# TC-Python Documentation

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**Thermo-Calc Software AB**

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CHAPTER

ONE

# TC-PYTHON QUICK INSTALL GUIDE

This quick 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 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.

### 1.1.1 Install Anaconda

1. Navigate to the Anaconda website: https://www.anaconda.com/download/.
2. Click to choose your OS (operating system) and then click **Download**. Follow the instructions. It is recommended you keep all the defaults.

## 1.2 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 Examples folder with Python files you can use in the IDE to understand and work with TC-Python.

   The installation location for this API is the same as for other SDKs and based on the OS. For details, see *Default Directory Locations* in the *Thermo-Calc Installation Guide*.

## 1.3 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
   ```

   For example, on a Windows OS Standalone custom installation the path to the TC-Python folder is `C:\Users\Public\Documents\Thermo-Calc\2020a\SDK\TC-Python\`

   Details for Mac and Linux installations are described in Default Directory Locations in the *Thermo-Calc Installation Guide*. Note that on Linux typically *pip3* is used.
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 dependency *py4j* in a special configuration:

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

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

## 1.4 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.

1. Navigate to the PyCharm website: https://www.jetbrains.com/pycharm/download.
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*.

## 1.5 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.

### 1.5.1 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 as done in Step 4.

   For example, on a Windows OS Standalone custom installation the path to the TC-Python folder is `C:\Users\Public\Documents\Thermo-Calc\2020a\SDK\TC-Python\`

   Details for Mac and Linux installations are described in the *Default Directory Locations* section in the *Thermo-Calc Installation Guide*.

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** .

### 1.5.2 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 *Best Practices* chapter.

## 1.6 Updating to a newer version

When updating to a newer version of Thermo-Calc, **you always need to also install the latest version of TC-Python**. It is not sufficient to run the installer of Thermo-Calc. The procedure is generally identical to *Step 3*:

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

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

```
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. Note that on Linux usually *pip3* is used.

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

```
pip show TC-Python
```

CHAPTER

TWO

# MAC OS: SETTING ENVIRONMENT VARIABLES

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

```
TC20A_HOME=/Applications/Thermo-Calc-2020a.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:**

```
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:

```
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:

```
# 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()`.

```
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.

---

```
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:**

```
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”.

**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:**

```
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")
        )
```

### 3.3.2 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:**

```
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:**

```
from tc_python import *

with TCPython() as start:
```

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```
    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:**

```
from tc_python import *

with TCPython() as start:
    temperature_vs_mole_fraction_of_solid = (
        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).
```

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```
                            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 *
```

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```
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")
```

## 3.4 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:**

```
# ...
# 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")
```

# CHAPTER FOUR

# BEST PRACTICES

## 4.1 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()*.

```
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:

```
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:

```
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)
```

## 4.2 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:

```
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 ...
```

## 4.3 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:

```
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.

## 4.4 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
```

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```
    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)
```

## 4.5 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))

        phase_fractions = []
        cr_contents = range(parameters["cr_min"],
                            parameters["cr_max"],
                            parameters["delta_cr"])
```

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```
        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 can be used to identify the process and its parameters
            params, phase_fractions_from_process = result_from_process
            bcc_phase_fraction.extend(phase_fractions_from_process)

    # use the result in `bcc_phase_fraction`, for example for plotting
```

## 4.6 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"]).
                    get_system().
                    with_isothermal_diffusion_calculation().
                        set_temperature(temperature).
                        set_simulation_time(108000.0).
                        add_region(Region("Austenite").
```

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```
                                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...')
```

## 4.7 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.

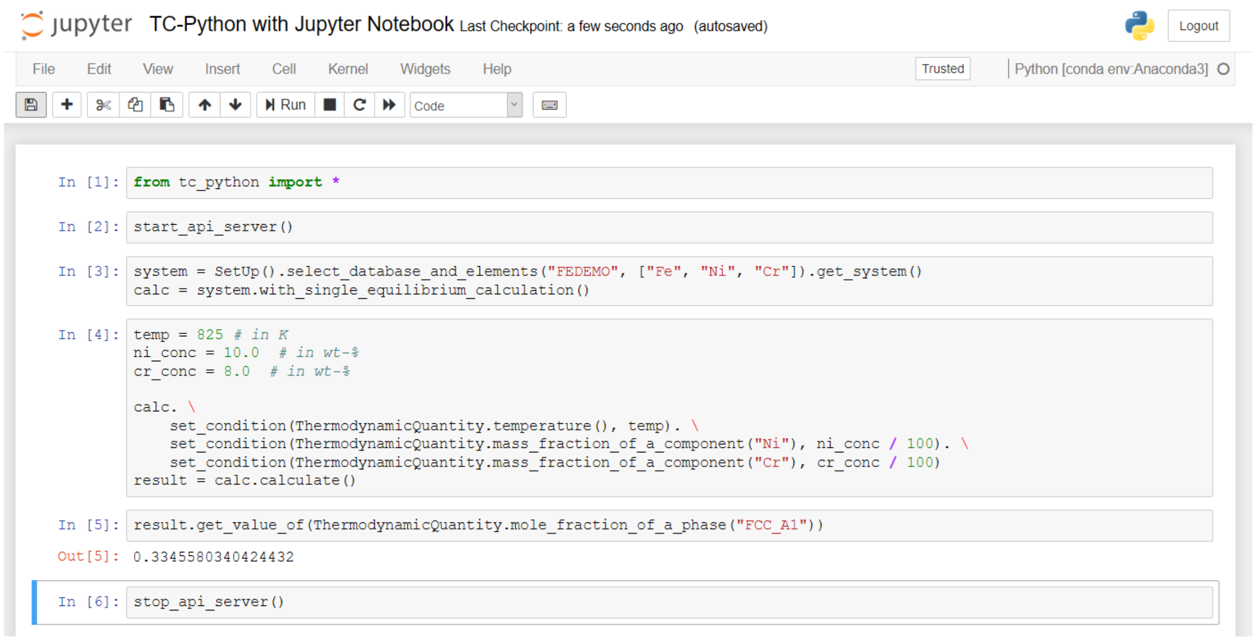
**You need to make sure that you execute the two functions** `tc_python.server.start_api_server()` and `tc_python.server.stop_api_server()` **exactly once within the Jupyter Notebook session**. If not stopping TC-Python, extra Java-processes might be present and the temporary disk-space is not cleared.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

| Operating system | Temporary directory |
|---|---|
| Windows | `C:\Users{UserName}\AppData\Local\Temp\TC_TMP4747588488953835507` |
| MacOS | `/var/folders/g7/7du81ti_b7mm84n184fn3k910000lg/T/TC_TMP4747588488953835507` |
| Linux | `/tmp/TC_TMP4747588488953835507` |

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.

**Example using TC-Python with a Jupyter Notebook**:


jupyter
TC-Python with Jupyter Notebook Last Checkpoint: a few seconds ago (autosaved)
Logout
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Trusted
Python [conda env:Anaconda3]
Run
Code

```
In [1]: from tc_python import *

In [2]: start_api_server()

In [3]: system = SetUp().select_database_and_elements("FEDEMO", ["Fe", "Ni", "Cr"]).get_system()
        calc = system.with_single_equilibrium_calculation()

In [4]: temp = 825 # in K
        ni_conc = 10.0  # in wt-%
        cr_conc = 8.0  # in wt-%

        calc. \
            set_condition(ThermodynamicQuantity.temperature(), temp). \
            set_condition(ThermodynamicQuantity.mass_fraction_of_a_component("Ni"), ni_conc / 100). \
            set_condition(ThermodynamicQuantity.mass_fraction_of_a_component("Cr"), cr_conc / 100)
        result = calc.calculate()

In [5]: result.get_value_of(ThermodynamicQuantity.mole_fraction_of_a_phase("FCC_A1"))
Out[5]: 0.3345580340424432

In [6]: stop_api_server()
```

CHAPTER

FIVE

# API REFERENCE

## 5.1 Calculations

### 5.1.1 Module "single_equilibrium"

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

Bases: *`tc_python.abstract_base.AbstractCalculation`*

Configuration for a single equilibrium calculation.

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

**`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 behaviour 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 will reflect the present state of the calculation during the whole lifetime of the object. This method comes with a performance and temporary disk space overhead. It should only be used if it is necessary to access the result object again later after the state has been changed. In most cases you should use the method *`calculate()`*.

**Returns** A new *`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.

**Returns** This *`SingleEquilibriumCalculation`* object

**`enable_global_minimization`**`()`

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

**Returns** This *`SingleEquilibriumCalculation`* 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 or whatsoever.

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.

**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 ThermodynamicQuantity to set as condition, a console syntax strings 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 POLY-module immediately in the engine.

**Parameters** **command** – The Thermo-Calc console 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*)
Sets the specified component to the status SUSPENDED, i.e. it is ignored in the calculation.

**Parameters** **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 ThermodynamicQuantity to set as condition, a console 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 or whatsoever.

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 = 'current_temperature'*, *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

**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 favourable 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, see Thermo-Calc documentation for details.

**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 favourable 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, see Thermo-Calc documentation for details.

**Default**: Enabled

**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*)

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 *`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 *`tc_python.single_equilibrium.SingleEquilibriumResult.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 *`tc_python.single_equilibrium.SingleEquilibriumResult.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

**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 ThermodynamicQuantity to get the value of, a console 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 POLY-module immediately in the engine. This will only affect the state of the result object.

**Parameters command** – The Thermo-Calc console 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).

**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 *SingleEquilibriumResult* object

**class** tc_python.single_equilibrium.**SingleEquilibriumTempResult**(*result*)

Bases: *tc_python.abstract_base.AbstractResult*

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 behaviour 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 *`tc_python.single_equilibrium.SingleEquilibriumResult.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 *`tc_python.single_equilibrium.SingleEquilibriumResult.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

**`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 ThermodynamicQuantity to get the value of, a console 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 POLY-module immediately in the engine.

**Parameters** **`command`** – The Thermo-Calc console 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"

**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).

**`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:

```
>>> 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.

**`disable_global_minimization`**()
Turns the global minimization completely off.

**Returns** This *`BatchEquilibriumCalculation`* object

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

**Returns** This *`BatchEquilibriumCalculation`* 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 or whatsoever.

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.

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

**Returns** This *`BatchEquilibriumCalculation`* object

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

**Parameters** **`quantity`** – the ThermodynamicQuantity to set as condition, a console syntax strings can be used as an alternative (for example "X(Cr)")

**Returns** This *`BatchEquilibriumCalculation`* object

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

**Parameters** **`command`** – The Thermo-Calc console 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).

**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

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

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

**Returns** This *BatchEquilibriumCalculation* object

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

**Parameters**

- **quantity** – The ThermodynamicQuantity to set as condition, a console syntax string can be used as an alternative (for example "X(Cr)")
- **value** – The value of the condition

**Returns** This *BatchEquilibriumCalculation* object

**set_conditions_for_equilibria**(*equilibria: List[List[Tuple[Union[tc_python.quantity_factory.ThermodynamicQuant 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:

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

You can use `ThermodynamicQuantity` instead of a console syntax string when specifying type of condition.

Example:

```
>>> [[(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 or whatsoever.

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 = 'current_temperature'*, *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

**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:

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

**Parameters** **`quantity`** – the ThermodynamicQuantity to get the value of, a console 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.`**`GrowthRateModel`**

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.

**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

**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 [-]

**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 [-]

**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 [-]

**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 [-]

**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 [-]

**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 [-]

**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 [-]

**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^-4]

**Returns** This *ParticleSizeDistribution* object

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

**Parameters**

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

**Returns** This *ParticleSizeDistribution* object

**set_volume_fraction_of_phase_type**(*volume_fraction_of_phase_type_enum: tc_python.precipitation.VolumeFractionOfPhaseType*)
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 *ParticleSizeDistribution* 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 *ParticleSizeDistribution* object

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

**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

**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

**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

**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

**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

**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**

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).

**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).

**disable_driving_force_approximation**()
Will disable driving force approximation for this precipitate class. **Default**: Driving force approximation is disabled.

**Returns** This *PrecipitatePhase* object

**enable_calculate_aspect_ratio_from_elastic_energy**()
Enables 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

**enable_driving_force_approximation**()
Will enable 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

**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 using 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 gets 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: interfacial_energy_estimation_prefactor = 2.5 => 2.5 * 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 [degrees]
- **`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 [degrees]
- **`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 [degrees]
- **`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*)
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) [m^-3]

**Returns** This *`PrecipitatePhase`* object

**`set_phase_boundary_mobility`** (*phase_boundary_mobility: float*)
Sets the phase boundary mobility. **Default**: 10.0 m^4/(Js).

**Parameters** **`phase_boundary_mobility`** – The phase boundary mobility [m^4/(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.TransformationStrainCalculationOpti*
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` has been 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`**() → 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

**`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 `PrecipitationCalculation` 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 `PrecipitationCalculation` 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 `PrecipitationCalculation` object

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

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

**Returns** This `PrecipitationCalculation` object

**class** tc_python.precipitation.**PrecipitationCalculationResult** (*result*)
Bases: *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 tha 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*)
Bases: *tc_python.precipitation.PrecipitationCalculationResult*

Result of a isothermal or non-isothermal precipitation calculation. This can be used to query for specific values. A detailed definition of the axis variables can be found in the Help.

**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**(*precipitate_id: str*, *time: float*) → [typing.List[float], 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 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 radius [m], aspect ratio)

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

Returns the (by R * 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_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 phase name or alias

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

**`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*) → [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*) → [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.**PrecipitationCalculationTTTorCCTResult**(*result*)

Bases: *tc_python.precipitation.PrecipitationCalculationResult*

Result of a TTT or CCT precipitation calculation.

**get_result_for_precipitate**(*precipitate_id: str*) → [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**() → 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

**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 `PrecipitationCalculation` 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 `PrecipitationCalculation` 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 `PrecipitationCalculation` object

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

**Parameters** **`numerical_parameters`** – The parameters

**Returns** This `PrecipitationCalculation` 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

**`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 `PrecipitationCalculation` 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 `PrecipitationCalculation` 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 `PrecipitationCalculation` object

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

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

**Returns** This `PrecipitationCalculation` 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**() → 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.

**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 `PrecipitationCalculation` 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 `PrecipitationCalculation` 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 unset 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 `PrecipitationCalculation` object

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

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

**Returns** This `PrecipitationCalculation` object

**class** tc_python.precipitation.**TransformationStrainCalculationOption**
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`**

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 * 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 * 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_n`**(*n: float = 0.33*)

Sets the exponent `n` in the governing equation `c * 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 behaviour 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_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 behaviour 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: `object`

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 * 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_approximate_driving_force_for_metastable_phases**()

> **Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 favourable 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 `ScheilCalculation` object

**disable_global_minimization**()

Disables global minimization.

**Default**: Disabled

**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_approximate_driving_force_for_metastable_phases**()

> **Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 favourable 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 `ScheilCalculation` object

**`enable_global_minimization`**()
Enables global minimization.

**Default**: Disabled

---

**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

**`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.

**Default**: No fast-diffusing elements.

**Parameters** **`element_names`** – The elements

**Returns** This `ScheilCalculation` object

**`set_liquid_phase`**(*phase_name: str = 'LIQUID'*)

**Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

Sets the phase used as the liquid phase.

**Default**: The phase "LIQUID".

**Parameters** **`phase_name`** – The phase name

**Returns** This `ScheilCalculation` object

**`set_max_no_of_iterations`**(*max_no_of_iterations: int = 500*)

**Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 `ScheilCalculation` object

**`set_required_accuracy`**(*accuracy: float = 1e-06*)

**Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 `ScheilCalculation` object

**`set_smallest_fraction`**(*smallest_fraction: float = 1e-12*)

> **Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 `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

**`set_temperature_step`**(*temperature_step_in_kelvin: float = 1.0*)

> **Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 `ScheilCalculation` object

**`terminate_on_fraction_of_liquid_phase`**(*fraction_to_terminate_at: float = 0.01*)

> **Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 `ScheilCalculation` object

**`terminate_on_temperature`**(*temperature_in_kelvin: float*)

> **Warning:** *Deprecated in version 2019b:* This function has been moved to `ScheilOptions` which you can set with the method `with_options()`. It will be removed in release 2020b.

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 `ScheilCalculation` object

**`with_back_diffusion`**(*scheil_back_diffusion: tc_python.scheil.ScheilBackDiffusion*)
Enables 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 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_options`**(*options: tc_python.scheil.ScheilOptions*)
Sets the Scheil-simulation options.

**Parameters** **`options`** – The Scheil-simulation options

**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 syntax strings can be used as an alternative (for example "T")
- **y_quantity** – The second Scheil quantity ("y-axis"), console 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** Dict containing the `ResultValueGroup` dataset objects with their *quantity labels* as keys

**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 syntax strings can be used as an alternative (for example "T")
- **y_quantity** – The second Scheil quantity ("y-axis"), console 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** Dict containing the `ResultValueGroup` dataset objects with their *"stable phases" labels* as keys

**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 syntax strings can be used as an alternative (for example "T")
- **y_quantity** – The second Scheil quantity ("y-axis"), console syntax strings can be used as an alternative (for example "NV")

**Returns** A tuple containing the x- and y-data in lists

**save_to_disk**(*path: str*)
Saves the result to disc. Note tha 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.**ScheilOptions**
Bases: `object`

Options for the Scheil-simulation.

**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 favourable 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_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, see Thermo-Calc documentation for details.

**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 favourable 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_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, see Thermo-Calc documentation for details.

**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_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

## 5.1.5 Module "step_or_map_diagrams"

**class** tc_python.step_or_map_diagrams.**AbstractAxisType**

Bases: object

The abstract base class for all axis types.

**get_type**() → str

Convenience method for getting the axis type.

**Returns** The type

**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.ThermodynamicQuar 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`**
Bases: `enum.Enum`

An enumeration.

**`DECREASE_FIRST_AXIS = 3`**

**`DECREASE_SECOND_AXIS = 4`**

**`INCREASE_FIRST_AXIS = 0`**

**`INCREASE_SECOND_AXIS = 1`**

**`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

**class** `tc_python.step_or_map_diagrams.`**`Linear`**

Bases: *tc_python.step_or_map_diagrams.AbstractAxisType*

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*

**Note:** Either *maximum step size* or *minimum number of steps* can be used but not both at the same time.

**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)

**Note:** Either *maximum step size* or *minimum number of steps* can be used but not both at the same time.

**Parameters** **`min_nr_of_steps`** – The minimum number of steps

**Returns** This *Linear* object

**class** `tc_python.step_or_map_diagrams.`**`Logarithmic`**(*scale_factor: float = 1.1*)

Bases: *tc_python.step_or_map_diagrams.AbstractAxisType*

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.abstract_base.AbstractCalculation*

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 POLY module 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**()

Dont 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**() → 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 or whatsoever.

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.

**keep_default_equilibria**()

Keep the initial equilibria added by default. This is only relevant in combination with add_initial_equilibrium

Default behaviour 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 *PhaseDiagramCalculation* to set as condition, a console syntax strings 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 POLY-module immediately in the engine.

**Parameters** **command** – The Thermo-Calc console 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 ThermodynamicQuantity to set as condition, a console 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 or whatsoever.

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 = 'current_temperature'*, *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

**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 favourable 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

**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, see Thermo-Calc documentation for details.

**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 favourable 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, see Thermo-Calc documentation for details.

**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 will not be 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 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 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.ThermodynamicQuantit 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 will not be 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 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 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 tha 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.ResultValueGroup

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.ResultValueGroup]

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** Dict 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.ResultValueGroup

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**(*x: float, y: float, text: str*)

Bases: object

Represents a *phase label at a plot coordinate*, i.e. the stable phases that are present at that *plot* coordinate.

**Variables**

- **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]

- **`text`** – The label (i.e. the stable phases at that point in the phase diagram, for example "LIQUID + FCC_A1")

**class** `tc_python.step_or_map_diagrams.`**`PhaseNameStyle`**

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.abstract_base.AbstractCalculation`*

Configuration for a property diagram calculation.

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

**`calculate`**(*keep_previous_results: bool = False*) → 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`**`()` → 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 or whatsoever.

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.

**`remove_all_conditions`**`()`

Removes all set conditions.

**Returns** This `PropertyDiagramCalculation` object

**`remove_condition`**`(`*quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str]*`)`

Removes the specified condition.

**Parameters** **`quantity`** – The `ThermodynamicQuantity` to set as condition, a console syntax strings can be used as an alternative (for example *X(Cr)*)

**Returns** This `PropertyDiagramCalculation` object

**`run_poly_command`**`(`*command: str*`)`

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

**Parameters** **`command`** – The Thermo-Calc console 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_condition**(*quantity: Union[tc_python.quantity_factory.ThermodynamicQuantity, str], value: float*)
Sets the specified condition.

**Parameters**

- **quantity** – The ThermodynamicQuantity to set as condition, a console 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 or whatsoever.

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 = 'current_temperature'*, *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

**class** tc_python.step_or_map_diagrams.**PropertyDiagramOptions**

Bases: object

Simulation options for the property 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 favourable 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, see Thermo-Calc documentation for details.

**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 favourable 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, see Thermo-Calc documentation for details.

**Default**: Enabled

**Returns** This *PropertyDiagramOptions* 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 *PropertyDiagramOptions* 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 *PropertyDiagramOptions* 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 *PropertyDiagramOptions* 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 *PropertyDiagramOptions* 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 *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:** 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 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 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** Dict containing the datasets with the quantities as their keys

**get_values_grouped_by_stable_phases_of**(*x_quantity: Union[tc_python.quantity_factory.ThermodynamicQuantit 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:** 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 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 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** Dict containing the datasets with the quantities as their keys

**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:** 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 Thermodynamic quantity ("x-axis"), console 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 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 tha 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 `PropertyDiagramResult` 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 *`PropertyDiagramResult`* object

### 5.1.6 Module "diffusion"

**class** `tc_python.diffusion.`**`AbstractBoundaryCondition`**

Bases: `object`

The abstract base class for all boundary conditions.

**`get_type`**`()` → str

Convenience method for getting the boundary condition type.

**Returns** The type

**class** `tc_python.diffusion.`**`AbstractCalculatedGrid`**

Bases: *`tc_python.diffusion.AbstractGrid`*

**`get_type`**`()` → str

Convenience method for getting the grid type.

**Returns** The type

**class** `tc_python.diffusion.`**`AbstractElementProfile`**

Bases: `object`

The abstract base class for all initial composition profile types.

**`get_type`**`()` → str

Convenience method for getting the initial concentration profile type.

**Returns** The type

**class** `tc_python.diffusion.`**`AbstractGrid`**

Bases: `object`

The abstract base class for all grids.

**`get_type`**`()` → str

Convenience method for getting the grid type.

**Returns** The type

**class** `tc_python.diffusion.`**`AbstractSolver`**

Bases: `object`

Abstract base class for the solvers (Classic, Homogenization and Automatic).

**`get_type`**`()` → str

Convenience method for getting the boundary condition type.

**Returns** The type

**class** `tc_python.diffusion.`**`AutomaticSolver`**

Bases: *`tc_python.diffusion.AbstractSolver`*

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.

**get_type**() → str

The type of the solver.

**Returns** The type

**set_flux_balance_equation_accuracy**(*accuracy: float = 1e-16*)

**Only valid if the classic solver is actually used (i.e. not more than one phase in each region).**

Sets the required accuracy during the solution of the flux balance equations. **Default**: 1.0e-16

**Parameters** **accuracy** – The required accuracy

**Returns** A new *AutomaticSolver* object

**set_tieline_search_variable_to_activity**()

**Only valid if the classic solver is actually used (i.e. not more than one phase in each region).**

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

**set_tieline_search_variable_to_potential**()

**Only valid if the classic solver is actually used (i.e. not more than one phase in each region).**

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

**class** tc_python.diffusion.**BoundaryCondition**

Bases: *tc_python.diffusion.AbstractBoundaryCondition*

Contains factory methods for the the different boundary conditions available.

**classmethod closed_system**()

Returns a closed-system boundary condition.

**Returns** A new *ClosedSystem* object

**classmethod fixed_compositions**(*unit_enum: tc_python.diffusion.Unit = <Unit.MASS_PERCENT: 3>*)

Returns a fixed-composition boundary condition.

**Parameters** **unit_enum** – The composition unit

**Returns** A new *FixedCompositions* object

**classmethod mixed_zero_flux_and_activity**()

Returns a mixed zero-flux and activity boundary condition, i.e. for the defined species different conditions are used.

**Returns** A new *MixedZeroFluxAndActivity* 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.

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**classmethod double_geometric**(*no_of_points: int = 50*, *lower_geometrical_factor: float = 1.1*, *upper_geometrical_factor: float = 0.9*)

Creates a double geomtric 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

**classmethod geometric**(*no_of_points: int = 50*, *geometrical_factor: float = 1.1*)

Creates a 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

**classmethod linear**(*no_of_points: int = 50*)

Creates an equally spaced grid.

**Parameters** **no_of_points** – The number of points

**Returns** A new *LinearGrid* object

**class** tc_python.diffusion.**ClassicSolver**

Bases: *tc_python.diffusion.AbstractSolver*

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.

**get_type**() → str

Convenience method for getting the type of the solver.

**Returns** The type of the solver

**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

**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. Either activity or chemical potential are applied to reduce the degrees of freedom at the local equilibrium. **Default**: This is the default setting

**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

**class** tc_python.diffusion.**ClosedSystem**
Bases: *tc_python.diffusion.AbstractBoundaryCondition*

Represents a boundary for a closed system.

**get_type**() → str
Convenience method for getting the type of the boundary condition.

**Returns** The type of the boundary condition

**class** tc_python.diffusion.**CompositionProfile**(*unit_enum: tc_python.diffusion.Unit = <Unit.MASS_PERCENT: 3>*)
Bases: object

Contains initial concentration profiles for the elements.

**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

**class** tc_python.diffusion.**ConstantProfile**(*value: float*)
Bases: *tc_python.diffusion.AbstractElementProfile*

Represents a constant initial concentration profile.

**get_type**() → str
The type of the element profile.

**Returns** The type

**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. A detailed definition of the axis variables can be found in the 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)

**get_mass_fraction_at_upper_interface**(*region: str*, *component: str*) → [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)

**get_mass_fraction_of_component_at_time**(*component: str*, *time: Union[tc_python.diffusion.SimulationTime, float]*) → [typing.List[float], typing.List[float]]

Returns the mass 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], mass fraction of component at the specified time)

**get_mass_fraction_of_phase_at_time**(*phase: str*, *time: Union[tc_python.diffusion.SimulationTime, float]*) → [typing.List[float], typing.List[float]]

Returns the mass 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], mass fraction of hte phase at the specified time)

**get_mole_fraction_at_lower_interface**(*region: str*, *component: str*) → [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)

**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)

**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)

**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)

**`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])

**`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])

**`get_regions`**() → List[str]
Returns the regions of the diffusion simulation.

**Note:** Automatically generated regions (*R_###*) will be included in the list.

**Returns** The region names

**`get_time_steps`**() → List[float]
Returns the timesteps of the diffusion simulation.

**Returns** The timesteps [s]

**`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)

**`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)

**`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)

**`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)

**`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)

**`get_total_mole_fraction_of_phase`**(*phase: str*) → [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)

**`get_total_volume_fraction_of_phase`**(*phase: str*) → [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)

**`get_values_of`**(*x_axis: Union[tc_python.quantity_factory.DiffusionQuantity, str], y_axis: Union[tc_python.quantity_factory.DiffusionQuantity, str], plot_condition: Union[tc_python.quantity_factory.PlotCondition, str] = '', independent_variable: Union[tc_python.quantity_factory.IndependentVariable, str] = ''*) → [typing.List[float], typing.List[float]]

Returns the specified result from the simulation, allows all possible settings.

**Note:** As an alternative, DICTRA-console 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. 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]

**`get_velocity_of_lower_boundary_of_region`**(*region: str*) → [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])

**get_velocity_of_upper_boundary_of_region**(*region: str*) → [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 into a new TC-Python session 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

**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 command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands will be stored and used until explicitly deleted using `tc_python.diffusion.DiffusionIsoThermoCalculation.remove_all_console_commands()`.

**Parameters** **console_command** – The DICTRA console command

**Returns** This `DiffusionCalculation` 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.

**Parameters** **region** – The region to be added

**Returns** This `DiffusionCalculation` 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

**`remove_all_console_commands`**()

Removes all previously added console commands.

**Returns** This `DiffusionCalculation` object

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

Sets the simulation time.

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

**Returns** This `DiffusionCalculation` 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 modelling a tube geometry [m]

**Returns** This `DiffusionCalculation` object

**`with_left_boundary_condition`**(*boundary_condition: tc_python.diffusion.BoundaryCondition*)

Defines the boundary condition on the left edge of the system.

**Default**: A closed-system boundary condition

**Parameters** **`boundary_condition`** – The boundary condition

**Returns** This `DiffusionCalculation` object

**`with_options`**(*options: tc_python.diffusion.Options*)

Sets the general simulation conditions.

**Parameters** **`options`** – The general simulation conditions

**Returns** This `DiffusionCalculation` object

**`with_planar_geometry`**()

Sets geometry to *planar*.

**This is default.**

**Returns** This `DiffusionCalculation` object

**`with_reference_state`**(*element: str, phase: str = 'SER', temperature: float = 'current_temperature', 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

**`with_right_boundary_condition`**(*boundary_condition: tc_python.diffusion.BoundaryCondition*)
Defines the boundary condition on the right edge of the system.

**Default**: A closed-system boundary condition

**Parameters** **`boundary_condition`** – The boundary condition

**Returns** This `DiffusionCalculation` object

**`with_solver`**(*solver: tc_python.diffusion.Solver*)
Sets the solver to use (*Classic*, *Homogenization* or *Automatic*). **Default is Automatic**.

**Parameters** **`solver`** – The solver to use

**Returns** This `DiffusionCalculation` 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 modelling a hollow sphere geometry [m]

**Returns** This `DiffusionCalculation` object

**`with_timestep_control`**(*timestep_control: tc_python.diffusion.TimestepControl*)
Sets the timestep control options.

**Parameters** **`timestep_control`** – The new timestep control options

**Returns** This `DiffusionCalculation` 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 command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands will be stored and used until explicitly deleted using *`tc_python.diffusion.DiffusionNonIsoThermalCalculation.remove_all_console_commands()`*.

**Parameters** **`console_command`** – The DICTRA console command

**Returns** This `DiffusionCalculation` 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.

**Parameters** **`region`** – The region to be added

**Returns** This `DiffusionCalculation` 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

**`remove_all_console_commands`**()
Removes all previously added console commands.

**Returns** This `DiffusionCalculation` object

**`set_simulation_time`**(*simulation_time: float*)
Sets the simulation time.

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

**Returns** This `DiffusionCalculation` 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

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**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 modelling a tube geometry [m]

**Returns** This `DiffusionCalculation` object

**with_left_boundary_condition**(*boundary_condition: tc_python.diffusion.BoundaryCondition*)
Defines the boundary condition on the left edge of the system.

**Default**: A closed-system boundary condition

**Parameters** **boundary_condition** – The boundary condition

**Returns** This `DiffusionCalculation` object

**with_options**(*options: tc_python.diffusion.Options*)
Sets the general simulation conditions.

**Parameters** **options** – The general simulation conditions

**Returns** This `DiffusionCalculation` object

**with_planar_geometry**()
Sets geometry to *planar*.

**This is default.**

**Returns** This `DiffusionCalculation` object

**with_reference_state**(*element: str*, *phase: str = 'SER'*, *temperature: float = 'current_temperature'*, *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 `DiffusionNonIsoThermalCalculation` object

**`with_right_boundary_condition`**(*boundary_condition: tc_python.diffusion.BoundaryCondition*)
Defines the boundary condition on the right edge of the system.

**Default**: A closed-system boundary condition

**Parameters** **`boundary_condition`** – The boundary condition

**Returns** This `DiffusionCalculation` object

**`with_solver`**(*solver: tc_python.diffusion.Solver*)
Sets the solver to use (*Classic*, *Homogenization* or *Automatic*). **Default is Automatic**.

**Parameters** **`solver`** – The solver to use

**Returns** This `DiffusionCalculation` 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 modelling a hollow sphere geometry [m]

**Returns** This `DiffusionCalculation` 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*)
Sets the timestep control options.

**Parameters** **`timestep_control`** – The new timestep control options

**Returns** This `DiffusionCalculation` 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.AbstractCalculatedGrid*

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*)
Creates a constant initial concentration profile.

**Parameters** **value** – The constant composition in the region. [unit as defined in *CompositionProfile*].

**Returns** A new *ConstantProfile* object

**classmethod function**(*dictra_console_mode_function: str*)
Creates a initial concentration profile defined by a function in DICTRA-console syntax.

**Parameters** **dictra_console_mode_function** – The function, expressed in DICTRA-console mode syntax.

**Returns** A new *StepProfile* object

**Note:** This is an advanced feature, preferably a complex concentration profile should be generated using Python-libraries and added to the simulation using *tc_python.diffusion.PointByPointGrid*.

**classmethod linear**(*start: float*, *end: float*)
Creates a linear initial concentration profile.

**Parameters**

- **start** – Composition at the left side of the region [unit as defined in *CompositionProfile*].
- **end** – Composition at the right side of the region [unit as defined in *CompositionProfile*].

**Returns** A new *LinearProfile* object

**classmethod step**(*lower_boundary: float*, *upper_boundary: float*, *step_at: float*)
Creates an initial concentration profile with a step at the specified distance, otherwise the composition is constant at the specified values.

**Parameters**

- **lower_boundary** – Composition before the step [unit as defined in *CompositionProfile*].
- **upper_boundary** – Composition after the step [unit as defined in *CompositionProfile*].
- **step_at** – The distance where the step should be [m].

**Returns** A new *StepProfile* object

**class** tc_python.diffusion.**FixedCompositions**(*unit_enum: tc_python.diffusion.Unit = <Unit.MASS_PERCENT: 3>*)
Bases: *tc_python.diffusion.AbstractBoundaryCondition*

Represents a boundary having fixed composition values.

**get_type**() → str
The type of the boundary condition.

**Returns** The type

**set_composition**(*element_name: str*, *value: float*)
Sets the composition for the specified 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]

**class** `tc_python.diffusion.`**`FunctionProfile`**(*dictra_console_mode_function: str*)

Bases: *`tc_python.diffusion.AbstractElementProfile`*

Creates an initial concentration profile defined by a function in DICTRA-console syntax.

**Note:** This is an advanced feature, preferably a complex concentration profile should be generated using Python-libraries and added to the simulation using *`tc_python.diffusion.PointByPointGrid`*.

**`get_type`**() → str

The type of the element profile.

**Returns** The type

**class** `tc_python.diffusion.`**`GeometricGrid`**(*no_of_points: int = 50*, *geometrical_factor: float = 1.1*)

Bases: *`tc_python.diffusion.AbstractCalculatedGrid`*

Represents a geometric grid.

**`get_geometrical_factor`**() → float

Returns the geometrical factor.

**Returns** The geometrical factor

**`get_no_of_points`**() → int

Returns the number of grid points.

**Returns** The number of grid points

**`get_type`**() → str

Returns the type of grid.

**Returns** The type

**`set_geometrical_factor`**(*geometrical_factor: float = 1.1*)

Sets the geometrical factor.

**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

**Returns** This *`GeometricGrid`* 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 *`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.**HomogenizationFunction**

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.**HomogenizationSolver**

Bases: *tc_python.diffusion.AbstractSolver*

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 behaviour.

**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*.

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_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 *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

**class** tc_python.diffusion.**LinearGrid**(*no_of_points: int = 50*)
Bases: *tc_python.diffusion.AbstractCalculatedGrid*

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: float*, *end: float*)
Bases: *tc_python.diffusion.AbstractElementProfile*

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.AbstractBoundaryCondition*

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: float*)
Sets a fixed activity for an element at the boundary.

**Parameters**

- **element_name** – The name of the element
- **activity** – The activity

**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

**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_equilibrium_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: Optional[int] = None*)

Enables and configures saving of results to file during the simulation. They can be saved for every n-th or optionally for every timestep (*None*). **Default**: Saving of the results at every timestep

**Parameters** **every_nth_step** – *None* 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_interfaces**(*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

**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

**get_type**() → str

Type of the grid.

**Returns** The type

**class** tc_python.diffusion.**Region**(*name: str*)

Bases: `object`

Represents a region of the simulation domain that can contain more that 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=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 will be 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

**class** `tc_python.diffusion.`**`SimulationTime`**

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`**()

Returns an *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**()

Returns a *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**()

Returns a *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 behaviour.

**Returns** A new `HomogenizationSolver` object

**class** tc_python.diffusion.**StepProfile**(*lower_boundary: float, upper_boundary: float, step_at: float*)

Bases: `tc_python.diffusion.AbstractElementProfile`

Represents an initial constant concentration profile with a step at the specified position.

**get_type**() → str

The type of the element profile.

**Returns** The type

**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 '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 '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_simulat*
*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 smalles timestep allowed [s]

**Returns** This *TimestepControl* object

**class** tc_python.diffusion.**Unit**
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 command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands will be stored and used until explicitly deleted using `remove_all_poly_commands()`.

**Parameters** **poly_command** – The POLY console 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, . . . ).

**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.

**get_argument_default**(*argument_id*) → 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)

**get_argument_description**(*argument_id*) → 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

**get_arguments**() → Set[str]
Returns a list of the arguments of the property model.

**Note:** The arguments are the 'UI-panel components' defined in the property model interface method `provide_ui_panel_components()`. They have the same id as specified in the property model. The naming is different because there is no UI present in the context of TC-Python.

**Returns** The ids of the available arguments

**get_model_description**() → str

Returns the description text of the current model.

**Returns** the description

**get_model_parameter_value**(*model_parameter_id*) → float

Returns the current value of an optimizable model parameter. The id can be obtained with `get_model_parameters()`.

**Parameters** **model_parameter_id** – The model parameter id

**Returns** The current value [unit according to the parameter meaning]

**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

**remove_all_conditions**()

Removes all set classic POLY conditions.

**Note:** This does not affect the compositions set by `set_composition()`.

**Returns** This `PropertyModelCalculation` object

**remove_all_poly_commands**()

Removes all previously added POLY console commands.

**Returns** This `PropertyModelCalculation` object

**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 a 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: 1>*)

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*, *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

**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_value_of`**(*result_quantity_id: 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]

**`save_to_disk`**(*path: str*)
Saves the result to disk. The result can later be loaded into a new TC-Python session using `tc_python.server.SetUp.load_result_from_disk()`.

---

**Note:** The *result data* is represented by a whole folder possibly containing multiple files.

---

**Parameters** **`path`** – The path to the result folder, can be relative or absolute.

**Returns** This `PropertyModelResult` object

## 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.

**`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

**`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, they will be independent.

**Returns** A new `System` 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

**`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 is 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 = None*) → Dict[str, float]

Provides conversion between composition units for any combination of chemical compounds. It is fast because no thermodynamic equilibrium calculation is involved.

**Syntax of the chemical compounds**: "Al2O3", "FeO", "CO", "Fe", "C", . . .

**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 given as a dict (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

**`get_element_object`**`(`*element_name: str*`)` → tc_python.entities.Element
Returns the `Element` object of an element. This can be used to obtain detailed information about the element.

**Parameters** **`element_name`** – The element name

**Returns** A `Element`: object

**`get_elements_in_system`**`()` → List[str]
Returns the names of all elements present in the selected system.

**Note:** The list does not contain any elements or components that have been auto-selected by the database(s) in a calculator. Use the `get_components()` of the calculator object instead to get the complete information.

**Returns** A list of element names

**`get_ges_parameter`**`(`*parameter: str*`)` → str
Returns a GES-database parameter expression from the database. Example: *system.get_ges_parameter(“G(LIQUID,FE;0)”)* might return the expression *“+1.2*GFELIQ”*.

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

**Note:** Please consult the Thermo-Calc GES-system documentation for details about the syntax.

**Parameters** **`parameter`** – The GES-parameter (for example: *"G(LIQUID,FE;0)"*)

**Returns** The GES-expression (for example: *"+1.2*GFELIQ"*)

**`get_phase_object`**(*phase_name: str*) → tc_python.entities.Phase

Returns the `Phase` object of a phase. This can be used to obtain detailed information about the phase.

**Parameters** **`phase_name`** – The phase name

**Returns** A `Phase`: object

**`get_phases_in_system`**() → List[str]

Returns all phase names present in the system due to its configuration (selected elements, phases, etc.).

**Returns** A list of phase names

**`get_species_object`**(*species_name: str*) → tc_python.entities.Species

Returns the `Species` object of an species. This can be used to obtain detailed information about the species.

**Parameters** **`species_name`** – The species name

**Returns** A `Species`: object

**`run_ges_command`**(*command: str*)

Sends a command to the GES monitor. 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:** The current `System` is copied and the GES-command is executed on the new system, i.e. the returned `System` object is independent from the current one.

**Note:** Please consult the Thermo-Calc GES-system documentation for details about the syntax.

**Parameters** **`command`** – The GES-command (for example: *"AM-PH-DE FCC_A1 C_S 2 Fe:C"*)

**Returns** A new `System` object

**`set_ges_parameter`**(*parameter: str*, *expression: str*)

Resets a GES-database parameter expression. Example: *system.set_ges_parameter("G(LIQUID,FE;0)", "+1.2*GFELIQ").*

**Note:** The current `System` is copied and the GES-parameter is changed in the new system, i.e. the returned `System` object is independent from the current one.

**Note:** Please consult the Thermo-Calc GES-system documentation for details about the syntax.

**Parameters** **`parameter`** – The GES-parameter (for example: *"G(LIQUID,FE;0)"*)

**Returns** The GES-expression (for example: *"+1.2*GFELIQ"*)

**Returns** A new *`System`* object

**`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

**`with_cct_precipitation_calculation`**`()` → tc_python.precipitation.PrecipitationCCTCalculation

Creates a CCT-diagram calculation.

**Returns** A new `PrecipitationCCTCalculation` object

**`with_isothermal_diffusion_calculation`**`()` → tc_python.diffusion.DiffusionIsoThermalCalculation

Creates an isothermal diffusion calculation.

**Returns** A new `DiffusionIsoThermalCalculation` object

**`with_isothermal_precipitation_calculation`**`()` → tc_python.precipitation.PrecipitationIsoThermalCalculation

Creates an isothermal precipitation calculation.

**Returns** A new `PrecipitationIsoThermalCalculation` object

**`with_non_isothermal_diffusion_calculation`**`()` → tc_python.diffusion.DiffusionNonIsoThermalCalculation

Creates a non-isothermal precipitation calculation.

**Returns** A new `PrecipitationNonIsoThermalCalculation` object

**`with_non_isothermal_precipitation_calculation`**`()` → tc_python.precipitation.PrecipitationNonIsoThermalCalcula

Creates a non-isothermal precipitation calculation.

**Returns** A new `PrecipitationNonIsoThermalCalculation` object

**`with_phase_diagram_calculation`**(*default_conditions: bool = True, components: List[str] = []*) → 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: *[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 `PhaseDiagramCalculation` object

**`with_property_diagram_calculation`**(*default_conditions: bool = True, components: List[str] = []*) → 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: *[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 `PropertyDiagramCalculation` object

**`with_property_model_calculation`**(*model: str, path_to_models: str = ”*) → tc_python.propertymodel.PropertyModelCalculation

Creates a property model calculation.

**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 model folder used by the normal Thermo-Calc application is used.

**Returns** A new `PropertyModelCalculation` object

**`with_scheil_calculation`**() → 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] = []*) → 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: *[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 `SingleEquilibriumCalculation` object

**with_ttt_precipitation_calculation**() → tc_python.precipitation.PrecipitationTTTCalculation
Creates a TTT-diagram calculation.

**Returns** A new `PrecipitationTTTCalculation` object

**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.

**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

**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, they will be 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, they will be independent.

**Returns** A new *System* object

**select_database_and_elements**(*database_name: str, list_of_element_strings: List[str]*)
Selects 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_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).

**Parameters**

- **path_to_user_database** – The path to the database file (*.TDB), defaults to the current working directory. Only the filename is required if the database is located in the same folder as the Python script.
- **list_of_element_strings** – A list of one or more elements as strings, for example [“Fe”, “C”]

**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.**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

**class** tc_python.entities.**Phase**(*phase*)

Bases: `object`

Represents a phase, making detailed information about the phase accessible.

**get_name**() → str

Returns the name of the phase.

**Returns** The phase name

**get_species**() → Set[tc_python.entities.Species]

Returns the species of the phase.

**Returns** A set containing the species

**get_species_for_composition_profile**() → 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.

**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.

**Returns** Set with the species

**get_sublattices**() → List[tc_python.entities.Sublattice]

Returns the sublattices of the phase in a well-defined contiguous order.

**Returns** A list containing the `Sublattice` objects

**get_type**() → tc_python.entities.PhaseType

Returns the type of the phase (liquid, ionic liquid, solid, gas).

**Returns** The type of a phase

**has_diffusion_data**() → bool

Returns if diffusion data exists for the phase.

**Returns** If diffusion data exists for the phase

**has_molar_volume_data**() → bool
Returns if molar volume data exists for the phase.

**Returns** If molar volume data exists for the phase

**is_dilute_diffusion_model**() → bool
Returns if diffusion is described using the DILUTE model for the phase. This will always return *False* if no diffusion data is available.

**Returns** If the DILUTE model is used

**is_gas**() → bool
Returns if the phase is a gas phase.

**Returns** If the phase is a gas phase

**is_ionic_liquid**() → bool
Returns if the phase is an ionic liquid phase.

**Returns** If the phase is an ionic liquid phase

**is_liquid**() → bool
Returns if the phase is a liquid or ionic liquid phase.

**Returns** If the phase is a liquid phase

**is_solid**() → bool
Returns if the phase is a solid phase.

**Returns** If the phase is a solid phase

**class** `tc_python.entities.`**PhaseType**
Bases: `enum.Enum`

The type of a phase.

**GAS = 0**
Gas phase.

**IONIC_LIQUID = 2**
Ionic liquid phase.

**LIQUID = 1**
Liquid phase.

**SOLID = 3**
Solid phase.

**class** `tc_python.entities.`**Species**(*species*)
Bases: `object`

Represents an species, making detailed information about the species accessible.

**get_all_elements**() → List[Tuple[tc_python.entities.Element, float]]
Returns all the elements, that the species is composed of.

**Returns** List of all elements of the species and their stoichiometry

**get_charge**() → int
Returns the charge of the species.

**Returns** The charge of the species

**get_name**() → str
Returns the name of the species.

**Returns** The species name

**is_element**() → bool
Returns if the species actually represents an element.

**Returns** If the species represents an element

**is_interstitial**() → 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**
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 one TC-Python session, i.e. within one *with*-clause, caching will be anyway activated and used through the default temporary directory.

**Returns** This *SetUp* object

**`get_database_info`**(*database_short_name: str*) → 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*) → 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`**() → List[str]

Obtains the short names of all databases available in the used Thermo-Calc installation.

**Note:** Only databases with a valid license will be listed.

**Returns** List of the available databases

**`get_property_models`**(*path_to_models: str = ''*) → 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**()

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 with TC-Python.

**Returns** A new `ResultLoader` object

**select_database_and_elements**(*database_name: str, list_of_elements: List[str]*) → 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.MultiDatabaseSystemBui

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 "MFEDEMO"
- **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.

**Parameters**

- **path_to_user_database** – The path to the database file (*.TDB), defaults to the current working directory. Only filename is required if the database is located in the same folder as the Python 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 will be 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 python 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

**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

**set_log_level_to_debug**()
Sets log level to DEBUG

**Returns** This *SetUp* object

**set_log_level_to_info**()
Sets log level to INFO

**Returns** This *SetUp* object

**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*)
Bases: object

Starting point of the API. Typical syntax:

```
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.

---

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.*.

**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**.

`tc_python.server.`**`stop_api_server`**`()`

Clears 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(*)").

**classmethod activity_of_component**(*component: str*, *use_ser: bool = False*)

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 will be used when this setting is set to False.

**Returns** A new `ActivityOfComponent` object.

**classmethod chemical_diffusion_coefficient**(*phase: str*, *diffusing_element: str*, *gradient_element: str*, *reference_element: str*)

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.

**classmethod chemical_potential_of_component**(*component: str*, *use_ser: bool = False*)

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 will be used when this setting is set to False.

**Param** 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 `ChemicalPotentialOfComponent` object.

**classmethod distance**(*region: str = 'All'*)

Creates a quantity representing the distance [m].

**Parameters** **region** – The name of the region or *All* to choose global.

**classmethod intrinsic_diffusion_coefficient**(*phase: str*, *diffusing_element: str*, *gradient_element: str*, *reference_element: str*)

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.

**classmethod l_bis**(*phase: str*, *diffusing_element: str*, *gradient_element: str*, *reference_element: str*)

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.

**classmethod mass_fraction_of_a_component**(*component: str*)
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*)
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 mobility_of_component_in_phase**(*phase: str*, *component: str*)
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.

**classmethod mole_fraction_of_a_component**(*component: str*)
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*)
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 position_of_lower_boundary_of_region**(*region: str*)
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.

**classmethod position_of_upper_boundary_of_region**(*region: str*)
Creates a quantity representing the position of upper boundary of a region [m].

**Parameters** **region** – The name of the region

**Returns** A new `PositionOfUpperBoundaryOfRegion` object.

**classmethod temperature**()
Creates a quantity representing the temperature [K].

**Returns** A new `Temperature` object.

**classmethod thermodynamic_factor**(*phase: str*, *diffusing_element: str*, *gradient_element: str*, *reference_element: str*)
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`**`()`
Creates a quantity representing the time [s].

**`classmethod total_mass_fraction_of_component`**`(`*component: str*`)`
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*`)`
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*`)`
Creates a quantity representing the total mass fraction of a phase.

**Param** phase: The name of the phase.

**Returns** A new `TotalMassFractionOfPhase` object.

**`classmethod total_mole_fraction_of_component`**`(`*component: str*`)`
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*`)`
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*`)`
Creates a quantity representing the total volume fraction of a phase.

**Param** phase: The name of the phase.

**Returns** A new `TotalVolumeFractionOfPhase` object.

**`classmethod tracer_diffusion_coefficient`**`(`*phase: str*, *diffusing_element: str*`)`
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*)
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*)
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*)
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*)
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*)
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'*)
Creates an independent variable representing the distance [m].

**Returns** A new *Distance* object

**classmethod 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'*)

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**()

Creates an integral plot condition.

**Returns** A new *IntegralCondition* object

**classmethod interface**(*region: str*, *interface_position: tc_python.utils.InterfacePosition*)

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'*)

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**()

Creates a quantity representing the apparent heat capacity [J/g/K].

**Returns** A new `ApparentHeatCapacityPerGram` object.

**classmethod apparent_heat_capacity_per_mole**()

Creates a quantity representing the apparent heat capacity [J/mol/K].

**Returns** A new `ApparentHeatCapacityPerMole` object.

**classmethod apparent_volumetric_thermal_expansion_coefficient**()

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*)

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*)

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_solid_phase**(*phase: str*)

Creates a quantity representing the average density of a solid phase [g/cm^3].

**Parameters** **`phase`** – The name of the phase or *ALL_PHASES* to choose all solid phases

**Returns** A new `DensityOfSolidPhase` object.

**classmethod density_of_system**()

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*)

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**()

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**()

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**()

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**()

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*)

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**()

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**()

Creates a quantity representing the total mass fraction of all solid phases.

**Returns** A new `MassFractionOfAllSolidPhase` object.

**classmethod molar_volume_of_phase**(*phase: str*)

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**()

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*)
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**()
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**()
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 = None*)
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 do start with 1**.

**Returns** A new `SiteFractionOfComponentInPhase` object.

**classmethod 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*)
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 will be used when this setting is set to False.

**Param** 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 `ActivityOfComponent` object.

**classmethod chemical_diffusion_coefficient**(*phase: str*, *diffusing_element: str*, *gradient_element: str*, *reference_element: str*)

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.

**classmethod chemical_potential_of_component**(*component: str*, *use_ser: bool = False*)

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 will be used when this setting is set to False.

**Param** 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 `ChemicalPotentialOfComponent` object.

**classmethod composition_of_phase_as_mole_fraction**(*phase: str*, *component: str = 'All'*)

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*)

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*)
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*)
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*)
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*)
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*)
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*)
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**()
Creates a quantity representing the pressure [Pa].

**Returns** A new `Pressure` object.

**classmethod system_size**()
Creates a quantity representing the system size [mol].

**Returns** A new `SystemSize` object.

**classmethod temperature**()
Creates a quantity representing the temperature [K].

**Returns** A new `Temperature` object.

**classmethod tracer_diffusion_coefficient**(*phase: str*, *diffusing_element: str*)
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*)
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*)
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*)
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**
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**
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`**
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**

- **x** – list of floats representing the first quantity ("x-axis")
- **y** – list of floats representing the second quantity ("y-axis")

**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 "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.`**`raise_python_exceptions`**(*func*)

**Internal method of the API**: Usage of that decorator maps all relevant Java exceptions in the API to the appropriate Python exception.

## 5.8 Module "abstract_base"

**class** `tc_python.abstract_base.`**`AbstractCalculation`**(*calculator*)

Bases: `object`

Abstract base class for calculations.

**get_configuration_as_string**() → 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**.

**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.`**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.

CHAPTER

SIX

# TROUBLESHOOTING

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:

```
curl -O https://www2.thermocalc.com/downloads/support/diagnostics-py/tc-python-
↪diagnostic-script-2020a.py
```

```
"""
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 = '2020a'

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('')
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('')
print('Python executable path: (gives a hint about the used virtual / conda␣
↪environment, in case of Anaconda the corresponding \n'
      'environment name can be found by running `conda env list` on the Anaconda␣
↪command prompt, '
      'TC-Python must be installed into \nEACH separate environment used!)')
print(sys.executable)
```

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```
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 *TC-Python Quick Install 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 *TC-Python Quick Install 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 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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