantity.AbstractQuantity

Factory class providing quantities used for defining the plot condition in general diffusion result querying.

Note: In this factory class only the most common quantities are defined, you can always use the Console Mode syntax strings in the respective methods as an alternative (for example: “time last”).

classmethod distance(distancepoint: float, region: str = 'All') → tc_python.quantity.DistanceCondition

Creates a plot condition representing the distance [m].

Change in version 2019b: Mandatory parameter distancepoint added

Parameters

• distancepoint – The distance from the lower interface of the region
• region – The name of the region or All to choose global.

Returns A new DistanceCondition object
classmethod integral() → tc_python.quantity.IntegralCondition

Creates an integral plot condition.

Returns A new IntegralCondition object
classmethod interface(region: str, interface_position: tc_python.utils.InterfacePosition) → tc_python.quantity.InterfaceCondition

Creates a plot condition representing an interface between two regions.

Parameters

• region – The name of the region used for defining the interface
• interface_position – The position of the interface relative to that region (lower or upper)

Returns A new InterfaceCondition object
classmethod time(timepoint: Union[float, str] = 'Last') → tc_python.quantity.TimeCondition

Creates a plot condition representing the time [s].

Change in version 2019b: Lists of timepoints are no longer supported

Parameters timepoint – The timepoint. Optionally “Last” can be used for the end of the simulation
Returns A new `TimeCondition` object

class tc_python.quantity_factory.ScheilQuantity
Bases: tc_python.quantity.AbstractQuantity

Factory class providing quantities used for defining a Scheil calculation result (`tc_python.scheil.ScheilCalculationResult`).

classmethod apparent_heat_capacity_per_gram() → tc_python.quantity.ApparentHeatCapacityPerGram

Creates a quantity representing the apparent heat capacity [J/g/K].

Returns A new `ApparentHeatCapacityPerGram` object.

classmethod apparent_heat_capacity_per_mole() → tc_python.quantity.ApparentHeatCapacityPerMole

Creates a quantity representing the apparent heat capacity [J/mol/K].

Returns A new `ApparentHeatCapacityPerMole` object.

classmethod apparent_volumetric_thermal_expansion_coefficient() → tc_python.quantity.ApparentVolumetricThermalExpansionCoefficient

Creates a quantity representing the apparent volumetric thermal expansion coefficient of the system [1/K].

Returns A new `ApparentVolumetricThermalExpansionCoefficient` object.

classmethod composition_of_phase_as_mole_fraction(phase: str, component: str) → tc_python.quantity.CompositionOfPhaseAsMoleFraction

Creates a quantity representing the composition of a phase [mole-fraction].

Parameters

- **phase** – The name of the phase, use `ALL_PHASES` to choose all stable phases
- **component** – The name of the component, use `ALL_COMPONENTS` to choose all components

Returns A new `CompositionOfPhaseAsMoleFraction` object.

classmethod composition_of_phase_as_weight_fraction(phase: str, component: str) → tc_python.quantity.CompositionOfPhaseAsWeightFraction

Creates a quantity representing the composition of a phase [weight-fraction].

Parameters

- **phase** – The name of the phase, use `ALL_PHASES` to choose all stable phases
- **component** – The name of the component, use `ALL_COMPONENTS` to choose all components

Returns A new `CompositionOfPhaseAsWeightFraction` object.

classmethod density_of_phase(phase: str) → tc_python.quantity.DensityOfPhase

Creates a quantity representing the average density of a phase [g/cm^3].

Parameters **phase** – The name of the phase or `ALL_PHASES` to choose all phases

Returns A new `DensityOfPhase` object.

classmethod density_of_solid_phase(phase: str) → tc_python.quantity.DensityOfSolidPhase

Creates a quantity representing the average density of a solid phase [g/cm^3].

Note: Deprecated in version 2022a: This quantity has been renamed to `density_of_phase()`. It will be removed in release 2023a.

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Parameters phase – The name of the phase or ALL_PHASES to choose all solid phases

Returns A new DensityOfSolidPhase object.

classmethod density_of_system() → tc_python.quantity.DensityOfSystem

Creates a quantity representing the average density of the system [g/cm^3].

Returns A new DensityOfSystem object.

classmethod distribution_of_component_of_phase(phase: str, component: str) →
tc_python.quantity.DistributionOfComponentOfPhase

Creates a quantity representing the (molar) fraction of the specified component being present in the specified phase compared to the overall system [-]. This corresponds to the degree of segregation to that phase.

Parameters

• phase – The name of the phase

• component – The name of the component

Returns A new DistributionOfComponentOfPhase object.

classmethod heat_per_gram() → tc_python.quantity.HeatPerGram

Creates a quantity representing the total heat release from the liquidus temperature down to the current temperature [J/g].

Note: The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (latent_heat_per_mole() and latent_heat_per_gram()), and the other is the heat related to the specific heat of liquid and solid phases (heat_per_mole() and heat_per_gram()).

Returns A new HeatPerGram object.

classmethod heat_per_mole() → tc_python.quantity.HeatPerMole

Creates a quantity representing the total heat release from the liquidus temperature down to the current temperature [J/mol].

Note: The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (latent_heat_per_mole() and latent_heat_per_gram()), and the other is the heat related to the specific heat of liquid and solid phases (heat_per_mole() and heat_per_gram()).

Returns A new HeatPerMole object.

classmethod latent_heat_per_gram() → tc_python.quantity.LatentHeatPerGram

Creates a quantity representing the cumulated latent heat release from the liquidus temperature down to the current temperature [J/g].

Note: The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (latent_heat_per_mole() and latent_heat_per_gram()), and the other is the heat related to the specific heat of liquid and solid phases (heat_per_mole() and heat_per_gram()).

Returns A new LatentHeatPerGram object.
classmethod latent_heat_per_mole() → tc_python.quantity.LatentHeatPerMole

Creates a quantity representing the cumulated latent heat release from the liquidus temperature down to the current temperature [J/mol].

**Note:** The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (`latent_heat_per_mole()` and `latent_heat_per_gram()`), and the other is the heat related to the specific heat of liquid and solid phases (`heat_per_mole()` and `heat_per_gram()`).

**Returns** A new `LatentHeatPerMole` object.

classmethod mass_fraction_of_a_solid_phase(phase: str) → tc_python.quantity.MassFractionOfASolidPhase

Creates a quantity representing the mass fraction of a solid phase.

**Parameters** phase – The name of the phase or `ALL_PHASES` to choose all solid phases

**Returns** A new `MassFractionOfASolidPhase` object.

classmethod mass_fraction_of_all_liquid() → tc_python.quantity.MassFractionOfAllLiquid

Creates a quantity representing the total mass fraction of all the liquid phase.

**Returns** A new `MassFractionOfAllLiquid` object.

classmethod mass_fraction_of_all_solid_phases() → tc_python.quantity.MassFractionOfAllSolidPhases

Creates a quantity representing the total mass fraction of all solid phases.

**Returns** A new `MassFractionOfAllSolidPhases` object.

classmethod molar_volume_of_phase(phase: str) → tc_python.quantity.MolarVolumeOfPhase

Creates a quantity representing the molar volume of a phase [m^3/mol].

**Parameters** phase – The name of the phase or `ALL_PHASES` to choose all phases

**Returns** A new `MolarVolumeOfPhase` object.

classmethod molar_volume_of_system() → tc_python.quantity.MolarVolumeOfSystem

Creates a quantity representing the molar volume of the system [m^3/mol].

**Returns** A new `MolarVolumeOfSystem` object.

classmethod mole_fraction_of_a_solid_phase(phase: str) → tc_python.quantity.MoleFractionOfASolidPhase

Creates a quantity representing the molar fraction of a solid phase.

**Parameters** phase – The name of the phase or `ALL_PHASES` to choose all solid phases

**Returns** A new `MoleFractionOfASolidPhase` object.

classmethod mole_fraction_of_all_liquid() → tc_python.quantity.MoleFractionOfAllLiquid

Creates a quantity representing the total molar fraction of all the liquid phase.

**Returns** A new `MoleFractionOfAllLiquid` object.

classmethod mole_fraction_of_all_solid_phases() → tc_python.quantity.MoleFractionOfAllSolidPhases

Creates a quantity representing the total molar fraction of all solid phases.

**Returns** A new `MoleFractionOfAllSolidPhases` object.
classmethod site_fraction_of_component_in_phase(phase: str, component: str, sub_lattice_ordinal_no: int = 0) → tc_python.quantity.SiteFractionOfComponentInPhase

Creates a quantity representing the site fractions [-].

Parameters

- **phase** – The name of the phase, use `ALL_PHASES` to choose all stable phases
- **component** – The name of the component, use `ALL_COMPONENTS` to choose all components
- **sub_lattice_ordinal_no** – The ordinal number (i.e. 1, 2, ...) of the sublattice of interest, use None to choose all sublattices

Note: Detailed information about the sublattices can be obtained by getting the `Phase` object of a phase from the `System` object using `tc_python.system.System.get_phase_in_system`. For each phase the sublattices are obtained by using `tc_python.system.Phase.get_sublattices`. The order in the returned list is equivalent to the sublattice ordinal number expected, but note that the ordinal numbers start with 1.

Returns A new SiteFractionOfComponentInPhase object.

classmethod temperature() → tc_python.quantity.Temperature

Creates a quantity representing the temperature [K].

Returns A new Temperature object.

class tc_python.quantity_factory.ThermodynamicQuantity
Bases: tc_python.quantity.AbstractQuantity

Factory class providing quantities used for defining equilibrium calculations (single equilibrium, property and phase diagrams, ...) and their results.

Note: In this factory class only the most common quantities are defined, you can always use the Console Mode syntax strings in the respective methods as an alternative (for example: “NPM(*")

classmethod activity_of_component(component: str, use_ser: bool = False) → tc_python.quantity.ActivityOfComponent

Creates a quantity representing the activity of a component [-].

Parameters

- **component** – The name of the component, use `ALL_COMPONENTS` to choose all components
- **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state is used if this setting is set to `False`.

Returns A new ActivityOfComponent object.


Creates a quantity representing the chemical diffusion coefficient of a phase [m²/s].
Parameters

- **phase** – The name of the phase
- **diffusing_element** – The diffusing element
- **gradient_element** – The gradient element
- **reference_element** – The reference element (for example “Fe” in a steel)

Returns A new ChemicalDiffusionCoefficient object.

classmethod chemical_potential_of_component(component: str, use_ser: bool = False) → tc_python.quantity.ChemicalPotentialOfComponent

Creates a quantity representing the chemical potential of a component [J].

Parameters

- **component** – The name of the component, use ALL_COMPONENTS to choose all components
- **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state is used if this setting is set to False.

Returns A new ChemicalPotentialOfComponent object.

classmethod composition_of_phase_as_mole_fraction(phase: str, component: str = 'All') → tc_python.quantity.CompositionOfPhaseAsMoleFraction

Creates a quantity representing the composition of a phase [mole-fraction].

Parameters

- **phase** – The name of the phase, use ALL_PHASES to choose all stable phases
- **component** – The name of the component, use ALL_COMPONENTS to choose all components

Returns A new CompositionOfPhaseAsMoleFraction object.

classmethod composition_of_phase_as_weight_fraction(phase: str, component: str) → tc_python.quantity.CompositionOfPhaseAsWeightFraction

Creates a quantity representing the composition of a phase [weight-fraction].

Parameters

- **phase** – The name of the phase, use ALL_PHASES to choose all stable phases
- **component** – The name of the component, use ALL_COMPONENTS to choose all components

Returns A new CompositionOfPhaseAsWeightFraction object.

classmethod gibbs_energy_of_a_phase(phase: str, use_ser: bool = False) → tc_python.quantity.GibbsEnergyOfAPhase

Creates a quantity representing the Gibbs energy of a phase [J].

Parameters

- **phase** – The name of the phase or ALL_PHASES to choose all phases
- **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state will be used when this setting is set to False.

Returns A new GibbsEnergyOfAPhase object.
classmethod mass_fraction_of_a_component(component: str) → tc_python.quantity.MassFractionOfAComponent

Creates a quantity representing the mass fraction of a component.

Parameters component – The name of the component or ALL_COMPONENTS to choose all components

Returns A new MassFractionOfAComponent object.

classmethod mass_fraction_of_a_phase(phase: str) → tc_python.quantity.MassFractionOfAPhase

Creates a quantity representing the mass fraction of a phase.

Parameters phase – The name of the phase or ALL_PHASES to choose all phases.

Returns A new MassFractionOfAPhase object.

classmethod mole_fraction_of_a_component(component: str) → tc_python.quantity.MoleFractionOfAComponent

Creates a quantity representing the mole fraction of a component.

Parameters component – The name of the component or ALL_COMPONENTS to choose all components

Returns A new MoleFractionOfAComponent object.

classmethod mole_fraction_of_a_phase(phase: str) → tc_python.quantity.MoleFractionOfAPhase

Creates a quantity representing the mole fraction of a phase.

Parameters phase – The name of the phase or ALL_PHASES to choose all phases

Returns A new MoleFractionOfAPhase object.

classmethod normalized_driving_force_of_a_phase(phase: str) → tc_python.quantity.NormalizedDrivingForceOfAPhase

Creates a quantity representing normalized driving force of a phase [-].

Warning: A driving force calculation requires that the respective phase has been set to the state DORMANT. The parameter All is only reasonable if all phases have been set to that state.

Parameters phase – The name of the phase or ALL_PHASES to choose all phases

Returns A new DrivingForceOfAPhase object.

classmethod pressure() → tc_python.quantity.Pressure

Creates a quantity representing the pressure [Pa].

Returns A new Pressure object.

classmethod system_size() → tc_python.quantity.SystemSize

Creates a quantity representing the system size [mol].

Returns A new SystemSize object.

classmethod temperature() → tc_python.quantity.Temperature

Creates a quantity representing the temperature [K].

Returns A new Temperature object.

classmethod tracer_diffusion_coefficient(phase: str, diffusing_element: str) → tc_python.quantity.TracerDiffusionCoefficient

Creates a quantity representing tracer diffusion coefficient of a phase [m^2/s].
Parameters

- **phase** – The name of the phase
- **diffusing_element** – The diffusing element

Returns A new TracerDiffusionCoefficient object.

classmethod **u_fraction_of_a_component** (component: str) → tc_python.quantity.UFractionOfAComponent

Creates a quantity representing the u-fraction of a component.

Parameters **component** – The name of the component

Returns A new UFractionOfAComponent object.

classmethod **user_defined_function** (expression: str) → tc_python.quantity.Function

Creates a quantity representing a user-defined function.

Parameters **expression** – The function expression

Returns A new Function object

classmethod **volume_fraction_of_a_phase** (phase: str) → tc_python.quantity.VolumeFractionOfAPhase

Creates a quantity representing the volume fraction of a phase.

Parameters **phase** – The name of the phase or ALL_PHASES to choose all phases

Returns A new VolumeFractionOfAPhase object.

### 5.6 Module “utils”

class **tc_python.utils.CompositionUnit** (value)

    Bases: enum.Enum

    The composition unit.

    **MASS_FRACTION** = 2
    Mass fraction.

    **MASS_PERCENT** = 3
    Mass percent.

    **MOLE_FRACTION** = 0
    Mole fraction.

    **MOLE_PERCENT** = 1
    Mole percent.

class **tc_python.utils.ConversionUnit** (value)

    Bases: enum.Enum

    The composition unit used in a conversion.

    **MOLE_FRACTION** = 0
    Mole fraction.

    **MOLE_PERCENT** = 1
    Mole percent.

    **WEIGHT_FRACTION** = 2
    Weight fraction.
WEIGHT_PERCENT = 3
Weight percent.

class tc_python.utils.InterfacePosition(value)
Bases: enum.Enum
The position of an interface relative to its region. Only used for diffusion simulations.

LOWER = 0
The interface is on the lower side of its region.

UPPER = 1
The interface is on the upper side of its region.

class tc_python.utils.ResultValueGroup(result_line_group_java)
Bases: object
A x-y-dataset representing a line data calculation result (i.e. a Thermo-Calc quantity 1 vs. quantity 2).

Warning: Depending on the calculator, the dataset might contain NaN-values to separate the data between different subsets.

Variables

- **label** – a str describing what the data corresponds to
- **x** – list of floats representing the first quantity (“x-axis”)  
- **y** – list of floats representing the second quantity (“y-axis”)

    get_label() \(\rightarrow\) str
    Accessor for the line label :return the line label

    get_x() \(\rightarrow\) List[float]
    Accessor for the x-values :return the x values

    get_y() \(\rightarrow\) List[float]
    Accessor for the y-values :return the y values

class tc_python.utils.TemperatureProfile
Bases: object
Represents a time-temperature profile used by non-isothermal calculations.

Note: The total simulation time can differ from the defined temperature profile. Constant temperature is assumed for any timepoint after the end of the defined profile.

add_time_temperature(time: float, temperature: float)
Adds a time-temperature point to the non-isothermal temperature profile.

Parameters

- **time** – The time [s]
- **temperature** – The temperature [K]

Returns This *TemperatureProfile* object
5.7 Module “propertymodel_sdk”

class tc_python.propertymodel_sdk.CCTResult (quantity_id: str, description: str)
Bases: tc_python.propertymodel_sdk.ResultQuantity

Represents a Continuous Cooling (CCT) result.

Parameters

• quantity_id – The id of this result
• description – The description of this result

add_time_temperature (time_temperature_id: str, description: str)

Adds a time-temperature pair to the result.

Parameters

• time_temperature_id – The id of the time-temperature pair
• description – The description of the time-temperature pair

temperature_suffix = ' (T)'
The temperature suffix of a CCTResult

time_suffix = ' (t)'
The time suffix of a CCTResult

class tc_python.propertymodel_sdk.CCTResultValues (cooling_rate: float = -1.0,
cooling_rate_start_temperature: float = -1.0, cooling_rate_end_temperature: float = -1.0)

Bases: object

Represents Continuous Cooling (CCT) result values.

Parameters

• cooling_rate – The cooling rate [K/s]
• cooling_rate_start_temperature – The start temperature of cooling [K]
• cooling_rate_end_temperature – The end temperature of cooling [K]

set_result_time_temperature (time_temperature_id: str, time: float, temperature: float)

Sets a time-temperature pair of the result.

Parameters

• time_temperature_id – The id of the time-temperature pair
• time – The time [s]
• temperature – The temperature [K]

class tc_python.propertymodel_sdk.CalculationContext (system: tc_python.system.System,
model_utils=None)

Bases: object

Represents the interface of the Property Model with the Thermo-Calc application and the rest of the TC-Python functionality.

Parameters
- **system** – The system object of this calculation
- **model_utils** – The model utils object

### get_argument_ids() \(\rightarrow\) Set[str]

Returns a list with the arguments of the models. Including arguments created from dynamic parameters.

### get_dependent_component() \(\rightarrow\) str

Obtains the dependent component from the UI

**Note:** The dependent component is that which has no composition specified explicitly, typically this is the major element of the material (such as Fe, Al, Ni, …)

**Returns** The dependent component

### get_mass_fractions() \(\rightarrow\) Dict[str, float]

Obtains the current composition from the UI as mass-fraction.

**Note:** In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

**Returns** The composition (key: component, value: content) [mass-fraction]

### get_mass_percents() \(\rightarrow\) Dict[str, float]

Obtains the current composition from the UI in mass-percent.

**Note:** In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

**Returns** The composition (key: component, value: content) [mass-percent]

### get_mole_fractions() \(\rightarrow\) Dict[str, float]

Obtains the current composition from the UI as mole-fraction.

**Note:** In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

**Returns** The composition (key: component, value: content) [mole-fraction]

### get_mole_percents() \(\rightarrow\) Dict[str, float]

Obtains the current composition from the UI in mole-percent.

**Note:** In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

**Returns** The composition (key: component, value: content) [mole-percent]
get_temperature() → float
Obtains the current temperature from the UI.

Returns The temperature [K]

get_ui_boolean_value(component_id: str) → bool
Obtains the value from the specified checkbox UI component.

Parameters component_id – Id of the checkbox

Returns The setting of the checkbox

get_ui_condition_list(component_id: str) → tc_python.propertymodel_sdk.ConditionListEntry
Used to get the selected condition from components of type UIConditionListComponent
:param component_id: Id of the list UI component
:return: The selected condition

get_ui_float_value(component_id: str) → float
Obtains the value from the specified UI component.

Parameters component_id – Id of the UI component

Returns The value

get_ui_list_value(component_id: str) → str
Obtains the selected entry from a UI component list. If a special element (such as ANY, NONE, ...) is selected, the corresponding locale-independent placeholder is provided.

Parameters component_id – Id of the list UI component

Returns The selected entry

get_ui_string_value(component_id: str) → str
Obtains the selected entry from a UI component text field.

Parameters component_id – Id of the string UI component

Returns The selected entry

get_ui_temperature_value(component_id: str) → float
Obtains the temperature from the specified temperature UI component.

Parameters component_id – Id of the temperature UI component

Returns The temperature [K], note that input unit of the UI is specified in the model panel. If required, the temperature is automatically converted to K.

set_result_cct_values(quantity_id: str, r: tc_python.propertymodel_sdk.CCTResultValues)
Sets the value of a previously defined result quantity (of type CCTResultValues) for further usage in the Thermo-Calc application for plotting, etc.

Parameters

• quantity_id – unique id of the result quantity

• r – the CCTResultValues to be set

set_result_quantity_value(quantity_id: str, value: float, parameter: str = '')
Sets the value of a previously defined result quantity for further usage in the Thermo-Calc application for plotting, etc.

Parameters

Note: Any result quantity that remains unset is automatically set to NaN.
• **quantity_id** – Unique id of the result quantity
• **parameter** – Use if result is parameterized. f.i. “per phase”
• **value** – The value to be set

```
set_single_equilibrium_result(quantity_id: str, r: tc_python.single_equilibrium.SingleEquilibriumResult)
```

class tc_python.propertymodel_sdk.ConditionListEntry
Bases: object

Used in combination with components of type UIConditionListComponent.
Contains the element, if the selected condition is a composition
Contains the Console Mode syntax of the selected condition
Contains the unit of the selected condition

```
class tc_python.propertymodel_sdk.PropertyModel(_locale: str = 'en-US')
Bases: object

The abstract base class for all property models.
```

**Note:** Every Property Model needs to implement most of the abstract methods of this class. However, some abstract methods are optional and should only be implemented if required.

**Note:** If overwriting the constructor in a Property Model, the constructor of the implemented class must have the identical signature and should pass the parameters to this base class constructor.

**Tip:** It is possible to switch off internal INFO-log messages coming from the calculation engine by changing the log-level on the TC-Python log object like this: 
```
logging.getLogger("tc_python").setLevel(logging.ERROR)
```

**Parameters**

- **_locale** – The locale to be used, this is an internal parameter and is of no meaning to the end-user

**Variables**

- **logger** – logger object that is connected to the Thermo-Calc UI (INFO- and WARNING-level will be printed as INFO, ERROR-level as ERROR), it can be accessed like this: 
```
self.logger.info("Some message")
```

```
abstract add_button_callback(component_id: str, ui_component_ids: Dict[str, int]) → List[tc_python.propertymodel_sdk.UIComponent]
```

Implement this method if you have one or more UI components on which you called UICOMPONENT. enable_add_button(), which adds a + button next to the component.
This method will be executed when you press any such + button.
This method is typically used to add more UI components dynamically and the method must return a list of the UI components to be added.

**This method can optionally be implemented by a Property Model.**

**Parameters**

- **component_id** – The id of the UI component next to the pressed + button
- **ui_component_ids** – dict with the id:s and the index of the current ui components of the model. Including arguments created in previous calls to add_button_callback.

**Returns** A list of UICOMPONENT objects to be added
abstract after_evaluations()
    Called by the Thermo-Calc application immediately after the last model evaluation (using the method
    PropertyModel.evaluate_model()). Use this method for any required cleanup.

This method can optionally be implemented by a Property Model.

abstract before_evaluations(context: tc_python.propertymodel_sdk.CalculationContext)
    Called by the Thermo-Calc application immediately before the first model evaluation (using the method
    PropertyModel.evaluate_model()). Use this method for any required preparations.

This method can optionally be implemented by a Property Model.

Parameters
context – The calculation context

abstract evaluate_model(context: tc_python.propertymodel_sdk.CalculationContext)
    Called by the Thermo-Calc application when the model should be actually calculated. This is the main-
    method of the Property Model that contains the actual calculation code.

This method needs to be implemented by all property models.

Parameters
context – The calculation context, this provides access to the Thermo-Calc application and all other TC-Python modules

abstract get_license_key() → str
    Provides the license key of the model.

This method can optionally be implemented by a Property Model.

abstract provide_calculation_result_quantities() → List[tc_python.propertymodel_sdk.ResultQuantity]
    Called by the Thermo-Calc application when the model should provide its result quantity objects.

This method needs to be implemented by all property models.

Returns
Result quantity objects of the model (to be filled later with results in the method
    PropertyModel.evaluate_model() )

abstract provide_model_category() → List[str]
    Called by the Thermo-Calc application when the model should provide its category (shown in the Thermo-
    Calc model tree).

This method needs to be implemented by all property models.

Returns
Category of the model, it may be present in several categories

abstract provide_model_description() → str
    Called by the Thermo-Calc application when the model should provide its detailed description.

This method needs to be implemented by all property models.

Returns
Description text for the model

abstract provide_model_name() → str
    Called by the Thermo-Calc application when the model should provide its name (shown in the Thermo-
    Calc model tree).

This method needs to be implemented by all property models.

Returns
Name of the model

abstract provide_model_parameters() → Dict[str, float]
    Called by the Thermo-Calc application when the model should provide all model parameters and their
    current values.

This method can optionally be implemented by a Property Model.
Note: These are internal variables of the Property Model that are intended to be modified from the outside. Typically this is used to adjust their values in an optimizer during the development of the model.

Returns The model parameter ids and their current values [unit according to the parameter meaning]

**abstract provide_ui_panel_components** () → List[tc_python.propertymodel_sdk.UIComponent]
Called by the Thermo-Calc application when the model should provide its UI components for the model panel to be plotted. This happens also whenever a model gets checked in the model tree.

This method needs to be implemented by all property models.

Returns Model UI panel components in the order to be presented in the model panel

**abstract remove_button_callback** (component_id: str, ui_component_ids: Dict[str, int]) → List[str]
Implement this method if you have one or more UI components on which you called UIComponent.enable_remove_button(), which adds a - button next to the component.

This method will be executed when you press any such - button.

This method is typically used to remove UI components dynamically and the method must return a list of the ids of the components that are going to be removed.

This method can optionally be implemented by a Property Model.

Parameters

• component_id – the id of the UI component next to the pressed - button

• ui_component_ids – list with the id:s and the index of the current ui components of the model. Including arguments created in previous calls to add_button_callback.

Returns a list of UI component ids that are required to be removed

**abstract set_model_parameter** (model_parameter_id: str, value: float)
Called by the Thermo-Calc application when a model parameter should be reset.

This method can optionally be implemented by a Property Model.

Note: These are internal variables of the Property Model that are intended to be modified from the outside. Typically this is used to adjust their values in an optimizer during the development of the model.

Parameters

• model_parameter_id – The parameter id

• value – The value [unit according to the parameter meaning]

**class** tc_python.propertymodel_sdk.ResultQuantity
(quantity_id: str, description: str, quantity_type: tc_python.propertymodel_sdk.ResultQuantityType)

Bases: object

Defines a calculation result quantity of a Property Model that is identified by a unique id.

Parameters

• quantity_id – Unique id of the quantity
• **description** – Description of the quantity (shown in the Thermo-Calc UI)

• **quantity_type** – Type of the quantity (defines the unit)

```python
def get_description() -> str:
    """Obtains the description of the quantity."""
    Returns Description of the quantity

def get_id() -> str:
    """Obtains the id of the quantity."""
    Returns Unique id of the quantity

def get_type() -> tc_python.propertymodel_sdk.ResultQuantityType:
    """Obtains the type of quantity."""
    Returns Type of the quantity
```

```python
class tc_python.propertymodel_sdk.ResultQuantityType (value):
    """Defining the type of a result quantity."""
    Bases: enum.Enum

    CCT_QUANTITY = 5
        A cct quantity
    ENERGY_QUANTITY = 2
        An energy quantity
    GENERAL_QUANTITY = 0
        A general quantity
    LENGTH_QUANTITY = 7
        A length in quantity
    SINGLE_EQUILIBRIUM_QUANTITY = 6
        A cct quantity
    STRENGTH_QUANTITY = 8
        A strength quantity
    SURFACE_ENERGY_QUANTITY = 3
        A surface energy quantity
    TEMPERATURE_QUANTITY = 1
        A temperature quantity
    TIME_QUANTITY = 4
        A time quantity
```

```python
class tc_python.propertymodel_sdk.SpecialListMarkers (value):
    """Placeholders for special list elements that are locale-dependent. They will be provided by UI list components if a special marker has been selected."""
    Bases: object

    ANY_LIST_MARKER = 'ANY'
        Marker that represents "Any"
    NONE_LIST_MARKER = 'NONE'
        Marker that represents "None"
```

```python
class tc_python.propertymodel_sdk.UIBooleanComponent (component_id: str, name: str, description: str, setting: bool):
    Bases: tc_python.propertymodel_sdk.UIComponent
```

5.7. Module “propertymodel_sdk”
Checkbox UI component of the model panel.

**Parameters**

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **setting** – Initial setting of the checkbox

**connect_component_visibility**(*dependent_component_id: str*)

Connects the visibility of any other UI component of the model panel to the value of this boolean component.

**Parameters**

- **dependent_component_id** – Id of the UI element to be dependent on this boolean component

**enable_add_button**()

Adds a + button to the right of the UI component.

**Returns**

This UI component

**enable_remove_button**()

Adds a - button to the right of the UI component.

**Returns**

This UI component

**get_dependent_components**() → List[str]

Obtains a list containing all UI elements currently connected regarding their visibility.

**Returns**

A list with the component id of all UI elements currently connected

**get_setting**() → bool

Obtains the setting of the checkbox.

**Returns**

The setting of the checkbox

**remove_component_visibility**(*dependent_component_id: str*)

Removes the visibility connection to a UI component that has been previously connected.

**Parameters**

- **dependent_component_id** – Id of the previously connection UI element

**set_index**(*index: int = -1*)

Sets the position in the graphical user interface.

**Parameters**

- **index** – The position

**Returns**

This UI component

**class** `tc_python.propertymodel_sdk.UIComponent`(*component_id: str, name: str, description: str*)

**Bases:** object

Abstract Base class for all UI components of the model panel.

Never make an instance of UIComponent, always use the sub-classes. For instance UIStringComponent.

**Parameters**

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
**get_description()** → str
Obtains the additional description of the component.

**Returns** Additional description of the component

**get_id()** → str
Obtains the unique id of the component.

**Returns** Unique id of the component

**get_name()** → str
Obtains the name of the component.

**Returns** Name of the component, will be presented in the model panel

```python
class tc_python.propertymodel_sdk.UIConditionListComponent(component_id: str, name: str, description: str)
```

**Bases:** `tc_python.propertymodel_sdk.UIComponent`

System condition list UI component of the model panel.

**Parameters**

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component

```python
class tc_python.propertymodel_sdk.UIFloatComponent(component_id: str, name: str, description: str, value: float)
```

**Bases:** `tc_python.propertymodel_sdk.UIComponent`

General real value text field UI component of the model panel.

**Parameters**

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `value` – Initial setting of the text field

**enable_add_button()**

Adds a + button to the right of the UI component.

**Returns** This UI component

**enable_remove_button()**

Adds a - button to the right of the UI component.

**Returns** this UI component

**get_value()** → float
Obtains the setting of the text field.

**Returns** The setting of the text field

**set_index(index: int = -1)**

Sets the position in the graphical user interface.

**Parameters**

- `index` – The position

**Returns** This UI component
class tc_python.propertymodel_sdk.UIGeneralListComponent(component_id: str, name: str, description: str, content: List[Tuple[str, str]], selected_entry: str = '')

Bases: tc_python.propertymodel_sdk.UIComponent

General list UI component of the model panel that can contain any strings.

Parameters

- component_id – Unique id of the component
- name – Name of the component, will be presented in the model panel
- description – Additional description of the component
- content – Entries of the list, they need to contain a locale-independent id and a localized content string, for example: ["ENTRY_1_ID", "entry 1"], ["ENTRY_2_ID", "entry 2"]
- selected_entry – Entry to be initially selected. If omitted, by default the first element is selected.

customize_component_visibility(dependent_component_id: str, selected_item_to_set_visible: str)

Connects the visibility of any other UI component of the model panel to the selection of a certain entry of the list.

Parameters

- dependent_component_id – Id of the UI element to be dependent on the chosen element
- selected_item_to_set_visible – Entry (locale independent id) of the list to be chosen to set the dependent component visible

enable_add_button()

Adds a + button to the right of the UI component.

Returns This UI component

enable_remove_button()

Adds a - button to the right of the UI component.

Returns This UI component

get_content() → List[Tuple[str, str]]

Obtains the entries of the list.

Returns Entries of the list, they need to contain a locale-independent id and a localized content string, for example: ["ENTRY_1_ID", "entry 1"], ["ENTRY_2_ID", "entry 2"]

get_dependent_components() → Dict[str, List[str]]

Obtains a dictionary containing all UI elements currently connected regarding their visibility.

Returns All UI elements currently connected (key: dependent component id, value: required list entries to set it visible)

get_selected_entry() → str

Obtains the initially selected entry.

Returns Initially selected entry. If empty, the first element is selected.

remove_component_visibility(dependent_component_id: str)

Removes the visibility connection to a UI component that has been previously connected.
Parameters `dependent_component_id` – Id of the previously connection UI element

```python
def set_index(index: int = -1)
    # Sets the position in the graphical user interface.
    # Parameters index – The position
    # Returns This UI component
```

class `tc_python.propertymodel_sdk.UIPhaseListComponent`
```
    component_id: str, name: str, description: str, default_phase: str = '',
    any_marker_setting: bool = False
```

Bases: `tc_python.propertymodel_sdk.UIComponent`

Phase list UI component of the model panel.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `default_phase` – Default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. If an ANY-marker is added, this is chosen as the default element.
- `any_marker_setting` – Defines if an entry “ANY PHASE” should be added to the phase list, if set to true this overrides any default phase setting

```python
def enable_add_button()
    # Adds a + button to the right of the UI component.
    # Returns This UI component
```

def enable_remove_button()
    # Adds a - button to the right of the UI component.
    # Returns This UI component

```python
def get_any_marker_setting() -> bool
    # Obtains the setting if any entry “ANY PHASE” is added to the phase list.
    # Returns If an entry “ANY PHASE” is added to the phase list, if set to true this overrides any default phase setting
```

```python
def get_default_phase() -> str
    # Obtains the default phase.
    # Returns Default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. If an ANY-marker is added, this is chosen as the default element.
```

def set_index(index: int = -1)
    # Sets the position in the graphical user interface.
    # Parameters index – The position
    # Returns This UI component
```

class `tc_python.propertymodel_sdk.UIStringComponent`
```
    component_id: str, name: str, description: str, string: str
```

Bases: `tc_python.propertymodel_sdk.UIComponent`

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General text field UI component of the model panel.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `string` – Initial setting of the text field

`enable_add_button()`
Adds a + button to the right of the UI component.

Returns This UI component

`enable_remove_button()`
Adds a - button to the right of the UI component.

Returns This UI component

`get_value()` → `str`
Obtains the setting of the text field.

Returns The setting of the text field

`set_index` `(index: int = -1)`
Sets the position in the graphical user interface.

Parameters `index` – The position

Returns This UI component

```python
class tc.python.propertymodel_sdk.UITemperatureComponent (component_id: str, name: str, description: str, temp: float)
```

Bases: `tc.python.propertymodel_sdk.UIComponent`

Temperature value text field UI component of the model panel.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `temp` – Initial temperature to be set in the text field (unit defined by the user in the Thermo-Calc system)

`enable_add_button()`
Adds a + button to the right of the UI component.

Returns This UI component

`enable_remove_button()`
Adds a - button to the right of the UI component.

Returns This UI component

`get_temp()` → `float`
Obtains the temperature set in the text field.

Returns The temperature to be set in the text field (unit defined by the user in the Thermo-Calc system)
**set_index** *(index: int = -1)*
Sets the position in the graphical user interface.

**Parameters**
- **index** – The position

**Returns**
This UI component

```
tc_python.propertymodel_sdk.create_boolean_ui_component(component_id: str, name: str, description: str, initial_setting: bool) → tc_python.propertymodel_sdk.UIBooleanComponent
```

Creates a UI checkbox component for a boolean value. The value of that component can later be accessed during the model evaluation.

**Parameters**
- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **initial_setting** – Initial setting of the checkbox

**Returns**
The created component

```
tc_python.propertymodel_sdk.create_condition_list_ui_component(component_id: str, name: str, description: str) → tc_python.propertymodel_sdk.UIConditionListComponent
```

Creates a UI list component for all conditions defined in the system. The value of that component can later be accessed during the model evaluation.

**Parameters**
- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component

**Returns**
The created component

```
tc_python.propertymodel_sdk.create_energy_quantity(quantity_id: str, description: str) → tc_python.propertymodel_sdk.ResultQuantity
```

Creates a UI energy result quantity (in J). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

**Parameters**
- **quantity_id** – Unique id of the result quantity
- **description** – Additional description of the result quantity

**Returns**
The created result quantity

```
tc_python.propertymodel_sdk.create_float_ui_component(component_id: str, name: str, description: str, value: float) → tc_python.propertymodel_sdk.UIFloatComponent
```

Creates a UI text field component for a real number. The value of that component can later be accessed during the model evaluation.

**Parameters**
- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **value** – Initial setting of the text field

**Returns** The created component

tc_python.propertymodel_sdk.create_general_quantity(quantity_id: str, description: str) \[\rightarrow tc_python.propertymodel_sdk.ResultQuantity\]

Creates a general result quantity that can contain any type of result (without a unit). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

**Parameters**

- **quantity_id** – Unique id of the result quantity
- **description** – Additional description of the result quantity

**Returns** The created result quantity

tc_python.propertymodel_sdk.create_length_quantity(quantity_id: str, description: str) \[\rightarrow tc_python.propertymodel_sdk.ResultQuantity\]

Creates a length result quantity. When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

**Parameters**

- **quantity_id** – Unique id of the result quantity
- **description** – Additional description of the result quantity

**Returns** The created result quantity

tc_python.propertymodel_sdk.create_list_ui_component(component_id: str, name: str, description: str, entry_list: List[Tuple[str, str]], selected_entry: str = '') \[\rightarrow tc_python.propertymodel_sdk.UIGeneralListComponent\]

Creates a UI list component for string entries. The value of that component can later be accessed during the model evaluation.

**Parameters**

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **entry_list** – Entries of the list, they need to contain a locale-independent id and a localized content string, for example: [('ENTRY_1_ID', 'entry 1'), (ENTRY_2_ID', 'entry 2')]
- **selected_entry** – Entry to be initially selected. If omitted, by default the first element is selected.

**Returns** The created component
tc_python.propertymodel_sdk.create_phase_list_ui_component(component_id: str, name: str, description: str, default_phase: str = '', any_marker: bool = False) → tc_python.propertymodel_sdk.UIPhaseListComponent

Creates a UI list component for all phases defined in the system. It is possible to select a default phase that is supposed to be the expected phase selection for that list. The value of that component can later be accessed during the model evaluation.

A default phase is the phase that is initially selected and re-selected as soon as a currently selected phase is removed. If the default phase is not available, a “NONE”-marker will be created and used instead of the default phase. A typical use case for the default phase setting is a phase list that expects to contain the LIQUID-phase of a system.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **default_phase** – Default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. **If an ANY-marker is added, this is chosen as the default element.**
- **any_marker** – Defines if an entry “ANY PHASE” should be added to the phase list, if set to true this overrides any default phase setting

Returns The created component

---

tc_python.propertymodel_sdk.create_strength_quantity(quantity_id: str, description: str) → tc_python.propertymodel_sdk.ResultQuantity

Creates a strength result quantity. When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** – Unique id of the result quantity
- **description** – Additional description of the result quantity

Returns The created result quantity

---

tc_python.propertymodel_sdk.create_string_ui_component(component_id: str, name: str, description: str, string: str) → tc_python.propertymodel_sdk.UIStringComponent

Creates a UI text field component. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **string** – Initial setting of the text field
Returns  The created component

tc_python.propertymodel_sdk.create_surface_energy_quantity(quantity_id: str, description: str) → tc_python.propertymodel_sdk.ResultQuantity

Creates an energy result quantity (in J). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- quantity_id – Unique id of the result quantity
- description – Additional description of the result quantity

Returns  The created result quantity

tc_python.propertymodel_sdk.create_temperature_quantity(quantity_id: str, description: str) → tc_python.propertymodel_sdk.ResultQuantity

Creates a temperature result quantity (in K). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- quantity_id – Unique id of the result quantity
- description – Additional description of the result quantity

Returns  The created result quantity

tc_python.propertymodel_sdk.create_temperature_ui_component(component_id: str, name: str, description: str, initial_temp: float) → tc_python.propertymodel_sdk.UITemperature

Creates a UI text field component for a temperature value. The value of that component can later be accessed during the model evaluation.

Parameters

- component_id – Unique id of the component
- name – Name of the component, will be presented in the model panel
- description – Additional description of the component
- initial_temp – Initial temperature to be set in the text field. (The unit of initial_temp is Kelvin. The value in the text field will be automatically converted using the unit chosen by the user.)

Returns  The created component

tc_python.propertymodel_sdk.create_time_quantity(quantity_id: str, description: str) → tc_python.propertymodel_sdk.ResultQuantity

Creates a time result quantity (in s). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- quantity_id – Unique id of the result quantity
- description – Additional description of the result quantity

Returns  The created result quantity
5.8 Module “exceptions”

exception tc_python.exceptions.APIServerException
   Bases: tc_python.exceptions.GeneralException
   An exception that occurred during the communication with the API-server. It is normally not related to an error in the user program.

exception tc_python.exceptions.CalculationException
   Bases: tc_python.exceptions.TCException
   An exception that occurred during a calculation.

exception tc_python.exceptions.ComponentNotExistingException
   Bases: tc_python.exceptions.GeneralException
   The selected component is not existing.

exception tc_python.exceptions.DatabaseException
   Bases: tc_python.exceptions.CalculationException
   Error loading a thermodynamic or kinetic database, typically due to a misspelled database name or a database missing in the system.

exception tc_python.exceptions.DegreesOfFreedomNotZeroException
   Bases: tc_python.exceptions.CalculationException
   The degrees of freedom in the system are not zero, i.e. not all required conditions have been defined. Please check the conditions given in the exception message.

exception tc_python.exceptions.EquilibriumException
   Bases: tc_python.exceptions.CalculationException
   An equilibrium calculation has failed, this might happen due to inappropriate conditions or a very difficult problem that can not be solved.

exception tc_python.exceptions.GeneralCalculationException
   Bases: tc_python.exceptions.CalculationException
   General error occurring while a calculation is performed.

exception tc_python.exceptions.GeneralException
   Bases: tc_python.exceptions.TCException
   A general exception that might occur in different situations.

exception tc_python.exceptions.InvalidCalculationConfigurationException
   Bases: tc_python.exceptions.CalculationException
   Thrown when errors are detected in the configuration of the calculation.

exception tc_python.exceptions.InvalidCalculationStateException
   Bases: tc_python.exceptions.CalculationException
   Trying to access an invalid calculation object that was invalidated by calling invalidate on it.

exception tc_python.exceptions.InvalidNumberOfResultGroupsException
   Bases: tc_python.exceptions.ResultException
   A calculation result contains several result groups, which is not supported for the used method.

exception tc_python.exceptions.InvalidResultConfigurationException
   Bases: tc_python.exceptions.ResultException
   A calculation result configuration is invalid.
exception `tc_python.exceptions.InvalidResultStateException`  
Bases: `tc_python.exceptions.CalculationException`  
Trying to access an invalid result (for example a `SingleEquilibriumTempResult` object that got already invalidated by condition changes or a result that was invalidated by calling `invalidate` on it).

exception `tc_python.exceptions.LicenseException`  
Bases: `tc_python.exceptions.GeneralException`  
No valid license for the API or any Thermo-Calc product used by it found.

exception `tc_python.exceptions.NoDataForPhaseException`  
Bases: `tc_python.exceptions.ResultException`  
There is no result data available for a selected phase.

exception `tc_python.exceptions.NotAllowedOperationException`  
Bases: `tc_python.exceptions.CalculationException`  
The called method or operation is not allowed in the current mode of operation (i.e. debug or production mode).  
Production mode means that the Property Model is only present as an *.py.encrypted-file, while in debug mode it is available as *.py-file. Certain methods for obtaining internal model parameters are not available for encrypted models.

exception `tc_python.exceptions.PhaseNotExistingException`  
Bases: `tc_python.exceptions.GeneralException`  
The selected phase is not existing, so no data can be provided for it.

exception `tc_python.exceptions.ResultException`  
Bases: `tc_python.exceptions.TCException`  
An exception that occurred during the configuration of a calculation result.

exception `tc_python.exceptions_SyntaxException`  
Bases: `tc_python.exceptions.CalculationException`  
Syntax error in a Console Mode expression.

exception `tc_python.exceptions.TCException`  
Bases: Exception  
The root exception of TC-Python.

exception `tc_python.exceptions.UnrecoverableCalculationException`  
Bases: `tc_python.exceptions.CalculationException`  
The calculation reached a state where no further actions are possible, this happens most often due to a FORTRAN- hard crash in the API server backend.

Note: It is possible to catch that exception outside of the with-clause context and to continue by setting up a new context (i.e. by a new with `TCPython()` as session).

tc_python.exceptions.handle_exception(e)
5.9 Module “abstract_base”

```python
class tc_python.abstract_base.AbstractCalculation(calculator)
   Bases: object

   Abstract base class for calculations.

   get_configuration_as_string() \rightarrow str
       Returns detailed information about the current state of the calculation object.

   Warning: The structure of the calculator objects is an implementation detail and might change between releases without notice. Therefore do not rely on the internal object structure.

get_system_data() \rightarrow tc_python.abstract_base.SystemData
   Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using with_system_modifications().

   Note: Parameters can only be read from unencrypted (i.e. user) databases loaded as *.tdb-file.

   Returns The system data

invalidate()
   Invalidates the object and frees the disk space used by it. This is only required if the disk space occupied by the object needs to be released during the calculation. No data can be retrieved from the object afterwards.

with_system_modifications(system_modifications: tc_python.abstract_base.SystemModifications)
   Updates the system of this calculator with the supplied system modification (containing new phase parameters and system functions).

   Note: This is only possible if the system has been read from unencrypted (i.e. user) databases loaded as a *.tdb-file.

   Parameters system_modifications – The system modification to be performed

   Returns
```

```python
class tc_python.abstract_base.AbstractResult(result)
   Bases: object

   Abstract base class for results. This can be used to query for specific values .

   invalidate()
       Invalidates the object and frees the disk space used by it. This is only required if the disk space occupied by the object needs to be released during the calculation. No data can be retrieved from the object afterwards.

class tc_python.abstract_base.PhaseParameter(parameter_name: Union[str, object])
   Bases: object

   Database phase parameter expression used by SystemModifications.set().

   Parameters parameter_name – The phase parameter name

   get_intervals() \rightarrow List[tc_python.abstract_base.TemperatureInterval]
       Returns the list of all defined intervals.
```
Returns The defined temperature intervals

`get_lower_temperature_limit()` → float

Returns the lower temperature limit.

Returns The lower temperature limit in K

`get_name()` → str

Returns the name of the phase parameter.

Returns The name of the phase parameter.

`remove_all_intervals()`

Removes all previously defined temperature intervals.

Returns This `PhaseParameter` object

`remove_interval_with_upper_limit(upper_temperature_limit: float)`

Removes a previously defined temperature interval with matching upper temperature limit. If no such interval exists, an exception is thrown.

Returns This `PhaseParameter` object

`set_expression_with_upper_limit` (parameter_expression: str, upper_temperature_limit: float = 6000.0)

Adds/overwrites a parameter expression for a temperature interval.

Default value of the upper limit of the interval: 6000 K

Note: The lower temperature limit is either defined by the lower temperature limit given with `PhaseParameter.set_lower_temperature_limit()` or by the upper temperature limit of the adjacent interval.

Note: If there is an existing interval with exactly the same `upper_temperature_limit`, that interval is overwritten, otherwise the interval is added.

Parameters

- `parameter_expression` – The parameter expression, example: 
  \[+V34*T*LN(T)+V35*T**2+V36*T**(-1)+V37*T**3]\

- `upper_temperature_limit` – The upper temperature limit for which the expression should be used

Returns This `PhaseParameter` object

`set_interval(interval: tc_python.abstract_base.TemperatureInterval)`

Adds/overwrites a temperature interval.

Note: The lower temperature limit is either defined by the lower temperature limit given with `PhaseParameter.set_lower_temperature_limit()` or by the upper temperature limit of the adjacent interval.
Note: If there is an existing interval with exactly the same `upper_temperature_limit`, that interval is overwritten, otherwise the interval is added.

Returns This `PhaseParameter` object

```python
set_lower_temperature_limit(lower_temperature_limit: float = 298.15)
```
Sets the lower temperature limit of the phase parameter.

Default: 298.15 K

Parameters `lower_temperature_limit` – The lower temperature limit in K

Returns This `PhaseParameter` object

class tc_python.abstract_base.SystemData(system_data)
Bases: object

Provides information about the parameters and functions of a user database. The obtained objects can be used to modify the database using `with_system_modifications()` of all calculators.

Note: Parameters can only be read from unencrypted (i.e. `user`) databases loaded as `.tdb`-file.

```python
get_phase_parameter(parameter: str) → tc_python.abstract_base.PhaseParameter
```
Returns a phase parameter.

Example:

```
system_data.get_phase_parameter('G(HCP_A3,FE:VA;0)')
```

Note: Parameters can only be read from unencrypted (i.e. `user`) databases loaded as a `.tdb`-file.

Note: For details about the syntax search the Thermo-Calc help for `GES` (the name for the Gibbs Energy System module in Console Mode).

Parameters `parameter` – The name of the phase parameter (for example: “G(LIQUID,FE;0)"

Returns The phase parameter

```python
get_phase_parameter_names() → List[str]
```
Returns all phase parameters present in the current system.

Returns The list of phase parameters

```python
get_system_function(f: str) → tc_python.abstract_base.SystemFunction
```
Returns a system function.

Note: The parameter ‘f’ was previously called ‘function’ but was renamed.

Example:

```
system_data.get_system_function('GHSERCR')
```
Note: Functions can only be read from unencrypted (i.e. user) databases loaded as a *.tdb-file.

Note: For details about the syntax search the Thermo-Calc help for GES (the name for the Gibbs Energy System module in Console Mode).

Parameters  
- **f** – The name of the system function (for example: “GHSERCR”)

Returns  
The system function

get_system_function_names() → List[str]  
Returns all system functions present in the current system.

Returns  
The list of system functions

class tc_python.abstract_base.SystemFunction(function_name: Union[str, object])  
Bases: object

Database function expression used by SystemModifications.set().

Parameters  
- **function_name** – The function name

get_intervals() → List[tc_python.abstract_base.TemperatureInterval]  
Returns the list of all defined intervals.

Returns  
The defined temperature intervals

get_lower_temperature_limit() → float  
Returns the lower temperature limit.

Returns  
The lower temperature limit in K

get_name() → str  
Returns the name of the system function.

Returns  
The name of the system function

remove_all_intervals()  
Removes all previously defined temperature intervals.

Returns  
This SystemFunction object

remove_interval_with_upper_limit(upper_temperature_limit: float)  
Removes a previously defined temperature interval with matching upper temperature limit.

If no such interval exists, an exception is thrown.

Returns  
This SystemFunction object

set_expression_with_upper_limit(function_expression: str, upper_temperature_limit: float = 6000.0)  
Adds/overwrites a function expression for a temperature interval.

Default value of the upper limit of the interval: 6000 K

Note: The lower temperature limit is either defined by the lower temperature limit given with SystemFunction.set_lower_temperature_limit() or by the upper temperature limit of the adjacent interval.
Note: If there is an existing interval with exactly the same `upper_temperature_limit`, that interval is overwritten, otherwise the interval is added.

Parameters

- **function_expression** – The function expression, example:
  
  
  \[+V34*T*LN(T)+V35*T**2+V36*T**(-1)+V37*T**3]\n
- **upper_temperature_limit** – The upper temperature limit for which the expression should be used

Returns This `SystemFunction` object

**set_interval** *(interval: tc_python.abstract_base.TemperatureInterval)*

Sets/overwrites a temperature interval.

Note: The lower temperature limit is either defined by the lower temperature limit given with `SystemFunction.set_lower_temperature_limit()` or by the upper temperature limit of the adjacent interval.

Note: If there is an existing interval with exactly the same `upper_temperature_limit`, that interval is overwritten, otherwise the interval is added.

Returns This `SystemFunction` object

**set_lower_temperature_limit** *(lower_temperature_limit: float = 298.15)*

Sets the lower temperature limit of the system function.

Default: 298.15 K

Parameters **lower_temperature_limit** – The lower limit in K

Returns This `SystemFunction` object

**class** tc_python.abstract_base.SystemModifications

Bases: object

Functionality to modify a user database during a calculation by changing phase parameters and system functions.

The actual changes are only applied by using `tc_python.abstract_base.AbstractCalculation.with_system_modifications()` on a calculator object.

**run_ges_command** *(ges_command: str)*

Sends a GES-command. This is actually applied when running `with_system_modifications` on a calculator object.

Example: `run_ges_command("AM-PH-DE FCC_A1 C_S 2 Fe:C")` for adding a second composition set to the FCC_A1 phase with Fe as major constituent on first sublattice and C as major constituent on second sublattice.

Note: For details about the syntax search the Thermo-Calc help for GES (the name for the Gibbs Energy System module in Console Mode).
Note: It should not be necessary for most users to use this method, try to use the corresponding method implemented in the API instead.

Warning: As this method runs raw GES-commands directly in the engine, it may hang the program in case of spelling mistakes (e.g. forgotten parenthesis, ...).

Parameters ges_command – The GES-command (for example: “AM-PH-DE FCC_A1 C_S 2 Fe:C”)

Returns This SystemModifications object

set (parameter_or_function: Union[tc_python.abstract_base.PhaseParameter, tc_python.abstract_base.SystemFunction])

Overwrites or creates a phase parameter or system function.

Example: system_modifications.set(PhaseParameter(‘G(LIQUID,FE;0)’).set_expression_with_upper_limit(‘+1.2*GFELIQ’))


Note: The old parameter/function is overwritten and any temperature intervals not defined are lost.

Note: Please consult the Thermo-Calc GES-system documentation for details about the syntax.

Returns This SystemModifications object

class tc_python.abstract_base.TemperatureInterval (expression: Union[str, object], upper_temperature_limit: float)

Bases: object

Temperature interval expression used by the classes SystemFunction and PhaseParameter.

Parameters

• expression – The temperature function expressed in Thermo-Calc database syntax.

• upper_temperature_limit – The upper temperature limit in K

get_expression () → str

Returns the function expression of this temperature interval.

Returns The temperature function expression

get_upper_temperature_limit () → float

Returns the upper limit of this temperature interval.

Returns The upper temperature limit in K

set_expression (expression: str)

Sets the function expression of this temperature interval.

Parameters expression – The temperature function expression

set_upper_temperature_limit (upper_temperature_limit: float)

Sets the upper limit of this temperature interval.
Parameters `upper_temperature_limit` – The upper temperature limit in K
This section provides an FAQ for common problems that occur when using TC-Python.

### 6.1 Diagnostics script

If you have problems running TC-Python, run the diagnostics script below.

On Linux you can alternatively download the script directly into your current working directory by:

```
```

```
###
Run this script when troubleshooting TC-Python

It is important to run this script EXACTLY the same way as you run your TC-Python script
(In the same IDE, same project, same Python environment, same Jupyter notebook e.t.c)
###

```
version = '2022a'

print('Testing TC-Python version: ' + version)
print('Please make sure that the variable "version" above, matches the release that you want to test, if not change it and re-run this script."

# below this line, nothing needs to be manually updated.

import sys

print('Python version: (should be at least 3.5 and can NOT be older than 3.0)')
print(str(sys.version_info[0]) + '.' + str(sys.version_info[1]))
if sys.version_info[0] < 3 or sys.version_info[1] < 5:
    print('Wrong version of Python !!!!!')

print('Python executable path: (gives a hint about the used virtual / conda environment, in case of Anaconda the corresponding environment name can be found by running `conda env list` on the Anaconda command prompt, ')
print('TC-Python must be installed into \nEACH separate environment used!')
print(sys.executable)
```
import os
print('')
print('Thermo-Calc ' + version + ' installation directory: (must be a valid path to a complete installation of ' + version + ')')
tc_env_variable = 'TC' + version[2:].upper() + '_HOME'
try:
    print(os.environ[tc_env_variable])
except:
    print('No Thermo-calc environment variable for ' + version + ' was found. (' + tc_env_variable + ')')
print('')
print('Url of license server: (if license server is NO-NET, you need a local license file)')
try:
    print(os.environ['LSHOST'])
except:
    print('No Thermo-calc license server url was found. (LSHOST)')
print('')
print('Path to local license file: (only necessary if not using license server)')
try:
    print(os.environ['LSERVRC'])
except:
    print('No path to local license file was found. (LSERVRC)')

import tc_python
numerical_version = version[:-1]
if version[-1] == 'a':
    numerical_version += '.1.*'
elif version[-1] == 'b':
    numerical_version += '.2.*'
print('')
print('TC-Python version: (needs to be ' + numerical_version + ')')
print(tc_python.__version__)

with tc_python.TCPython() as session:
    print('')
    print('Lists the databases: (should be a complete list of the installed databases that you have license for or do not require license)')
    print(session.get_databases())
6.2 “No module named tc_python” error on first usage

This problem occurs because your used Python interpreter cannot find the TC-Python package. We expect that you have installed the TC-Python package in your Python system interpreter following the instructions in the Installation Guide.

Normally the error message “No module named tc_python” is caused by unintentionally configuring a PyCharm project to use a so-called Virtual Environment. This happens unfortunately by default when creating a new PyCharm project with not changing the default settings.

Note: A Virtual Environment is basically a separate and completely independent copy of the system-wide Python interpreter. It does not contain any packages.

On Windows systems we recommend to use the Anaconda Python Distribution as Python interpreter. However, the instructions given here are valid for any operating system and distribution.

Since TC-Python 2018b we do recommend to not use Virtual Environments unless there is a reasonable use case for that.

There are two possible solutions to fix the problem:

1. The quick fix for your problem is to run

   `pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl`

   within the Terminal window of the opened PyCharm project. This Terminal window automatically runs within the Virtual Environment configured for the project (if any). You can see the name of the Virtual Environment at the beginning of each command prompt line (here it is called venv):

   Microsoft Windows [Version 10.0.16299.431]
   (c) 2017 Microsoft Corporation. All rights reserved.

   (venv) C:\Users\User\Documents>

   The command will consequently install TC-Python also within that Virtual Environment automatically. The Terminal window can be found at the bottom of the IDE. Note that it might be necessary to enable these buttons first by selecting the menu entry View → Tool Buttons.

2. The better fix is to change your project to use the system interpreter. This is described in detail in the section Fixing potential issues with the environment in Step 5 of the Installation Guide.

   It is recommendable to use that approach also for all your future projects.

Both fixes will only change the configuration of the opened project. Further useful information can be found in the section Python Virtual Environments.
6.3 “pip install” fails with “Failed to establish a new network connection” or similar

If *pip install* fails with a network related error (might also be “socket not available”, “retrying after connection broken”, . . . ) it is often due to the computer being behind a proxy-server, this is common in large organizations. Of course also the network connection might be broken.

TC-Python has dependencies to a few other packages:

- py4j
- jproperties
- six (transient dependency of jproperties)

1. The recommended approach is to simply use *pip*. It will resolve the dependencies automatically by downloading them from the *PyPI*-repository server (https://pypi.org). If your computer is located behind a proxy-server, the connection to the repository will fail. In that case it is necessary to configure *pip* with the detailed configuration of the proxy server:

   ```
   pip install -proxy user:password@proxy_ip:port py4j jproperties
   ```

2. Another alternative is to manually download the latest *.whl*-file of each dependency from the repository server (https://pypi.org -> *Search projects*) and to install it manually using:

   ```
   pip install py4j-#.#.#-py2.py3-none-any.whl
   ...
   ```

The actual actual version number needs to be inserted into the file name. The downside of this approach is that updates to that package have to be fully manual also in the future. Additionally it is also necessary to install all transient dependencies in that way.
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