TC-Python Documentation

Release 2024a

Thermo-Calc Software AB

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CONTENTS

CHAPTER

ONE

INSTALLATION GUIDE

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

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

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

1.1 What type of installation should I choose?

There are two possibilities to install TC-Python:

1. *Using the Python-interpreter bundled to Thermo-Calc*: This interpreter has TC-Python preinstalled together with some popular Python-packages. **This is the recommended option for new users to TC-Python, but it is limited to the preinstalled packages**.
2. *Installing TC-Python into the Python-interpreter of your choice*: **This is the recommended option for any more advanced usage and provides full flexibility.**

1.2 Using the Python-interpreter bundled to Thermo-Calc

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

1.2.1 Limitations

The bundled Python 3.9.18 interpreter is containing the following major packages:

Package	Version
matplotlib	3.8
numpy	1.26.0
scikit-learn	1.3.1
scipy	1.11.3
pyvista	0.42.2
TC-Python	2024a

Please contact the Thermo-Calc support if you think that further packages might be useful in future releases.

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

- *pyex_M_01_Input_from_file.py*
- *pyex_M_02_Output_to_file.py*

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

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

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

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

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*.

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

Open PyCharm and configure the interpreter:

1. Go the menu **File**→**Settings**.
2. Navigate in the tree to **Project: YourProjectName** and choose **Project Interpreter**.
3. Click on the settings symbol close to the **Project Interpreter** dropdown menu and choose **Add**.
4. Now choose **System Interpreter** and add the bundled Thermo-Calc Python 3 interpreter. It is located in different places depending on the operating system:

Operating system	Path to the bundled Python-interpreter
Windows	`C:\Program Files\Thermo-Calc\2024a\python\python.exe`
Linux	`/home/UserName/Thermo-Calc/2024a/python/bin/python3`
MacOS	`/Applications/Thermo-Calc-2024a.app/Contents/Resources/python/bin/python3`

5. Select your added interpreter and confirm.

1.2.4 Step 3: Run a TC-Python Example

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

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

1.2.4.1 Open the TC-Python Project in PyCharm

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

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

Operating system	Path to the TC-Python folder
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2024a\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2024a/SDK/TC-Python`
MacOS	`/Users/Shared/Thermo-Calc/2024a/SDK/TC-Python`

2. Click on the `Examples` folder and then click **OK**.
3. From any subfolder:
   - Double-click to open an example file to examine the code.
   - Right-click an example and choose **Run** .

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

1.3 Installing TC-Python into the Python-interpreter of your choice

1.3.1 Step 1: Install a Python Distribution

If you already have a Python distribution installation, version 3.8 or higher, skip this step.

These instructions are based on using the Anaconda platform for the Python distribution. Install version 3.8 or higher to be able to work with TC-Python, although it is recommended that you use the most recent version.

Note: TC-Python requires Python 3.8 or newer.

1.3.1.1 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.

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

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

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

1.3.3 Step 3: Install TC-Python

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

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

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

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

Operating system	Path to the TC-Python folder
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2024a\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2024a/SDK/TC-Python`
MacOS	`/Users/Shared/Thermo-Calc/2024a/SDK/TC-Python`

3. Press <`Enter`>. When the process is completed, there is a confirmation that TC-Python is installed.

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

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

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

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

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

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

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*.

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

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

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

1.3.5.1 Open the TC-Python Project in PyCharm

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

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

Operating system	Path to the TC-Python folder
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2024a\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2024a/SDK/TC-Python`
MacOS	`/Users/Shared/Thermo-Calc/2024a/SDK/TC-Python`

2. Click on the `Examples` folder and then click **OK**.
3. From any subfolder:
   - Double-click to open an example file to examine the code.
   - Right-click an example and choose **Run** .

1.3.5.2 Fixing potential issues with the environment

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

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

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

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

1.4 Optional packages

Plotting results of Additive Manufacturing simulations requires the package *pyvista*. It is automatically installed if using the option *[am-plotting]* during the installation:

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

The bundled interpreter contains *pyvista* by default.

1.5 Updating to a newer version

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

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

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

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

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

However, that should normally not be required.

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

```
pip show TC-Python
```

CHAPTER

TWO

MAC OS: SETTING ENVIRONMENT VARIABLES

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

```
TC24A_HOME=/Applications/Thermo-Calc-2024a.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:
    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 *One axis* in Graphical Mode can also be configured in this calculation. In Console Mode the property diagram is created using the Step command. The minimum you need to specify are elements, conditions and the calculation axis. Everything else is set to default values, if you do not specify otherwise.

Example:

```
from tc_python import *

with TCPython() as start:
    property_diagram = (
        start.
            select_database_and_elements("FEDEMO", ["Fe", "C"]).
            get_system().
            with_property_diagram_calculation().
                with_axis(CalculationAxis(ThermodynamicQuantity.temperature()).
                    set_min(500).
                    set_max(3000)).
                set_condition(ThermodynamicQuantity.mole_fraction_of_a_component("C"), 0.
↪01).
                calculate().
                get_values_grouped_by_stable_phases_of(ThermodynamicQuantity.
↪temperature(),
                                                       ThermodynamicQuantity.volume_
↪fraction_of_a_phase("ALL"))
        )
```

3.3.6 Phase diagram calculations

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

Example:

```
from tc_python import *

with TCPython() as start:
    phase_diagram = (
        start.
            select_database_and_elements("FEDEMO", ["Fe", "C"]).
            get_system().
            with_phase_diagram_calculation().
                with_first_axis(CalculationAxis(ThermodynamicQuantity.temperature()).
                    set_min(500).
                    set_max(3000)).
                with_second_axis(CalculationAxis(ThermodynamicQuantity.mole_fraction_of_
↪a_component("C")).
                    set_min(0).
                    set_max(1)).
```

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```
                set_condition(ThermodynamicQuantity.mole_fraction_of_a_component("C"), 0.
↪01).
                calculate().
                get_values_grouped_by_stable_phases_of(ThermodynamicQuantity.mass_
↪fraction_of_a_component("C"),
                                                    ThermodynamicQuantity.
↪temperature())
        )
```

3.3.7 Diffusion calculations

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

Example:

```
from tc_python import *

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

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

3.3.8 Property Model calculations

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

Example:

```
from tc_python import *

with TCPython() as start:
```

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

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

    print("Available result quantities: {}".format(result.get_result_quantities()))
    driving_force = result.get_value_of("normalizedDrivingForce")
```

3.3.9 Material to Material calculations

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

Example:

```
from tc_python import *

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

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

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

3.3.10 Process Metallurgy calculations

Process Metallurgy calculations are specialized to support the convenient handling of component-based additions (i.e., slag compositions such as *50% Al2O3 - 30% CaO - 20% SiO2*), provide tailor-made result quantities, a framework for developing kinetic process simulations, and more useful features.

There are two distinct types of calculations:

- *tc_python.process_metallurgy.equilibrium.EquilibriumCalculation*: isothermal and adiabatic equilibrium calculations
- *tc_python.process_metallurgy.process.ProcessSimulationCalculation*: a kinetic process simulation framework, based on an *Effective Equilibrium Reaction Zone* (EERZ) approach

Equilibrium calculation example:

Equilibrium calculations are useful in a large range of situations when considering the kinetics of a process is unnecessary.

```
from tc_python import *

with TCPython() as session:
    metal = EquilibriumAddition({"Fe": None, "C": 4.5, "Si": 1.0}, 100e3,␣
↪temperature=1650 + 273.15)
    slag = EquilibriumAddition({"CaO": 75, "Al2O3": 25}, 3e3, temperature=1600 + 273.15)
    gas = EquilibriumGasAddition({"O2": 100}, 1000, amount_unit=GasAmountUnit.NORM_CUBIC_
↪METER)
    calc = session.with_metallurgy().with_adiabatic_equilibrium_
↪calculation(ProcessDatabase.OXDEMO)

    (calc
     .add_addition(metal)
     .add_addition(slag)
     .add_addition(gas))

    result = calc.calculate()

    print(f"Stable phases: {result.get_stable_phases()}, temperature: {result.get_
↪temperature()} K")
```

Process simulation example:

TC-Python is providing a *framework* for modelling in principle any process in metallurgy, especially steel-making. It is up to the user to actually develop a concrete model for the process in question. The framework is in the current release limited to one reaction zone connecting two bulk zones. These bulk zones are typically the steel melt and the top slag, but not limited to that. The framework in its current version has proven to be useful to model industrial ladle furnaces, AOD- and VOD-converters and more. Process features such as heating and cooling, heat transfer between the bulk zones, inclusion formation and their flotation, etc., can be modelled.

This is a very simplified minimal but complete model mimicking a BOF process:

```
from tc_python import *

with TCPython() as session:
    calc = (session.with_metallurgy()
            .with_adiabatic_process_calculation(ProcessDatabase.OXDEMO)
            .set_end_time(15 * 60))

    steel_zone = MetalBulkZone(density=7800)
    slag_zone = SlagBulkZone(density=4500)

    steel_zone.add_addition(SingleTimeAddition({"Fe": None, "C": 4.5, "Si": 1.0}, 120e3,
                                               temperature=1600 + 273.15), time=0)
    slag_zone.add_addition(SingleTimeAddition({"CaO": 75, "SiO2": 25}, 1.2e3,
                                              temperature=1500 + 273.15,
                                              composition_unit=CompositionUnit.MOLE_
↪PERCENT), time=0)

    steel_zone.add_continuous_addition(ContinuousGasAddition({"O2": 100}, 1,
                                                             rate_unit=GasRateUnit.NORM_
↪CUBIC_METER_PER_SEC))

    calc.with_reaction_zone(ReactionZone(area=10.0,
                                         left_zone=steel_zone, mass_transfer_coefficient_
↪left=1.0e-5,
                                         right_zone=slag_zone, mass_transfer_coefficient_
↪right=1.0e-6))

    result = calc.calculate()

    print(f"Stable phases in the steel melt: {result.get_stable_phases(steel_zone)}")
    print(f"C-content in steel vs. time: {result.get_composition_of_phase_group(steel_
↪zone,
                                                                                         ␣
↪PhaseGroup.ALL_METAL)['C']}")
```

3.3.11 Additive Manufacturing calculations

For Additive Manufacturing calculations, everything that you can configure in the *AM Calculator* in Graphical Mode can also be configured in this calculation. In the minimal case, you do not need to specify any options (the material used by default is *IN625*).

```
from tc_python import *

with TCPython() as start:
    am_result = (start.with_additive_manufacturing()
                 .with_steady_state_calculation()
                 .calculate())

    print(f"Melt pool depth: {am_result.get_meltpool_depth()}")
    plotter, mesh = am_result.get_pyvista_plotter()
    plotter.add_mesh(mesh)
    plotter.show()
```

With several custom settings a basic calculation looks like this:

```
from tc_python import *

with TCPython() as start:
    am_result = (start.with_additive_manufacturing()
                 .with_steady_state_calculation()
                 .disable_fluid_flow_marangoni()
                 .disable_separate_materials()
                 .with_material_properties(MaterialProperties.from_library("IN718"))
                 .set_powder_density(90)
                 .set_ambient_temperature(15 + 273.15)
                 .set_base_plate_temperature(25 + 273.15)
                 .with_top_boundary_conditions(TopBoundaryConditions().set_radiation_
↪emissivity(0.2))
                 .with_heat_source(HeatSource.conical()
                                   .set_power(210)
                                   .set_absorptivity(80.0))
                 .calculate())

    print(f"Melt pool depth: {am_result.get_meltpool_depth()}")
    plotter, mesh = am_result.get_pyvista_plotter()
    plotter.add_mesh(mesh)
    plotter.show()
```

Tip: The graphical visualization and extraction of data from the 3D result dataset requires the package *pyvista*. More details are provided in the section *Optional packages*.

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")
```

3.4.1 DiffusionResult

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

Example:

```
# ...
# some code to set up a Diffusion calculation
# ...
first_diffusion_result = diffusion_calculation.calculate()

continued_calculation = first_diffusion_result.with_continued_calculation()

continued_calculation.set_simulation_time(110000.0)
continued_calculation.with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_
↪activity().set_activity_for_element('C', 1.0))
second_result = continued_calculation.calculate()
# ...
# Now you can use get second_result to get calculated values, just as normal.
# You can also use first_diffusion_result even after second_result is created.
# You can also use second_result (and even first_diffusion_result) to create a new␣
↪ContinuedDiffusionCalculation by calling with_continued_calculation.
```

3.5 Property Model Framework

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

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

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

3.5.1 Property models vs. TC-Python

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

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

3.5.2 Architecture

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

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

```
from tc_python import *


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

    def provide_model_name(self) -> str:
        return "My Demo Model"

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

    def provide_ui_panel_components(self) -> List[UIComponent]:
```

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```
        return [UIBooleanComponent("CHECKBOX", "Should this be checked?", "Simple␣
↪checkbox", setting=False)]

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

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

        # obtain the entered values from the GUI
        composition_as_mass_fraction = context.get_mass_fractions()
        temp_in_k = context.get_temperature()
        calc = context.system.with_single_equilibrium_calculation()
        # continue with a TC-Python calculation now ...

        context.set_result_quantity_value("RESULT", 5.0)  # the value would normally␣
↪have been calculated
```

The basic building blocks of the Property Model API are:

- *tc_python.propertymodel_sdk.ResultQuantity*: Defines a calculation result of a Property Model that will be provided to the UI after each model evaluation
- *tc_python.propertymodel_sdk.CalculationContext*: Provides access to the data from the UI (such as the entered composition and temperature) and to the current TC-Python system object which is the entrypoint for using TC-Python from within the Property Model
- *tc_python.propertymodel_sdk.UIComponent*: These are the UI-components that create the user interface of the Property Model within the model panel of the Thermo-Calc application UI. Different components are available (for example checkboxes, text fields and lists).

3.5.3 Property Model directory

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

Operating system	Default Property Model directory
Windows	`C:\Program Files\Thermo-Calc\2024a\PropertyModels`
Linux	`/home/UserName/Thermo-Calc/2024a/PropertyModels` or: `/opt/Thermo-Calc/2024a/PropertyModels`
MacOS	`/Applications/Thermo-Calc-2024a.app/Contents/Resources/PropertyModels`

Note: The Property Model directory location has been changed in the release 2023b.

CHAPTER FOUR

BEST PRACTICES

4.1 Re-use of the single equilibrium calculation state

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

- Improving the convergence speed in case of very complicated equilibria if a similar equilibrium had been calculated already before. Similarity refers here primarily to composition, temperature and entered phase set. This case can occur for example with the Nickel-database TCNi.
- Convenient and fast switching between states that have changed a lot (for example regarding suspended phases, numerical settings, . . .)

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

```
from tc_python import *

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

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

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

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

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```
    result_fixed_phase = calc.set_state_to_bookmark(bookmark_fixed_phase_condition)
    print("Conditions do not contain temperature: {}".format(result_fixed_phase.get_
↪conditions()))
    # this calculation had **not yet** been performed
    print("Stable phases (do contain BCC): {}".format(calc.calculate().get_stable_
↪phases()))
```

4.2 Re-use and saving of results

Before a calculation is run in TC-Python, a check is made to see if the exact same calculation has run before, and if that is the case, the result from the calculation can be loaded from disk instead of being re-calculated.

This functionality is always enabled within a script running TC-Python, but you can make it work the same way when re-running a script, or even when running a completely different script.

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

This is controlled by the method *tc_python.server.SetUp.set_cache_folder()*.

```
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)
```

4.3 All TC-Python objects are non-copyable

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

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

```python
from tc_python import *

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

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

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

4.4 Python Virtual Environments

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

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

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

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

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

4.5 Using *with TCPython()* efficiently

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

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

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

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

Example:

```python
from tc_python import *

# ...

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

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


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

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

4.6 Parallel calculations

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

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

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

Example:

```python
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().
```

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```
                        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"])
        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
```

4.7 Handling crashes of the calculation engine

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

```
UnrecoverableCalculationException
```

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

Example:

```
from tc_python import *

for temperature in range(900, 1100, 10):
    try:
```

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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(temperature).
                        set_simulation_time(108000.0).
                        add_region(Region("Austenite").
                            set_width(1E-4).
                            with_grid(CalculatedGrid.linear().set_no_of_points(50)).
                            with_composition_profile(CompositionProfile().
                                add("Ni", ElementProfile.linear(10.0, 50.0))
                            ).
                        add_phase("FCC_A1")).
                calculate())

            distance, ni_fraction = diffusion_result.get_mass_fraction_of_component_at_
↪time("Ni", 108000.0)
            print(ni_fraction)

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

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

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

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

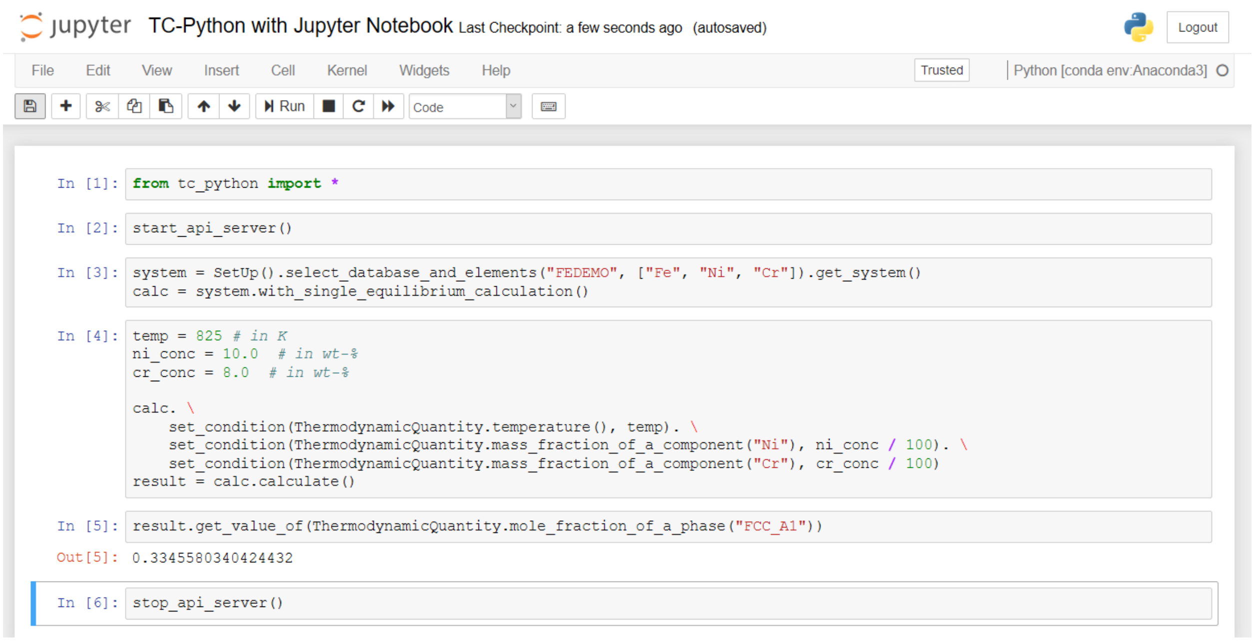
You need to make sure that you execute the two functions *tc_python.server.start_api_server()* and *tc_python.server.stop_api_server()* **exactly once within the Jupyter Notebook session**. If not stopping TC-Python, extra Java-processes might be present and the temporary disk-space is not cleared. However,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

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

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

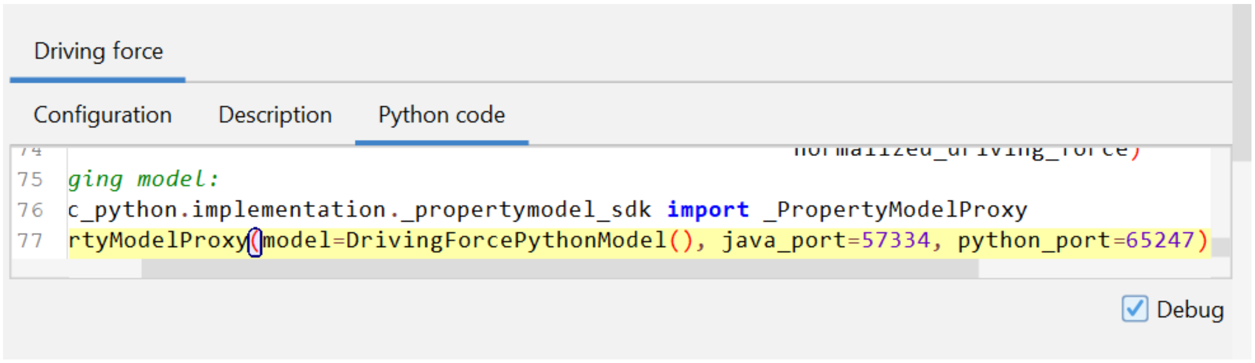
```
In [1]: from tc_python import *

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()
```

4.9 Property Model Framework

4.9.1 Debugging Property Model code

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

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



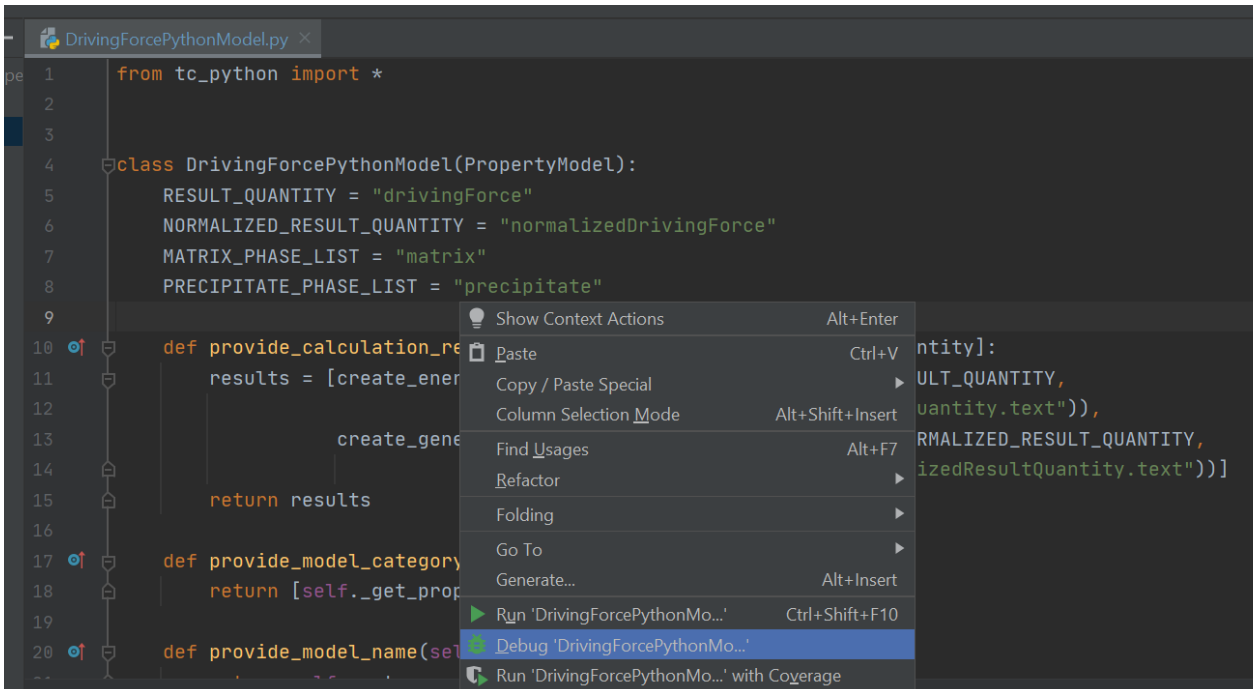
```
ging model:
c_python.implementation._propertymodel_sdk import _PropertyModelProxy
rtyModelProxy(model=DrivingForcePythonModel(), java_port=57334, python_port=65247)
```

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

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

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

In PyCharm it looks like this:


DrivingForcePythonModel.py
Show Context Actions Alt+Enter
Paste Ctrl+V
Copy / Paste Special
Column Selection Mode Alt+Shift+Insert
Find Usages Alt+F7
Refactor
Folding
Go To
Generate... Alt+Insert
Run 'DrivingForcePythonMo...' Ctrl+Shift+F10
Debug 'DrivingForcePythonMo...'
Run 'DrivingForcePythonMo...' with Coverage

```
from tc_python import *


class DrivingForcePythonModel(PropertyModel):
    RESULT_QUANTITY = "drivingForce"
    NORMALIZED_RESULT_QUANTITY = "normalizedDrivingForce"
    MATRIX_PHASE_LIST = "matrix"
    PRECIPITATE_PHASE_LIST = "precipitate"

    def provide_calculation_re                                ntity]:
        results = [create_ener                                ULT_QUANTITY,
                                                              uantity.text")),
                   create_gene                                RMALIZED_RESULT_QUANTITY,
                                                              izedResultQuantity.text"))]
        return results

    def provide_model_category
        return [self._get_prop

    def provide_model_name(sel
```

Note: When your IDE and Thermo-Calc have sucessfully connected, you will see this in the Thermo-Calc log:

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

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

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

```
from tc_python import *

with TCPython() as start:
    property_model = (
        start.
            select_database_and_elements("FEDEMO", ["Fe", "C"]).
            get_system().
            with_property_model_calculation("my own Driving Force", debug_model=True).
            set_composition("C", 1.0).
            )
    property_model.calculate()

    ...
```

4.9.2 Developing Property Models in several files

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

- *side-by-side* modules
- *common* modules

Side-by-side modules are Python files located in the same folder as the Property Model.

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

4.9.2.1 *side-by-side* modules

You are required to:

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

Example:

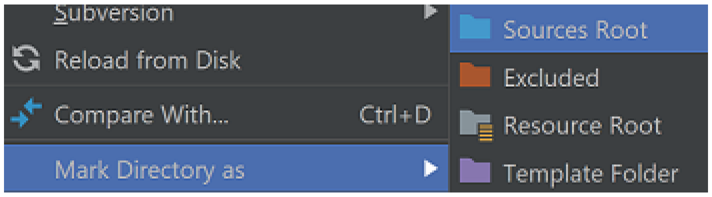
`CriticalTemperaturesPythonModel.py` (The main Property Model file):

```
from CriticalTemperaturesPython import CriticalTemperatures
from tc_python import *
import numpy as np

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

`__init__.py`:

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

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



critical_temperatures_library.py:

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

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

Note: Modules installed in the Python interpreter such as *numpy*, *scipy*, etc can be imported as normal. This only concerns files imported as *side-by-side* modules.

4.9.2.2 *common* modules

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

You are required to:

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

Example:

`CriticalTemperaturesPythonModel.py` (The main Property Model file):

```
from PropertyModels import Martensite
from tc_python import *

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

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

```
from PropertyModels import Martensite
```

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

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

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

critical_temperatures_library.py:

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

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

Note: *common* modules must be located in folder called `common`.

4.9.3 Alternative Python for Property Models

4.9.3.1 Default bundled Python interpreter

Thermo-Calc is by default using a Python 3.9.18 interpreter bundled to the software for running the property models. It is containing the following major packages:

Package	Version
matplotlib	3.8
numpy	1.26.0
scikit-learn	1.3.1
scipy	1.11.3
pyvista	0.42.2
TC-Python	2024a

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

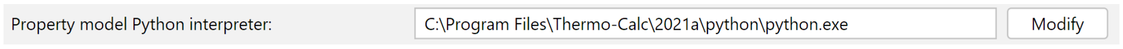
Please contact the Thermo-Calc support if you think that further packages might be useful in future releases. If these packages are insufficient for you, it is possible to use another Python-interpreter: *Configuring another Python interpreter*.

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

Operating system	Path to the bundled Python-interpreter
Windows	`C:\Program Files\Thermo-Calc\2024a\python\python.exe`
Linux	`/home/UserName/Thermo-Calc/2024a/python/bin/python3`
MacOS	`/Applications/Thermo-Calc-2024a.app/Contents/Resources/python/bin/python3`

4.9.3.2 Configuring another Python interpreter

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


Property model Python interpreter: C:\Program Files\Thermo-Calc\2021a\python\python.exe

4.10 Process Metallurgy Calculations

4.10.1 Equilibrium calculations with changing elements between calculations

It is possible to add, change or remove additions after performing an equilibrium calculation using *tc_python.process_metallurgy.equilibrium.EquilibriumCalculation.calculate()*. This will change the elements being present in the system if the elements of the additions are differing. The Process Metallurgy Module will handle this situation by reloading the database with the latest set of elements. While this is an appropriate approach in most cases, there can be some disadvantages: reloading the database takes some time and the internal engine state is lost, which may lead to successive calculations failures in some situations.

To avoid the database reload, it is possible **to add the respective elements to additions being present in all calculations (with a zero-fraction)**:

```
from tc_python import *

with TCPython() as session:
    calc = session.with_metallurgy().with_adiabatic_equilibrium_
↪calculation(ProcessDatabase.OXDEMO)

    # add the element Al with zero-fraction already
    steel = EquilibriumAddition({'Fe': None, 'C': 4, 'Al': 0}, amount=100.0e3,␣
↪temperature=1700 + 273.15)
    slag = EquilibriumAddition({'CaO': 70, 'SiO2': 30}, amount=3.0e3, temperature=1700 +␣
↪273.15)

    al_addition = EquilibriumAddition({'Al': 100}, amount=1.0e3)

    (calc
     .add_addition(steel)
     .add_addition(slag))

    result_1 = calc.calculate()

    calc.add_addition(al_addition)

    result_2 = calc.calculate()
    # evaluate the result as required ...
```

Or **to add a later addition already before the first call to** `calculate()` **with a zero amount**:

```
from tc_python import *

with TCPython() as session:
```

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(continued from previous page)

```
    calc = session.with_metallurgy().with_adiabatic_equilibrium_
↪calculation(ProcessDatabase.OXDEMO)

    steel = EquilibriumAddition({'Fe': None, 'C': 4}, amount=100.0e3, temperature=1700 +␣
↪273.15)
    slag = EquilibriumAddition({'CaO': 70, 'SiO2': 30}, amount=3.0e3, temperature=1700 +␣
↪273.15)

    # add the addition for now with zero-amount
    al_addition = EquilibriumAddition({'Al': 100}, amount=0)

    (calc
     .add_addition(al_addition)
     .add_addition(steel)
     .add_addition(slag))

    result_1 = calc.calculate()

    calc.update_addition(al_addition.set_amount(1.0e3))

    result_2 = calc.calculate()
    # evaluate the result as required ...
```

4.10.2 Zones

TC-Python is providing a *framework* for building time-dependent kinetic simulations of industrial and academic metallurgical processes where liquid phases are important. It is based on an *Effective Equilibrium Reaction Zone* (EERZ) approach which is separating a process into different zones. These zones have identical temperature and composition and are called *bulk zones*. Such zones can be in contact and react with each other by *reaction zones*. That means a *reaction zone* is modelling the interface between two *bulk zones*. One bulk zone is typically the steel melt and another bulk zone the top slag.

4.10.3 Applications

While this approach can in principle be extended to any number of zones, in the current release TC-Python is providing **only one reaction zone**. Practical work has however proven that this limitation is not critical for a lot of industrial processes, including ladle furnaces, AOD- and VOD-converters. Even more processes can be modelled with some limit of accuracy.

The reason for the power of the current implementation is that a number of important process features can be included:

- heating (*tc_python.process_metallurgy.process.Zone.add_power()*)
- cooling (*tc_python.process_metallurgy.process.Zone.add_power()*)
- heat transfer between bulk zones (*tc_python.process_metallurgy.process.ReactionZone.add_heat_transfer()*)
- inclusion formation
- inclusion flotation and other transfer of phase groups between bulk zones (*tc_python.process_metallurgy.process.ReactionZone.add_transfer_of_phase_group()*)

- addition of material and gas at any time in any zone (`tc_python.process_metallurgy.process.Zone.add_addition()` / `tc_python.process_metallurgy.process.Zone.add_continuous_addition()`)
- an exhaust gas zone collecting all formed gas (`tc_python.process_metallurgy.process.ProcessSimulationResult.get_exhaust_gas()`)
- time-dependent definition of most parameters (e.g., mass transfer coefficient, transfer of phase group, heating, etc.)

Please note that many of these features are called as well a *reaction zone* in other EERZ model implementations.

4.10.4 Implementation of practical process models

The Process Metallurgy Module has been successfully applied to a number of industrial processes.

Due to the broad range of industrial metallurgical processes, TC-Python is not providing ready-to-use models for certain processes. There are however examples available for common processes and this collection will be extended over time. The implementation of a model is an abstraction of the real process and should always be kept as simple as possible. Practical experience has proven that in many situations not more than one *reaction zone* is required.

The mass transfer coefficient is a fundamental parameter describing the kinetics in a *reaction zone* and is generally an empirical parameter. It depends however mostly on the geometry and stirring conditions in the process and not on the material compositions. Further on, the mass transfer coefficient has usually typical values for a given process - regardless of the actual furnace. That means that existing suggestions from the literature can be used as a starting point to derive the actual mass transfer coefficient for the process of interest.

CHAPTER

FIVE

API REFERENCE

5.1 Calculations

5.1.1 Module "single_equilibrium"

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

Bases: *`AbstractCalculation`*

Abstract configuration required for a single equilibrium calculation.

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

`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, etc.

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

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

Returns
Gibbs energy addition to G per mole formula unit.

`get_system_data()` → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

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

Returns
The system data

`run_poly_command`(*command: str*)

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

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

Returns
This `SingleEquilibriumCalculation` object

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

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

`set_component_to_entered`(*component: str*)

Sets the specified component to the status ENTERED, that is the default state.

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

Returns
This `SingleEquilibriumCalculation` object

`set_component_to_suspended`(*component: str*, *reset_conditions: bool = False*)

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

Parameters

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

Returns
This `SingleEquilibriumCalculation` object

`set_gibbs_energy_addition_for`(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This *`SingleEquilibriumCalculation`* object

`set_phase_to_dormant`(*phase: str*)

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

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

Returns
This *`SingleEquilibriumCalculation`* object

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

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

Parameters

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

Returns
This *`SingleEquilibriumCalculation`* object

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

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

Parameters

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

Returns
This *`SingleEquilibriumCalculation`* object

`set_phase_to_suspended`(*phase: str*)

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

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

Returns
This *`SingleEquilibriumCalculation`* object

`with_options`(*options:* SingleEquilibriumOptions)

Sets the simulation options.

Parameters
`options` – The simulation options

Returns
This *`SingleEquilibriumCalculation`* object

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

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

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

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

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

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

Parameters

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

Returns

This *`SingleEquilibriumCalculation`* object

`with_system_modifications`(*system_modifications:* SystemModifications)

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

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

Parameters

`system_modifications` – The system modification to be performed

Returns

This *`SingleEquilibriumCalculation`* object

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

Bases: *`AbstractSingleEquilibriumCalculation`*

Configuration for a single equilibrium calculation.

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

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

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

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

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

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

Returns
The bookmark id

calculate() → *SingleEquilibriumTempResult*

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

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

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

calculate_with_state(*timeout_in_minutes: float = 0.0*) → *SingleEquilibriumResult*

Performs the calculation and provides a result object that reflects the present state of the calculation during the whole lifetime of the object.

Note: Because this method has performance and temporary disk space overhead (i.e. it is resource heavy), only use it when it is necessary to access the result object after the state is changed. In most cases you should use the method `calculate()`.

Parameters
timeout_in_minutes – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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, etc.

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

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

Returns
Gibbs energy addition to G per mole formula unit.

get_interfacial_energy(*matrix_phase: str*, *precipitate_phases: List[str]*, *zero_volume_elements: List[str] = ['C', 'N']*) → Dict[str, float]

Estimates the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. The approximation model is based on Becker's bond energy approach.

Default: elements with no contribution to volume are C and N.

Parameters

- **matrix_phase** – The matrix phase.
- **precipitate_phases** – The list of precipitate phases for which interfacial energy between them and the matrix phase is to be calculated.
- **zero_volume_elements** – The elements that are assumed to not contribute to the volume.

Returns
A dictionary containing interfacial energy per precipitate phase.

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

remove_all_conditions()

Removes all set conditions.

Returns
This *SingleEquilibriumCalculation* object

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

Removes the specified condition.

Parameters

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

Returns

This *`SingleEquilibriumCalculation`* object

`run_poly_command`(*command: str*)

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

Parameters

`command` – The Thermo-Calc Console Mode command

Returns

This *`SingleEquilibriumCalculation`* object

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

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

`set_component_to_entered`(*component: str*)

Sets the specified component to the status ENTERED, that is the default state.

Parameters

`component` – The component name or *ALL_COMPONENTS*

Returns

This *`SingleEquilibriumCalculation`* object

`set_component_to_suspended`(*component: str, reset_conditions: bool = False*)

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

Parameters

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

Returns

This *`SingleEquilibriumCalculation`* object

`set_condition`(*quantity: Union[*ThermodynamicQuantity*, str], value: float*)

Sets the specified condition.

Parameters

- `quantity` – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example "X(Cr)")
- `value` – The value of the condition

Returns

This *`SingleEquilibriumCalculation`* object

set_gibbs_energy_addition_for(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This *SingleEquilibriumCalculation* object

set_phase_to_dormant(*phase: str*)

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

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

Returns
This *SingleEquilibriumCalculation* object

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

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

Parameters

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

Returns
This *SingleEquilibriumCalculation* object

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

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

Parameters

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

Returns
This *SingleEquilibriumCalculation* object

set_phase_to_suspended(*phase: str*)

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

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

Returns
This *SingleEquilibriumCalculation* object

`set_state_to_bookmark`(*bookmark_id: str*) → *SingleEquilibriumTempResult*

Resets the calculation state to a previously bookmarked state.

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

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

Parameters
`bookmark_id` – The bookmark id of the state to return to.

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

`with_options`(*options:* SingleEquilibriumOptions)

Sets the simulation options.

Parameters
`options` – The simulation options

Returns
This *`SingleEquilibriumCalculation`* object

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

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

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

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

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

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

Parameters

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

Returns
This *`SingleEquilibriumCalculation`* object

with_system_modifications(*system_modifications:* SystemModifications)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This *SingleEquilibriumCalculation* object

class tc_python.single_equilibrium.**SingleEquilibriumOptions**

Bases: `object`

General simulation conditions for the thermodynamic calculations.

disable_approximate_driving_force_for_metastable_phases()

Disables the approximation of the driving force for metastable phases.

Default: Enabled

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

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

Returns
This *SingleEquilibriumOptions* object

disable_control_step_size_during_minimization()

Disables stepsize control during minimization (non-global).

Default: Enabled

Returns
This *SingleEquilibriumOptions* object

disable_force_positive_definite_phase_hessian()

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

Default: Enabled

Returns
This *SingleEquilibriumOptions* object

enable_approximate_driving_force_for_metastable_phases()

Enables the approximation of the driving force for metastable phases.

Default: Enabled

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

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

Returns
This *SingleEquilibriumOptions* object

enable_control_step_size_during_minimization()

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

Default: Enabled

Returns
This *SingleEquilibriumOptions* object

enable_force_positive_definite_phase_hessian()

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

Default: Enabled

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: *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 *get_value_of()* to obtain them.

Parameters
`pressure` – The pressure [Pa]

Returns
This *SingleEquilibriumCalculation* object

change_temperature(*temperature: float*)

Change the temperature and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with high performance. The properties are calculated at the new temperature using the phase amount, pressure and composition of phases from the initial equilibrium. Use *get_value_of()* to obtain them.

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

Parameters
`temperature` – The temperature [K]

Returns
This `SingleEquilibriumCalculation` object

`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[*ThermodynamicQuantity*, str]*) → float

Returns a value from a single equilibrium calculation.

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

Returns
The requested value

`run_poly_command`(*command: str*)

Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine. This affects only the state of the result object.

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

Returns
This `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: *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 behavior to use that object after something has been changed in the state of the calculation, this will result in an `InvalidResultStateException` exception being raised.

`change_pressure`(*pressure: float*)

Change the pressure and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with higher performance. The properties are calculated at the new pressure using the phase amount, temperature and composition of phases from the initial equilibrium. Use *get_value_of()* to obtain them.

Parameters
`pressure` – The pressure [Pa]

Returns
This *SingleEquilibriumCalculation* object

`change_temperature`(*temperature: float*)

Change the temperature and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with high performance. The properties are calculated at the new temperature using the phase amount, pressure and composition of phases from the initial equilibrium. Use *get_value_of()* to obtain them.

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

Parameters
`temperature` – The temperature [K]

Returns
This *SingleEquilibriumCalculation* object

`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[*ThermodynamicQuantity*, str]*) → float

Returns a value from a single equilibrium calculation.

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

Returns
The requested value

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

`run_poly_command`(*command: str*)

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

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

Returns
This *`SingleEquilibriumCalculation`* object

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

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

5.1.2 Module "batch_equilibrium"

`class tc_python.batch_equilibrium.`**`BatchEquilibriumCalculation`**`(`*calculator*`)`

Bases: `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[*ThermodynamicQuantity*, str]], logging_frequency: int = 10, timeout_in_minutes: float = 0.0*`)` → *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

- **`quantities`** – A list of the quantities to be calculated.
- **`logging_frequency`** – Determines how often logging should be done.
- **`timeout_in_minutes`** – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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, etc.

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

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

Returns
Gibbs energy addition to G per mole formula unit.

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

remove_all_conditions()

Removes all set conditions.

Returns
This *BatchEquilibriumCalculation* object

remove_condition(*quantity: Union[*ThermodynamicQuantity*, str]*)

Removes the specified condition.

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

Returns
This *BatchEquilibriumCalculation* object

run_poly_command(*command: str*)

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

Parameters
command – The Thermo-Calc Console Mode command

Returns
This *BatchEquilibriumCalculation* object

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

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

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*, *reset_conditions: bool = False*)

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

Parameters

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

Returns

This *BatchEquilibriumCalculation* object

set_condition(*quantity: Union[ThermodynamicQuantity, str]*, *value: float*)

Sets the specified condition.

Parameters

- **quantity** – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example "X(Cr)")
- **value** – The value of the condition

Returns

This *BatchEquilibriumCalculation* object

set_conditions_for_equilibria(*equilibria: List[List[Tuple[Union[ThermodynamicQuantity, str], float]]]*)

Set the conditions of the equilibria to be calculated.

This is done by sending a list of equilibria at once.

Each equilibrium itself is a list of conditions that will be changed for that equilibrium.

A condition is described by a tuple containing:

1. A Console Mode syntax string or a `ThermodynamicQuantity` instance,
2. A float value specifying the value of the condition.

Example:

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

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

Example:

```
>>> [[(ThermodynamicQuantity.temperature(), 800), (ThermodynamicQuantity.mole_
→fraction_of_a_component('Cr'), 0.1)], [(ThermodynamicQuantity.temperature(),␣
→850), (ThermodynamicQuantity.mole_fraction_of_a_component('Cr'), 0.15)]]
```

Parameters
`equilibria` – The list of equilibria

Returns
This *`BatchEquilibriumCalculation`* object

`set_gibbs_energy_addition_for`(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This *`BatchEquilibriumCalculation`* object

`set_phase_to_dormant`(*phase: str*)

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

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

Returns
This *`BatchEquilibriumCalculation`* object

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

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

Parameters

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

Returns
This *`BatchEquilibriumCalculation`* object

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

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

Parameters

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

Returns
This *BatchEquilibriumCalculation* object

set_phase_to_suspended(*phase: str*)

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

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

Returns
This *BatchEquilibriumCalculation* object

with_options(*options:* SingleEquilibriumOptions)

Sets the simulation options.

Parameters
options – The simulation options

Returns
This *BatchEquilibriumCalculation* object

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

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

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

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

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

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

Parameters

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

Returns
This *BatchEquilibriumCalculation* object

with_system_modifications(*system_modifications: SystemModifications*)

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

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

Parameters
system_modifications – The system modification to be performed

Returns
This *BatchEquilibriumCalculation* object

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

Bases: `object`

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

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

invalidate()

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

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

5.1.3 Module “precipitation”

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

Bases: *GrainGrowthModel*

set_grain_aspect_ratio(*grain_aspect_ratio: float = 1.0*)

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

Parameters
grain_aspect_ratio – The grain aspect ratio [-]

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

Bases: *`GrainGrowthModel`*

`disable_zener_pinning`()

Disable Zener pinning to ignore the particle pinning effect on the grain growth. Zener pinning is by default disabled when no grain size distribution is defined, i.e. a single constant grain size is used. The setting is by default enabled when a grain size distribution is defined.

Returns
This *`GrainSizeDistribution`* object

`enable_zener_pinning`()

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

Returns
This *`GrainSizeDistribution`* object

`set_grain_boundary_energy`(*energy: float = 0.5*)

Set the energy of the grain boundary.

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

Returns
This *`GrainSizeDistribution`* object

`set_grain_boundary_mobility_activation_energy`(*activation_energy: float = 242000.0*)

Set the grain boundary mobility activation energy where the mobility is defined by an Arrhenius type of equation.

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

Returns
This *`GrainSizeDistribution`* object

`set_grain_boundary_mobility_pre_factor`(*pre_factor: float = 0.004*)

Set the grain boundary mobility prefactor where the mobility is defined by an Arrhenius type of equation.

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

Returns
This *`GrainSizeDistribution`* object

class `tc_python.precipitation.`**`GrainGrowthModel`**

Bases: `object`

Factory class providing objects representing a grain growth model.

classmethod **`fixed_grain_size`**(*grain_radius: float = 0.0001*)

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

Parameters
`grain_radius` – The grain radius / size [m]

classmethod **`grain_growth`**(*grain_size_distribution:* GrainSizeDistribution)

Sets the initial grain size distribution for the matrix. **Default**: If the initial grain size distribution is not explicitly provided, a constant average grains size will be used and no grain growth evaluated during the simulation.

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

Parameters
`grain_size_distribution` – grain size distribution

`class tc_python.precipitation.GrainSizeDistribution`

Bases: `object`

Represents the grain size distribution at a certain time.

`add_radius_and_number_density`(*radius: float*, *number_density: float*)

Adds a radius and number density pair to the grain size distribution.

Parameters

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

Returns
This *GrainSizeDistribution* object

`class tc_python.precipitation.GrowthRateModel`(*value*)

Bases: `Enum`

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.

`PE_AUTOMATIC = 12`

The PE Automatic model enables the smooth transition from Paraequilibrium growth rate model to Simplified growth rate model. The rate of transition process is dependent on the relative differences in diffusion between C and substitutional elements, as well as the differences in driving force between paraequilibrium and ortho-equilibrium.

`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:* 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_mobility_adjustment(`*element: str = 'all', prefactor: float = 1.0, activation_energy: float = 0.0*`)`

A value that adds to the activation energy of mobility data from the database.

Parameters

- `element` – The alement to apply the adjustment for. If "all" is given, adjustment will apply to all elements.
- `prefactor` – A parameter that multiplies to the mobility data from a database. This value scales the mobility by a constant amount. This can be useful, for example, when the material has a higher than normal vacancy concentration at the start of the precipitation simulation (e.g. from a prior solutionizing and quenching treatment).
- `activation_energy` – A value that adds to the activation energy of mobility data from a database. It scales the mobility by a temperature dependent amount. Similar usage as mobility adjustment prefactor. [J/mol]

set_mobility_enhancement_activation_energy(*mobility_enhancement_activation_energy: float = 0.0*)

A value that adds to the activation energy of mobility data from the database. **Default**: 0.0 J/mol

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

set_mobility_enhancement_prefactor(*mobility_enhancement_prefactor: float = 1.0*)

A parameter that multiplies to the mobility data from database. **Default**: 1.0

Parameters
mobility_enhancement_prefactor – The mobility enhancement factor [-]

set_molar_volume(*volume: float*)

Sets the molar volume of the phase.

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

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

with_elastic_properties_cubic(*c11: float*, *c12: float*, *c44: float*)

Sets the elastic properties to "cubic" and specifies the elastic stiffness tensor components. **Default**: if not chosen, the default is DISREGARD

Parameters

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

with_elastic_properties_disregard()

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

with_elastic_properties_isotropic(*shear_modulus: float*, *poisson_ratio: float*)

Sets elastic properties to isotropic. **Default**: if not chosen, the default is DISREGARD

Parameters

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

with_grain_growth_model(*grain_growth_model:* GrainGrowthModel)

Sets the model for grain growth. Either fixed size or with a starting distribution

Default: Fixed grain radius size 1.0E-4 m

Parameters
grain_growth_model – the grain growth model

class tc_python.precipitation.**NumericalParameters**

Bases: object

Numerical parameters

`set_max_overall_volume_change`(*max_overall_volume_change: float = 0.001*)

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

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

`set_max_radius_points_per_magnitude`(*max_radius_points_per_magnitude: float = 200.0*)

Sets the maximum number of grid points over one order of magnitude in radius. **Default**: 200.0

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

`set_max_rel_change_critical_radius`(*max_rel_change_critical_radius: float = 0.1*)

Used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step. **Default**: 0.1

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

`set_max_rel_change_nucleation_rate_log`(*max_rel_change_nucleation_rate_log: float = 0.5*)

This parameter ensures accuracy for the evolution of effective nucleation rate. **Default**: 0.5

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

`set_max_rel_radius_change`(*max_rel_radius_change: float = 0.01*)

The maximum value allowed for relative radius change in one time step. **Default**: 0.01

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

`set_max_rel_solute_composition_change`(*max_rel_solute_composition_change: float = 0.01*)

Set a limit on the time step by controlling solute depletion or saturation, especially at isothermal stage. **Default**: 0.01

Parameters
`max_rel_solute_composition_change` – The limit for the relative solute composition change [-]

`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: 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_option()`*. 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`(*value*)

Bases: `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()

Disables 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()

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

Returns
This *PrecipitatePhase* object

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 is automatically calculated using a broken-bond model.

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

Returns
This `PrecipitatePhase` object

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

`set_interfacial_energy_estimation_prefactor`(*interfacial_energy_estimation_prefactor: float*)

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

Parameters
`interfacial_energy_estimation_prefactor` – The prefactor for the calculated interfacial energy

Returns
This `PrecipitatePhase` object

Note: The interfacial energy prefactor is an amplification factor for the automatically calculated interfacial energy. Example: *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
- `number_density` – Number density of nucleation sites. If not set, the value is calculated based on the matrix settings (grain size) [m^-3].

Returns
This *PrecipitatePhase* object

`set_nucleation_at_grain_corners`(*wetting_angle: float = 90*, *number_density: float = -1*)

Activates nucleation at grain corners for this class of precipitates. Calling the method overrides any other nucleation setting for this class of precipitates. **Default**: If not set, by default bulk nucleation is chosen.

Parameters

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

Returns
This *PrecipitatePhase* object

`set_nucleation_at_grain_edges`(*wetting_angle=90*, *number_density=-1*)

Activates nucleation at the grain edges for this class of precipitates. Calling the method overrides any other nucleation setting for this class of precipitates. **Default**: If not set, by default bulk nucleation is chosen.

Parameters

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

Returns
This *PrecipitatePhase* object

`set_nucleation_in_bulk`(*number_density: float = -1.0*)

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

Parameters
`number_density` – Number density of nucleation sites. If not set, the value is calculated based on the matrix settings (molar volume) [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:* PrecipitateMorphology)

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

Parameters
precipitate_morphology_enum – The precipitate morphology

Returns
This *PrecipitatePhase* object

set_trans_interface_mobility_adjustment(*element: str = 'all', prefactor: float = 1.0, activation_energy: float = 0.0*)

Trans-interface mobility adjustment Only relevant when growth rate model is PE Automatic A value that adds to the activation energy of mobility data from the database.

Parameters

- **element** – The element to apply the adjustment for. If "all" is given, adjustment will apply to all elements.
- **prefactor** – A parameter that multiplies to the mobility data from a database. The value scales the mobility by a constant amount. This results in the trans-interface mobility that controls the kinetics of Para-Equilibrium to Ortho-Equilibrium transition.
- **activation_energy** – A value that adds to the activation energy of mobility data from a database.It scales the mobility by a temperature dependent amount. Similar usage as trans-interface mobility adjustment prefactor. [J/mol]

set_transformation_strain_calculation_option(*transformation_strain_calculation_option_enum:* TransformationStrainCalculationOption)

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

Parameters
transformation_strain_calculation_option_enum – The chosen option

Returns
This *PrecipitatePhase* object

set_zener_pinning_parameters(*cutoff_size: float = 7e-07, kinetic_prefactor: float = 0.5, exponent: float = 0.93*)

These parameters are only relevant when zener pinning is enabled in the matrix phase

Parameters

- **cutoff_size** – Precipitates with radius smaller than this value are neglected in pinning force calculation.
- **kinetic_prefactor** – Dimensionless kinetic coefficient in Zener equation.
- **exponent** – Exponent of precipitate volume fraction in Zener equation.

Returns
This *PrecipitatePhase* object

with_elastic_properties(*elastic_properties:* PrecipitateElasticProperties)

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

Parameters
elastic_properties – The elastic properties object

Returns
This *PrecipitatePhase* object

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

with_growth_rate_model(*growth_rate_model_enum: 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: 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: *AbstractCalculation*

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

calculate(*timeout_in_minutes: float = 0.0*) → *PrecipitationCalculationTTTorCCTResult*

Runs the CCT diagram calculation.

Parameters
timeout_in_minutes – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

set_composition(*element_name: str, value: float*)

Sets the composition of the elements. The unit for the composition can be changed using *set_composition_unit()*. **Default**: Mole percent (`CompositionUnit.MOLE_PERCENT`)

Parameters

- **`element_name`** – The element
- **`value`** – The composition (fraction or percent depending on the composition unit)

Returns

This *`PrecipitationCCTCalculation`* object

`set_composition_unit`(*unit_enum: CompositionUnit*)

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

Parameters

`unit_enum` – The new composition unit

Returns

This *`PrecipitationCCTCalculation`* object

`set_cooling_rates`(*cooling_rates: List[float]*)

Sets all cooling rates for which the CCT diagram should be calculated.

Parameters

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

Returns

This *`PrecipitationCCTCalculation`* object

`set_max_temperature`(*max_temperature: float*)

Sets maximum temperature of the CCT diagram.

Parameters

`max_temperature` – the maximum temperature [K]

Returns

This *`PrecipitationCCTCalculation`* object

`set_min_temperature`(*min_temperature: float*)

Sets the minimum temperature of the CCT diagram.

Parameters

`min_temperature` – the minimum temperature [K]

Returns

This *`PrecipitationCCTCalculation`* object

`stop_at_volume_fraction_of_phase`(*stop_criterion_value: float*)

Sets the stop criterion as a volume fraction of the phase. This setting is applied to all phases.

Parameters

`stop_criterion_value` – the volume fraction of the phase (a value between 0 and 1)

Returns

This *`PrecipitationCCTCalculation`* object

`with_matrix_phase`(*matrix_phase: MatrixPhase*)

Sets the matrix phase.

Parameters

`matrix_phase` – The matrix phase

Returns

This *`PrecipitationCCTCalculation`* object

with_numerical_parameters(*numerical_parameters: NumericalParameters*)

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

Parameters
numerical_parameters – The parameters

Returns
This *PrecipitationCCTCalculation* object

with_system_modifications(*system_modifications: SystemModifications*)

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

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

Parameters
system_modifications – The system modification to be performed

Returns
This *PrecipitationCCTCalculation* object

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

Bases: *AbstractResult*

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

save_to_disk(*path: str*)

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

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

Returns
this *PrecipitationCalculationResult* object

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

Bases: *PrecipitationCalculationResult*

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

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

get_aspect_ratio_distribution_for_particle_length_of(*precipitate_id: str, time: float*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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_grain_critical_radius()` → [List[float], List[float]]

Returns the critical radius of grains in dependency of the time.

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

`get_grain_mean_radius()` → [List[float], List[float]]

Returns the mean grain size of the matrix phase in dependency of the time.

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

`get_grain_number_density()` → [List[float], List[float]]

Returns the grain number density (concentration) in dependency of the time.

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

`get_grain_number_density_distribution_for_length`(*time: float*) → [List[float], List[float]]

Returns the number density distribution of grains in terms of length at the requested time(s).

Parameters
`time` – The time [s]

Returns
A tuple of two lists of floats (grain length[m], number of grains per unit volume in a size class [m^-3])

`get_grain_number_density_distribution_for_radius`(*time: float*) → [List[float], List[float]]

Returns the number density distribution of a grains in terms of grain radius at the requested time(s).

Parameters
`time` – The time [s]

Returns
A tuple of two lists of floats (radius [m], number of grains per unit volume in a size class [m^-3])

`get_grain_size_distribution`(*time: float*) → [List[float], List[float]]

Returns the size distribution of the matrix phase in dependency of its grain radius at the requested time(s).

Parameters
`time` – The time [s]

Returns
A tuple of two lists of floats (grain radius[m], number density of grains[m^-4])

`get_matrix_composition_in_mole_fraction_of`(*element_name: str*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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_2d_of`(*precipitate_id: str*) → [List[float], List[float]]

Returns the mean radius of cross-sections taken through the dispersion 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_mean_radius_of`(*precipitate_id: str*) → [List[float], 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_normalized_grain_size_distribution`(*time: float*) → [List[float], List[float]]

Returns the normalized number density distribution with the grain radius normalized by the mean radius, for the requested time(s).

Parameters
`time` – The time [s]

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

`get_normalized_number_density_distribution_2d_of`(*precipitate_id: str*, *time: float*) → [List[float], List[float]]

Returns the normalized number density distribution of a precipitate in terms of the radius of cross-sections created by taking a plane through the dispersion, normalized by the mean radius of the cross-section, for the requested time(s).

Parameters

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

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

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

Returns the normalized number density distribution with the particle radius normalized by the mean radius, for the requested time(s).

Parameters

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

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

`get_nucleation_rate_of`(*precipitate_id: str*) → [List[float], 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_2d_for_particle_length_of`(*precipitate_id: str*, *time: float*) → [List[float], List[float]]

Returns the number density distribution of a precipitate considering the radius of cross-sections created by taking a plane through the dispersion, approximating the particles as spherical, for the requested time(s).

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 area within a size class [m^-2])

`get_number_density_distribution_2d_for_radius_of`(*precipitate_id: str*, *time: float*) → [List[float], List[float]]

Returns the number density distribution of a precipitate considering the radius of cross-sections created by taking a plane through the dispersion for the requested time(s).

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 area within a size class [m^-2])

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

Returns the number density distribution of a precipitate in terms of length for the requested time(s).

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 in the size class per unit volume [m^-3])

`get_number_density_distribution_for_radius_of`(*precipitate_id: str*, *time: float*) → [List[float], List[float]]

Returns the number density distribution of a precipitate in terms of radius for the requested time(s).

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 in the size class per unit volume [m^-3])

`get_number_density_of`(*precipitate_id: str*) → [List[float], List[float]]

Returns the particle number density (concentration) 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*) → [List[float], 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*) → [List[float], 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_2d_for_particle_length_of`(*precipitate_id: str*, *time: float*) → [List[float], List[float]]

Returns the size distribution of a precipitate considering the radius of cross-sections created by taking a plane through the dispersion, approximating the particles as spherical, for the requested time(s).

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 area per unit length [m^-3])

`get_size_distribution_2d_for_radius_of`(*precipitate_id: str*, *time: float*) → [List[float], List[float]]

Returns the size distribution of a precipitate considering the radius of cross-sections created by taking a plane through the dispersion for the requested time(s).

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 area per unit length [m^-3])

`get_size_distribution_for_particle_length_of`(*precipitate_id: str*, *time: float*) → [List[float], List[float]]

Returns the size distribution of a precipitate in terms of length for the requested time(s).

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*) → [List[float], List[float]]

Returns the size distribution of a precipitate in terms of radius for the requested time(s).

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*) → [List[float], 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: *PrecipitationCalculationResult*

Result of a TTT or CCT precipitation calculation.

`get_result_for_precipitate`(*precipitate_id: str*) → [List[float], 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: *AbstractCalculation*

Configuration for an isothermal precipitation calculation.

`calculate`(*timeout_in_minutes: float = 0.0*) → *PrecipitationCalculationSingleResult*

Runs the isothermal precipitation calculation.

Parameters
`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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

`get_system_data`() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

`set_composition`(*element_name: str*, *value: float*)

Sets the composition of the elements. The unit for the composition can be changed using *set_composition_unit()*. **Default**: Mole percent (`CompositionUnit.MOLE_PERCENT`)

Parameters

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

Returns
This *PrecipitationIsoThermalCalculation* object

set_composition_unit(*unit_enum: CompositionUnit = CompositionUnit.MOLE_PERCENT*)

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

Parameters
unit_enum – The new composition unit

Returns
This *PrecipitationIsoThermalCalculation* object

set_simulation_time(*simulation_time: float*)

Sets the simulation time.

Parameters
simulation_time – The simulation time [s]

Returns
This *PrecipitationIsoThermalCalculation* object

set_temperature(*temperature: float*)

Sets the temperature for the isothermal simulation.

Parameters
temperature – the temperature [K]

Returns
This *PrecipitationIsoThermalCalculation* object

with_matrix_phase(*matrix_phase: MatrixPhase*)

Sets the matrix phase.

Parameters
matrix_phase – The matrix phase

Returns
This *PrecipitationIsoThermalCalculation* object

with_numerical_parameters(*numerical_parameters: NumericalParameters*)

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

Parameters
numerical_parameters – The parameters

Returns
This *PrecipitationIsoThermalCalculation* object

with_system_modifications(*system_modifications: SystemModifications*)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This *PrecipitationIsoThermalCalculation* object

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

Bases: *AbstractCalculation*

Configuration for a non-isothermal precipitation calculation.

`calculate``(`*timeout_in_minutes: float = 0.0*`)` → *PrecipitationCalculationSingleResult*

Runs the non-isothermal precipitation calculation.

Parameters
`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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

`get_system_data``()` → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

`set_composition``(`*element_name: str*, *value: float*`)`

Sets the composition of the elements. The unit for the composition can be changed using *set_composition_unit()*. **Default**: Mole percent (`CompositionUnit.MOLE_PERCENT`)

Parameters

- `element_name` – The element
- `value` – The composition (fraction or percent depending on the composition unit)

Returns
This *PrecipitationIsoThermalCalculation* object

`set_composition_unit``(`*unit_enum:* CompositionUnit`)`

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

Parameters
`unit_enum` – The new composition unit

Returns
This *PrecipitationIsoThermalCalculation* object

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

Sets the simulation time.

Parameters
`simulation_time` – The simulation time [s]

Returns
This `PrecipitationNonThermalCalculation` object

`with_matrix_phase`(*matrix_phase: MatrixPhase*)

Sets the matrix phase.

Parameters
`matrix_phase` – The matrix phase

Returns
This *`PrecipitationIsoThermalCalculation`* object

`with_numerical_parameters`(*numerical_parameters: NumericalParameters*)

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

Parameters
`numerical_parameters` – The parameters

Returns
This *`PrecipitationIsoThermalCalculation`* object

`with_system_modifications`(*system_modifications: SystemModifications*)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This `PrecipitationNonThermalCalculation` object

`with_temperature_profile`(*temperature_profile: 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: *`AbstractCalculation`*

Configuration for a TTT (Time-Temperature-Transformation) precipitation calculation.

`calculate`(*timeout_in_minutes: float = 0.0*) → *PrecipitationCalculationTTTorCCTResult*

Runs the TTT diagram calculation.

Parameters
`timeout_in_minutes` – Used to prevent the calculation from running longer than what is

wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

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

Returns
The system data

set_composition(*element_name: str*, *value: float*)

Sets the composition of the elements. The unit for the composition can be changed using `set_composition_unit()`. **Default**: Mole percent (`CompositionUnit.MOLE_PERCENT`)

Parameters

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

Returns
This `PrecipitationTTTCalculation` object

set_composition_unit(*unit_enum:* CompositionUnit)

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

Parameters
unit_enum – The new composition unit

Returns
This `PrecipitationTTTCalculation` object

set_max_annealing_time(*max_annealing_time: float*)

Sets the maximum annealing time, i.e. the maximum time of the simulation if the stopping criterion is not reached.

Parameters
max_annealing_time – the maximum annealing time [s]

Returns
This `PrecipitationTTTCalculation` object

set_max_temperature(*max_temperature: float*)

Sets the maximum temperature for the TTT diagram.

Parameters
max_temperature – the maximum temperature [K]

Returns
This `PrecipitationTTTCalculation` object

`set_min_temperature`(*min_temperature: float*)

Sets the minimum temperature for the TTT diagram.

Parameters
`min_temperature` – the minimum temperature [K]

Returns
This *PrecipitationTTTCalculation* object

`set_temperature_step`(*temperature_step: float*)

Sets the temperature step for the TTT diagram. If not set, the default value is 10 K.

Parameters
`temperature_step` – the temperature step [K]

Returns
This *PrecipitationTTTCalculation* object

`stop_at_percent_of_equilibrium_fraction`(*percentage: float*)

Sets the stop criterion to a percentage of the overall equilibrium phase fraction, alternatively a required volume fraction can be specified (using *stop_at_volume_fraction_of_phase()*).

Parameters
`percentage` – the percentage to stop at (value between 0 and 100)

Returns
This *PrecipitationTTTCalculation* object

`stop_at_volume_fraction_of_phase`(*volume_fraction: float*)

Sets the stop criterion as a volume fraction of the phase, alternatively a required percentage of the equilibrium phase fraction can be specified (using `stop_at_percent_of_equilibria_fraction()`). Stopping at a specified volume fraction is the default setting.

This setting is applied to all phases.

Parameters
`volume_fraction` – the volume fraction to stop at (a value between 0 and 1)

Returns
This *PrecipitationTTTCalculation* object

`with_matrix_phase`(*matrix_phase:* MatrixPhase)

Sets the matrix phase.

Parameters
`matrix_phase` – The matrix phase

Returns
This *PrecipitationTTTCalculation* object

`with_numerical_parameters`(*numerical_parameters:* NumericalParameters)

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

Parameters
`numerical_parameters` – The parameters

Returns
This *PrecipitationTTTCalculation* object

with_system_modifications(*system_modifications: SystemModifications*)

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

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

Parameters
system_modifications – The system modification to be performed

Returns
This *PrecipitationTTTCalculation* object

class tc_python.precipitation.**TransformationStrainCalculationOption**(*value*)

Bases: `Enum`

Options for calculating the transformation strain.

CALCULATE_FROM_MOLAR_VOLUME = 2

Calculates the transformation strain from the molar volume, obtains a purely dilatational strain.

DISREGARD = 1

Ignores the transformation strain, **this is the default setting**.

USER_DEFINED = 3

Transformation strain to be specified by the user.

class tc_python.precipitation.**VolumeFractionOfPhaseType**(*value*)

Bases: `Enum`

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: *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.

disable_delta_ferrite_to_austenite_transition()

Turns off the delta ferrite BCC to austenite FCC transition.

Default: Delta ferrite to austenite transition is off. :return: This *CalculateSecondaryDendriteArmSpacing* object

enable_delta_ferrite_to_austenite_transition()

Turns on the delta ferrite BCC to austenite FCC transition.

Default: Delta ferrite to austenite transition is off. :return: This `CalculateSecondaryDendriteArmSpacing` object

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_fast_diffusing_elements(*element_names: List[str]*)

Sets elements as fast diffusing. This allows redistribution of these elements in both the solid and liquid parts of the alloy.

Default: No fast-diffusing elements.

Parameters
`element_names` – The elements

Returns
This `CalculateSecondaryDendriteArmSpacing` object

set_n(*n: float = 0.33*)

Sets the exponent `n` in the governing equation `c * cooling_rate^(-n)`.

Default: 0.33

Parameters
`n` – The exponent [-]

Returns
This `CalculateSecondaryDendriteArmSpacing` object

set_primary_phasename(*primary_phase_name: str = 'AUTOMATIC'*)

Sets the name of the primary phase.

The primary phase is the phase where the back diffusion takes place. If *AUTOMATIC* is selected, the program tries to find the phase which will give the most back diffusion. That behavior can be overridden by selecting a specific primary phase.

Default: *AUTOMATIC*

Parameters
`primary_phase_name` – The phase name (or *AUTOMATIC*)

Returns
This `CalculateSecondaryDendriteArmSpacing` object

class `tc_python.scheil.`**`ConstantSecondaryDendriteArmSpacing`**(*secondary_dendrite_arm_spacing: float = 5e-05*)

Bases: `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.

`disable_delta_ferrite_to_austenite_transition()`

Turns off the delta ferrite BCC to austenite FCC transition.

Default: Delta ferrite to austenite transition is off. :return: This `ConstantSecondaryDendriteArmSpacing` object

`enable_delta_ferrite_to_austenite_transition()`

Turns on the delta ferrite BCC to austenite FCC transition.

Default: Delta ferrite to austenite transition is off. :return: This `ConstantSecondaryDendriteArmSpacing` 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 `ConstantSecondaryDendriteArmSpacing` object

`set_fast_diffusing_elements`(*element_names: List[str]*)

Sets elements as fast diffusing. This allows redistribution of these elements in both the solid and liquid parts of the alloy.

Default: No fast-diffusing elements.

Parameters
`element_names` – The elements

Returns
This `ConstantSecondaryDendriteArmSpacing` object

`set_primary_phasename`(*primary_phase_name: str = 'AUTOMATIC'*)

Sets the name of the primary phase.

The primary phase is the phase where the back diffusion takes place. If *AUTOMATIC* is selected, the program tries to find the phase which will give the most back diffusion. That behavior can be overridden by selecting a specific primary phase.

Default: *AUTOMATIC*

Parameters
`primary_phase_name` – The phase name (or *AUTOMATIC*)

Returns
This `ConstantSecondaryDendriteArmSpacing` object

class `tc_python.scheil.`**`ScheilBackDiffusion`**

Bases: *`ScheilCalculationType`*

Configuration for *back diffusion in the solid primary phase*.

> **Warning:** This feature has only effect on systems with diffusion data (typically a mobility database). If used for a system without diffusion data, a normal Scheil calculation is done.

classmethod **`calculate_secondary_dendrite_arm_spacing`**`()`

Calculate the secondary dendrite arm spacing based on the following equation: `c * 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: *`AbstractCalculation`*

Configuration for a Scheil solidification calculation.

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

`calculate``(`*timeout_in_minutes: float = 0.0*`)` → *ScheilCalculationResult*

Runs the Scheil calculation.

Parameters
`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns
A *`ScheilCalculationResult`* which later can be used to get specific values from the simulation.

`disable_global_minimization``()`

Disables global minimization.

Default: Enabled

Note: When enabled, a global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

Returns
This *ScheilCalculation* object

enable_global_minimization()

Enables global minimization.

Default: Enabled

Note: When enabled, a global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

Returns
This *ScheilCalculation* object

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

set_composition(*component_name: str*, *value: float*)

Sets the composition of a component. The unit for the composition can be changed using *set_composition_unit()*.

Default: Mole percent (`CompositionUnit.MOLE_PERCENT`)

Parameters

- **component_name** – The component
- **value** – The composition value [composition unit defined for the calculation]

Returns
This *ScheilCalculation* object

set_composition_unit(*unit_enum:* CompositionUnit *= CompositionUnit.MOLE_PERCENT*)

Sets the composition unit.

Default: Mole percent (`CompositionUnit.MOLE_PERCENT`).

Parameters
unit_enum – The new composition unit

Returns
This *ScheilCalculation* object

`set_start_temperature`(*temperature_in_kelvin: float = 2500.0*)

Sets the start temperature.

> **Warning:** The start temperature needs to be higher than the liquidus temperature of the alloy.

Default: 2500.0 K

Parameters
`temperature_in_kelvin` – The temperature [K]

Returns
This *`ScheilCalculation`* object

`with_calculation_type`(*scheil_calculation_type:* ScheilCalculationType)

Chooses a specific Scheil calculation. ClassicScheil for only setting fast diffusers, ScheilBackDiffusion enables back diffusion in the solid primary phase and optionally fast diffusers in all solid phases, and ScheilSoluteTrapping enables solute trapping in the solid primary phase. :param scheil_type: Type of Scheil calculation, either ScheilClassic, ScheilBackDiffusion or ScheilSoluteTrapping :return: This *`ScheilCalculation`* object

`with_options`(*options:* ScheilOptions)

Sets the Scheil simulation options.

Parameters
`options` – The Scheil simulation options

Returns
This *`ScheilCalculation`* object

`with_system_modifications`(*system_modifications:* SystemModifications)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This *`ScheilCalculation`* object

class `tc_python.scheil.`**`ScheilCalculationResult`**(*result*)

Bases: *`AbstractResult`*

Result of a Scheil calculation.

`get_solid_phase_with_largest_mole_fraction`() → str

Returns the name of the solid phase with the largest amount in terms of mole fraction at the end of the Scheil simulation.

Returns
Phase name

get_stable_phases() → List[str]

Returns all phases that were stable during a Scheil simulation.

Returns
The list of stable phases

get_values_grouped_by_quantity_of(*x_quantity: Union[*ScheilQuantity*, str]*, *y_quantity: Union[*ScheilQuantity*, str]*, *sort_and_merge: bool = True*) → Dict[str, *ResultValueGroup*]

Returns x-y-line data grouped by the multiple datasets of the specified quantities (for example in dependency of phases or components). Use *get_values_of()* instead if you need no separation. The available quantities can be found in the documentation of the factory class `ScheilQuantity`.

Note: The different datasets might contain *NaN*-values between different subsections and might not be sorted **even if the flag `sort_and_merge` has been set** (because they might be unsortable due to their nature).

Parameters

- **x_quantity** – The first Scheil quantity ("x-axis"), Console Mode syntax strings can be used as an alternative (for example "T")
- **y_quantity** – The second Scheil quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example "NV")
- **sort_and_merge** – If *True*, the data is sorted and merged into as few subsections as possible (divided by *NaN*)

Returns
Containing the `ResultValueGroup` dataset objects with their *quantity labels* as keys

get_values_grouped_by_stable_phases_of(*x_quantity: Union[*ScheilQuantity*, str]*, *y_quantity: Union[*ScheilQuantity*, str]*, *sort_and_merge: bool = True*) → Dict[str, *ResultValueGroup*]

Returns x-y-line data grouped by the sets of "stable phases" (for example "LIQUID" or "LIQUID + FCC_A1"). Use *get_values_of()* instead if you need no separation. The available quantities can be found in the documentation of the factory class `ScheilQuantity`.

Note: The different datasets might contain *NaN*-values between different subsections and might not be sorted **even if the flag `sort_and_merge` has been set** (because they might be unsortable due to their nature).

Parameters

- **x_quantity** – The first Scheil quantity ("x-axis"), Console Mode syntax strings can be used as an alternative (for example "T")
- **y_quantity** – The second Scheil quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example "NV")
- **sort_and_merge** – If *True*, the data will be sorted and merged into as few subsections as possible (divided by *NaN*)

Returns
Containing the `ResultValueGroup` dataset objects with their *"stable phases" labels* as keys

get_values_of(*x_quantity: Union[*ScheilQuantity*, str]*, *y_quantity: Union[*ScheilQuantity*, str]*) → [List[float], List[float]]

Returns sorted x-y-line data without any separation. Use *get_values_grouped_by_quantity_of()* or *get_values_grouped_by_stable_phases_of()* instead if you need such a separation. The available quantities can be found in the documentation of the factory class `ScheilQuantity`.

Note: This method will always return sorted data without any *NaN*-values. In case of ambiguous quantities (for example: CompositionOfPhaseAsWeightFraction("FCC_A1", "All")) that can give data that is hard to interpret. In such a case you need to choose the quantity in another way or use one of the other methods.

Parameters

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

Returns

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

save_to_disk(*path: str*)

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

Parameters

path – the path to the folder you want the result to be saved in.

Returns

this *ScheilCalculationResult* object

class tc_python.scheil.**ScheilCalculationType**

Bases: `object`

Specific configuration for the different Scheil calculation types

classmethod **scheil_back_diffusion**()

Configuration for *back diffusion in the solid primary phase*.

Warning: This feature has only effect on systems with diffusion data (typically a mobility database). If used for a system without diffusion data, a normal Scheil calculation is done. :return: A *ScheilBackDiffusion*

classmethod **scheil_classic**()

Configuration for Classic Scheil with fast diffusers. :return: A *ScheilClassic*

classmethod **scheil_solute_trapping**()

Configures the Scheil solute trapping settings. The used solidification speed equation is *Scanning speed * cos(angle)* with *Scanning speed* and *angle* being provided either by the user or taken from the defaults. :return: A *ScheilSoluteTrapping*

class tc_python.scheil.**ScheilClassic**

Bases: *ScheilCalculationType*

Configuration for Classic Scheil with fast diffusers.

disable_delta_ferrite_to_austenite_transition()

Turns off the delta ferrite BCC to austenite FCC transition.

Default: Delta ferrite to austenite transition is off. :return: This *ScheilClassic* object

enable_delta_ferrite_to_austenite_transition()

Turns on the delta ferrite BCC to austenite FCC transition.

Default: Delta ferrite to austenite transition is off. :return: This *ScheilClassic* 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 *ScheilClassic* object

class tc_python.scheil.**ScheilOptions**

Bases: object

Options for the Scheil simulation.

calculate_from_gas()

Calculates the evaporation temperature if a gas phase is selected in the system, and then calculates equilibria in the gas+liquid and liquid regions until liquidus temperature is reached.

Default: Calculation starts from liquidus temperature.

Returns
This *ScheilOptions* object

calculate_from_liquidus()

Solidification calculation starting from the liquidus temperature. Liquid properties between start temperature and liquidus are not obtainable.

Default: Calculation starts from liquidus temperature.

Returns
This *ScheilOptions* object

calculate_from_start_temperature()

Calculation of equilibria from start temperature at 50 K intervals until liquidus temperature is reached. This option makes it possible to obtain properties of the liquid phase before the solidification starts.

Default: Calculation starts from liquidus temperature.

Returns
This *ScheilOptions* object

calculate_to_end_of_scheil()

Stops the calculation when the Scheil calculation is finished.

Default: Calculation stops when the Scheil calculation is finished.

Returns
This *ScheilOptions* object

calculate_to_temperature_below_solidus(*number_of_steps: int = 50*, *final_temperature: float = 298.15*)

Calculates properties in the solid state, for the phase compositions and fractions at the end of the Scheil calculation.

Default: Calculation stops when the Scheil calculation is finished.

Parameters

- **number_of_steps** – Calculates properties for the given number of temperatures, down to the final temperature.
- **final_temperature** – The final (lowest) temperature where the calculation is performed.

Returns
This *ScheilOptions* object

disable_approximate_driving_force_for_metastable_phases()

Disables the approximation of the driving force for metastable phases.

Default: Enabled

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

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

Returns
This *ScheilOptions* object

disable_control_step_size_during_minimization()

Disables stepsize control during minimization (non-global).

Default: Enabled

Returns
This *ScheilOptions* object

disable_equilibrium_solidification_calculation()

Skips the property (one axis) diagram calculation of solidification under equilibrium conditions, before the Scheil solidification calculation starts.

In general it is not necessary to perform this calculation.

Default: Disabled. The equilibrium solidification calculation is skipped.

Returns
This *ScheilOptions* object

disable_evaporation_property_calculation()

Disables calculation of evaporation properties.

Default: Disabled. The evaporation properties are not calculated.

Returns
This *ScheilOptions* object

disable_force_positive_definite_phase_hessian()

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

Default: Enabled

Returns
This `ScheilOptions` object

enable_approximate_driving_force_for_metastable_phases()

Enables the approximation of the driving force for metastable phases.

Default: Enabled

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

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

Returns
This `ScheilOptions` object

enable_control_step_size_during_minimization()

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

Default: Enabled

Returns
This `ScheilOptions` object

enable_equilibrium_solidification_calculation()

Performs a property (one axis) diagram calculation of solidification under equilibrium conditions, before the Scheil solidification calculation starts, in the same way as is typically done in graphical and console mode.

In general it is not necessary to perform this calculation.

Default: Disabled. The equilibrium solidification calculation is skipped.

Returns
This `ScheilOptions` object

enable_evaporation_property_calculation()

Enables calculation of the properties molar mass of gas, driving force for evaporation and evaporation enthalpy. The calculation requires the gas phase to be selected.

Default: Disabled. The evaporation properties are not calculated.

Returns
This `ScheilOptions` object

enable_force_positive_definite_phase_hessian()

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

Default: Enabled

Returns
This *ScheilOptions* object

`set_gas_phase`(*phase_name: str = 'GAS'*)

Sets the phase used as the gas phase.

Default: The phase "GAS".

Parameters
`phase_name` – The phase name

Returns
This *ScheilOptions* object

`set_global_minimization_max_grid_points`(*max_grid_points: int = 2000*)

Sets the maximum number of grid points in global minimization. ** Only applicable if global minimization is actually used**.

Default: 2000 points

Parameters
`max_grid_points` – The maximum number of grid points

Returns
This *ScheilOptions* object

`set_global_minimization_test_interval`(*global_test_interval: int = 10*)

Sets the interval for the global test.

Default: 10

Parameters
`global_test_interval` – The global test interval

Returns
This *ScheilOptions* object

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

Sets the phase used as the liquid phase.

Default: The phase "LIQUID".

Parameters
`phase_name` – The phase name

Returns
This *ScheilOptions* object

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

Set the maximum number of iterations.

Default: max. 500 iterations

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

Parameters
`max_no_of_iterations` – The max. number of iterations

Returns
This *ScheilOptions* object

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

Sets the required relative accuracy.

Default: 1.0E-6

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

Parameters
`accuracy` – The required relative accuracy

Returns
This *ScheilOptions* object

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

Sets the smallest fraction for constituents that are unstable.

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

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

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

Returns
This *ScheilOptions* object

set_temperature_step(*temperature_step_in_kelvin: float = 1.0*)

Sets the temperature step. Decreasing the temperature step increases the accuracy, but the default value is usually adequate.

Default step: 1.0 K

Parameters
`temperature_step_in_kelvin` – The temperature step [K]

Returns
This *ScheilOptions* object

terminate_on_fraction_of_liquid_phase(*fraction_to_terminate_at: float = 0.01*)

Sets the termination condition to a specified remaining fraction of liquid phase.

Default: Terminates at 0.01 fraction of liquid phase.

Note: Either the termination criterion is set to a temperature or fraction of liquid limit, both together are not possible.

Parameters
`fraction_to_terminate_at` – the termination fraction of liquid phase (value between 0 and 1)

Returns
This *ScheilOptions* object

`terminate_on_temperature`(*temperature_in_kelvin: float*)

Sets the termination condition to a specified temperature.

Default: Terminates at 0.01 fraction of liquid phase, i.e. not at a specified temperature.

Note: Either the termination criterion is set to a temperature or fraction of liquid limit, both together are not possible.

Parameters
`temperature_in_kelvin` – the termination temperature [K]

Returns
This *ScheilOptions* object

class tc_python.scheil.**ScheilSoluteTrapping**

Bases: *ScheilCalculationType*

Configures the Scheil solute trapping settings. The used solidification speed equation is *Scanning speed * cos(angle)* with *Scanning speed* and *angle* being provided either by the user or taken from the defaults.

`set_angle`(*alpha: float = 45.0*)

Sets the transformation angle alpha between the solid/liquid boundary and laser scanning direction.

Default: 45.0

Parameters
`alpha` – The transformation angle [degree]

Returns
This *ScheilSoluteTrapping* object

`set_primary_phasename`(*primary_phase_name: str = 'AUTOMATIC'*)

Sets the name of the primary phase.

The primary phase is the phase where solute trapping takes place. A necessary condition for this phase is that the phase definition contains all of the elements that are chosen in the system. When *AUTOMATIC* is selected, the program tries to find a suitable primary phase that fills this condition.

Default: *AUTOMATIC*

Parameters
`primary_phase_name` – The phase name (or *AUTOMATIC*)

Returns
This *ScheilSoluteTrapping* object

`set_scanning_speed`(*scanning_speed: float = 1.0*)

Sets the scanning speed.

Default: 1 m/s

Parameters
`scanning_speed` – The scaling factor [m/s]

Returns
This *ScheilSoluteTrapping* object

5.1.5 Module "step_or_map_diagrams"

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

Bases: `object`

The abstract base class for all axis types.

class `tc_python.step_or_map_diagrams.`**`AbstractPhaseDiagramCalculation`**(*calculator*)

Bases: *`AbstractCalculation`*

Abstract configuration required for a property diagram calculation.

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

`add_initial_equilibrium`(*initial_equilibrium:* InitialEquilibrium)

Add initial equilibrium start points from which a phase diagram is calculated.

Scans along the axis variables and generates start points when the scan procedure crosses a phase boundary.

It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the core remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria.

Parameters
`initial_equilibrium` – The initial equilibrium

Returns
This *`PhaseDiagramCalculation`* object

abstract **`calculate`**(*keep_previous_results: bool = False*, *timeout_in_minutes: float = 0.0*) → *PhaseDiagramResult*

`disable_global_minimization`()

Disables global minimization.

Default: Enabled

Returns
This *`PhaseDiagramCalculation`* object

`dont_keep_default_equilibria`()

Do not keep the initial equilibria added by default.

This is only relevant in combination with *`add_initial_equilibrium()`*.

This is the default behavior.

Returns
This *`PhaseDiagramCalculation`* object

`enable_global_minimization`()

Enables global minimization.

Default: Enabled

Returns
This *`PhaseDiagramCalculation`* object

`get_components()` → List[str]

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

Returns
The component names

`get_gibbs_energy_addition_for`(*phase: str*) → float

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

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

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

Returns
Gibbs energy addition to G per mole formula unit.

`get_system_data()` → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *`with_system_modifications()`*.

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

Returns
The system data

`keep_default_equilibria()`

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

Default behavior is to not keep default equilibria.

Returns
This *`PhaseDiagramCalculation`* object

`remove_all_initial_equilibria()`

Removes all previously added initial equilibria.

Returns
This *`PhaseDiagramCalculation`* object

`run_poly_command`(*command: str*)

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

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

Returns
This *`PhaseDiagramCalculation`* object

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

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

`set_gibbs_energy_addition_for`(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This *`PhaseDiagramCalculation`* object

`set_phase_to_dormant`(*phase: str*)

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

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

Returns
This *`PhaseDiagramCalculation`* object

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

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

Parameters

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

Returns
This *`PhaseDiagramCalculation`* object

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

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

Parameters

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

Returns
This *`PhaseDiagramCalculation`* object

`set_phase_to_suspended`(*phase: str*)

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

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

Returns
This *`PhaseDiagramCalculation`* object

with_options(*options:* PhaseDiagramOptions)

Sets the simulation options.

Parameters

`options` – The simulation options

Returns

This *PhaseDiagramCalculation* object

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

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

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

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

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

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

Parameters

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

Returns

This *PhaseDiagramCalculation* object

with_system_modifications(*system_modifications:* SystemModifications)

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

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

Parameters

`system_modifications` – The system modification to be performed

Returns
This *PhaseDiagramCalculation* object

class tc_python.step_or_map_diagrams.**AbstractPropertyDiagramCalculation**(*calculator*)

Bases: *AbstractCalculation*

Abstract configuration required for a property diagram calculation.

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

abstract calculate(*keep_previous_results: bool = False*, *timeout_in_minutes: float = 0.0*)

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, etc.

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

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

Returns
Gibbs energy addition to G per mole formula unit.

`get_system_data`() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

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

Returns
The system data

`run_poly_command`(*command: str*)

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

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

Returns
This `PropertyDiagramCalculation` object

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

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

`set_gibbs_energy_addition_for`(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This `PropertyDiagramCalculation` object

`set_phase_to_dormant`(*phase: str*)

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

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

Returns
This *PropertyDiagramCalculation* object

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

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

Parameters

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

Returns
This *PropertyDiagramCalculation* object

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

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

Parameters

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

Returns
This *PropertyDiagramCalculation* object

`set_phase_to_suspended`(*phase: str*)

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

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

Returns
This *PropertyDiagramCalculation* object

`with_options`(*options:* PropertyDiagramOptions)

Sets the simulation options.

Parameters
`options` – The simulation options

Returns
This *PropertyDiagramCalculation* object

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

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

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

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

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

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

Parameters

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

Returns

This *`PropertyDiagramCalculation`* object

`with_system_modifications`(*system_modifications: SystemModifications*)

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

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

Parameters

`system_modifications` – The system modification to be performed

Returns

This *`PropertyDiagramCalculation`* object

class `tc_python.step_or_map_diagrams.`**`AxisType`**

Bases: *`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[ThermodynamicQuantity, str]*)

Bases: `object`

A calculation axis used for property and phase diagram calculations.

Note: A calculation axis is defining the varied condition and the range of variation. It is the same concept as in Thermo-Calc *Graphical Mode* or *Console Mode*.

Default: A *Linear* axis with a *minimum number of 40 steps*

set_max(*max: float*)

Sets the maximum quantity value of the calculation axis.

There is no default value set, it always needs to be defined.

Parameters
max – The maximum quantity value of the axis [unit according to the axis quantity]

Returns
This *CalculationAxis* object

set_min(*min: float*)

Sets the minimum quantity value of the calculation axis.

There is no default value set, it always needs to be defined.

Parameters
min – The minimum quantity value of the axis [unit according to the axis quantity]

Returns
This *CalculationAxis* object

set_start_at(*at: float*)

Sets the starting point of the calculation on the axis.

Default: The default starting point is the center between the minimum and maximum quantity value

Parameters
at – The starting point on the axis [unit according to the axis quantity]

Returns
This *CalculationAxis* object

`with_axis_type`(*axis_type:* AxisType)

Sets the type of the axis.

Default: A *`Linear`* axis with a *minimum number of 40 steps*

Parameters
`axis_type` – The axis type (linear or logarithmic)

Returns
This *`CalculationAxis`* object

`class tc_python.step_or_map_diagrams.`**`Direction`**(*value*)

Bases: `Enum`

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:* 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: *`AxisType`*

Represents a linear axis.

`get_type()` → str

Convenience method for getting axis type.

Returns
The type

`set_max_step_size`(*max_step_size: float*)

Sets the axis to use the *maximum step size* configuration.

Default: This is not the default which is *minimum number of steps*

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: `AxisType`

Represents a logarithmic axis.

Note: A logarithmic axis is useful for low fractions like in a gas phase where 1E-7 to 1E-2 might be an interesting range. For the pressure a logarithmic axis is often also useful.

`get_type()` → str

Convenience method for getting axis type.

Returns
The type

`set_scale_factor`(*scale_factor: float = 1.1*)

Sets the scale factor.

Default: 1.1

Parameters
`scale_factor` – The scale factor setting the maximum factor between two calculated values, must be larger than 1.0

Returns
This `Logarithmic` object

`class tc_python.step_or_map_diagrams.PhaseDiagramCalculation(calculator)`

Bases: `AbstractPhaseDiagramCalculation`

Configuration for a phase diagram calculation.

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

`add_initial_equilibrium(initial_equilibrium: InitialEquilibrium)`

Add initial equilibrium start points from which a phase diagram is calculated.

Scans along the axis variables and generates start points when the scan procedure crosses a phase boundary.

It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the core remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria.

Parameters
initial_equilibrium – The initial equilibrium

Returns
This `PhaseDiagramCalculation` object

`calculate(keep_previous_results: bool = False, timeout_in_minutes: float = 0.0) → 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.
- **timeout_in_minutes** – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns
A new `PhaseDiagramResult` object which later can be used to get specific values from the calculated result.

`disable_global_minimization()`

Disables global minimization.

Default: Enabled

Returns
This `PhaseDiagramCalculation` object

dont_keep_default_equilibria()

Do not keep the initial equilibria added by default.

This is only relevant in combination with *add_initial_equilibrium()*.

This is the default behavior.

Returns
This *PhaseDiagramCalculation* object

enable_global_minimization()

Enables global minimization.

Default: Enabled

Returns
This *PhaseDiagramCalculation* object

get_components() → List[str]

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

Returns
The component names

get_gibbs_energy_addition_for(*phase: str*) → float

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

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

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

Returns
Gibbs energy addition to G per mole formula unit.

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

keep_default_equilibria()

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

Default behavior is to not keep default equilibria.

Returns
This *PhaseDiagramCalculation* object

remove_all_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[*ThermodynamicQuantity*, str]*)

Removes the specified condition.

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

Returns
This `ThermodynamicCalculation` object

run_poly_command(*command: str*)

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

Parameters
command – The Thermo-Calc Console Mode command

Returns
This *PhaseDiagramCalculation* object

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

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

set_condition(*quantity: Union[*ThermodynamicQuantity*, str]*, *value: float*)

Sets the specified condition.

Parameters

- **quantity** – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example *X(Cr)*)
- **value** – The value of the condition

Returns
This *PhaseDiagramCalculation* object

set_gibbs_energy_addition_for(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This *PhaseDiagramCalculation* object

`set_phase_to_dormant`(*phase: str*)

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

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

Returns
This *PhaseDiagramCalculation* object

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

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

Parameters

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

Returns
This *PhaseDiagramCalculation* object

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

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

Parameters

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

Returns
This *PhaseDiagramCalculation* object

`set_phase_to_suspended`(*phase: str*)

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

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

Returns
This *PhaseDiagramCalculation* object

`with_first_axis`(*axis:* CalculationAxis)

Sets the first calculation axis.

Parameters
`axis` – The axis

Returns
This *PhaseDiagramCalculation* object

`with_options`(*options:* PhaseDiagramOptions)

Sets the simulation options.

Parameters
`options` – The simulation options

Returns
This *PhaseDiagramCalculation* object

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

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

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

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

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

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

Parameters

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

Returns
This *PhaseDiagramCalculation* object

`with_second_axis`(*axis:* CalculationAxis)

Sets the second calculation axis.

Parameters
`axis` – The axis

Returns
This *PhaseDiagramCalculation* object

`with_system_modifications`(*system_modifications:* SystemModifications)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This *PhaseDiagramCalculation* object

`class tc_python.step_or_map_diagrams.`**`PhaseDiagramOptions`**

Bases: `object`

Simulation options for phase diagram calculations.

`disable_approximate_driving_force_for_metastable_phases()`

Disables the approximation of the driving force for metastable phases.

Default: Enabled

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

If it is important that these driving forces are correct, use *`disable_approximate_driving_force_for_metastable_pha`* 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. For details, search the Thermo-Calc documentation for “Hessian minimization”.

Default: Enabled

Returns
This *PhaseDiagramOptions* object

`dont_use_auto_start_points()`

Switches the usage of automatic starting points for the mapping off.

Default: Switched on

Returns
This *PhaseDiagramOptions* object

`dont_use_inside_mesh_points()`

Switches the usage of inside meshing points for the mapping off.

Default: Switched off

Returns
This *PhaseDiagramOptions* object

`enable_approximate_driving_force_for_metastable_phases()`

Enables the approximation of the driving force for metastable phases.

Default: Enabled

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

If it is important that these driving forces are correct, use *`disable_approximate_driving_force_for_metastable_pha`* to force the calculation to converge for the metastable phases.

Returns
This *`PhaseDiagramOptions`* object

`enable_control_step_size_during_minimization()`

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

Default: Enabled

Returns
This *`PhaseDiagramOptions`* object

`enable_force_positive_definite_phase_hessian()`

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

Default: Enabled

Returns
This *`PhaseDiagramOptions`* object

`set_global_minimization_max_grid_points`(*max_grid_points: int = 2000*)

Sets the maximum number of grid points in global minimization. ** Only applicable if global minimization is actually used**.

Default: 2000 points

Parameters
`max_grid_points` – The maximum number of grid points

Returns
This *`PhaseDiagramOptions`* object

`set_global_minimization_test_interval`(*global_test_interval: int = 0*)

Sets the interval for the global test.

Default: 0

Parameters
`global_test_interval` – The global test interval

Returns
This *`PhaseDiagramOptions`* object

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

Set the maximum number of iterations.

Default: max. 500 iterations

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

Parameters
`max_no_of_iterations` – The max. number of iterations

Returns
This *PhaseDiagramOptions* object

`set_no_of_mesh_along_axis`(*no_of_mesh_along_axis: int = 3*)

Sets the number of meshes along an axis for the mapping.

Default: 3

Parameters
`no_of_mesh_along_axis` – The number of meshes

Returns
This *PhaseDiagramOptions* object

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

Sets the required relative accuracy.

Default: 1.0E-6

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

Parameters
`accuracy` – The required relative accuracy

Returns
This *PhaseDiagramOptions* object

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

Sets the smallest fraction for constituents that are unstable.

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

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

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

Returns
This *PhaseDiagramOptions* object

`use_auto_start_points`()

Switches the usage of automatic starting points for the mapping on.

Default: Switched on

Returns
This *PhaseDiagramOptions* object

use_inside_mesh_points()

Switches the usage of inside meshing points for the mapping off.

Default: Switched off

Returns
This *PhaseDiagramOptions* object

class tc_python.step_or_map_diagrams.**PhaseDiagramResult**(*result*)

Bases: *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[ThermodynamicQuantity, str]*, *y_quantity: Union[ThermodynamicQuantity, str]*) → *PhaseDiagramResultValues*

Returns x-y-line data grouped by the multiple datasets of the specified quantities (for example in dependency of components). The available quantities can be found in the documentation of the factory class `ThermodynamicQuantity`. Usually the result data represents the phase diagram.

Note: The different datasets will contain *NaN*-values between different subsections and are not sorted (because they are unsortable due to their nature).

Note: Its possible to use functions as axis variables, either by using *ThermodynamicQuantity.user_defined_function*, or by using an expression that contains '='.

Example *get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))*

Example *get_values_grouped_by_quantity_of('T', 'CP=HM.T')*

Parameters

- **x_quantity** – The first quantity ("x-axis"), Console Mode syntax strings can be used as an alternative (for example *'T'*), or even a function (for example *'f=T*1.01'*)
- **y_quantity** – The second quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), or even a function (for example *'CP=HM.T'*)

Returns
The phase diagram data

`get_values_grouped_by_stable_phases_of`(*x_quantity: Union[*ThermodynamicQuantity*, str]*, *y_quantity: Union[*ThermodynamicQuantity*, str]*) → *PhaseDiagramResultValues*

Returns x-y-line data grouped by the sets of "stable phases" (for example "LIQUID" or "LIQUID + FCC_A1"). The available quantities can be found in the documentation of the factory class `ThermodynamicQuantity`. Usually the result data represents the phase diagram.

Note: The different datasets will contain *NaN*-values between different subsections and are not sorted (because they are unsortable due to their nature).

Note: Its possible to use functions as axis variables, either by using *ThermodynamicQuantity.user_defined_function*, or by using an expression that contains '='.

Example *get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))*

Example *get_values_grouped_by_quantity_of('T', 'CP=HM.T')*

Parameters

- **`x_quantity`** – The first quantity ("x-axis"), Console Mode syntax strings can be used as an alternative (for example *'T'*), or even a function (for example *'f=T*1.01'*)
- **`y_quantity`** – The second quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), or even a function (for example *'CP=HM.T'*)

Returns
The phase diagram data

`remove_phase_labels`()

Erases all added coordinates for phase labels.

Returns
This *`PhaseDiagramResult`* object

`save_to_disk`(*path: str*)

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

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

Returns
this *`PhaseDiagramResult`* object

`set_phase_name_style`(*phase_name_style_enum:* PhaseNameStyle = *PhaseNameStyle.NONE*)

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() → *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, *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
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[*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() → *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**(*phase_label_java*)

Bases: object

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

get_text() → str

Accessor for the phase label :return: the phase label

get_x() → List[float]

Accessor for the x-value :return: the x value

get_y() → List[float]

Accessor for the y-value :return: the y value

class tc_python.step_or_map_diagrams.**PhaseNameStyle**(*value*)

Bases: `Enum`

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: *AbstractPropertyDiagramCalculation*

calculate(*keep_previous_results: bool = False*, *timeout_in_minutes: float = 0.0*) → *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.
- **timeout_in_minutes** – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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, etc.

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

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

Returns
Gibbs energy addition to G per mole formula unit.

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

remove_all_conditions()

Removes all set conditions.

Returns
This *PropertyDiagramCalculation* object

remove_condition(*quantity: Union[ThermodynamicQuantity, str]*)

Removes the specified condition.

Parameters

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

Returns

This *PropertyDiagramCalculation* object

run_poly_command(*command: str*)

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

Parameters

command – The Thermo-Calc Console Mode command

Returns

This *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[ThermodynamicQuantity, str]*, *value: float*)

Sets the specified condition.

Parameters

- **quantity** – The thermodynamic quantity to set as condition; a Console Mode syntax string can be used as an alternative (for example *X(Cr)*)
- **value** – The value of the condition

Returns

This *PropertyDiagramCalculation* object

set_gibbs_energy_addition_for(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns

This *PropertyDiagramCalculation* object

set_phase_to_dormant(*phase: str*)

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

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

Returns
This `PropertyDiagramCalculation` object

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

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

Parameters

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

Returns
This `PropertyDiagramCalculation` object

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

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

Parameters

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

Returns
This `PropertyDiagramCalculation` object

`set_phase_to_suspended`(*phase: str*)

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

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

Returns
This `PropertyDiagramCalculation` object

`with_axis`(*axis:* CalculationAxis)

Sets the calculation axis.

Parameters
`axis` – The axis

Returns
This `PropertyDiagramCalculation` object

`with_options`(*options:* PropertyDiagramOptions)

Sets the simulation options.

Parameters
`options` – The simulation options

Returns
This `PropertyDiagramCalculation` object

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

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

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

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

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

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

Parameters

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

Returns

This *`PropertyDiagramCalculation`* object

`with_system_modifications`(*system_modifications:* SystemModifications)

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

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

Parameters

`system_modifications` – The system modification to be performed

Returns

This *`PropertyDiagramCalculation`* object

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

Bases: `object`

Simulation options for the property diagram calculations.

`disable_approximate_driving_force_for_metastable_phases`()

Disables the approximation of the driving force for metastable phases.

Default: Enabled

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

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

Returns
This `PropertyDiagramOptions` object

`disable_control_step_size_during_minimization()`

Disables stepsize control during minimization (non-global).

Default: Enabled

Returns
This `PropertyDiagramOptions` object

`disable_force_positive_definite_phase_hessian()`

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

Default: Enabled

Returns
This `PropertyDiagramOptions` object

`enable_approximate_driving_force_for_metastable_phases()`

Enables the approximation of the driving force for metastable phases.

Default: Enabled

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

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

Returns
This `PropertyDiagramOptions` object

`enable_control_step_size_during_minimization()`

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

Default: Enabled

Returns
This `PropertyDiagramOptions` object

`enable_force_positive_definite_phase_hessian()`

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

Default: Enabled

Returns
This `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: *AbstractResult*

Result of a property diagram. This can be used to query for specific values.

`get_values_grouped_by_quantity_of`(*x_quantity: Union[ThermodynamicQuantity, str]*, *y_quantity: Union[ThermodynamicQuantity, str]*, *sort_and_merge: bool = True*) → Dict[str, *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 Mode syntax strings can be used as an alternative (for example *'T'*), or even a function (for example *'f=T*1.01'*)
- **`y_quantity`** – The second quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), or even a function (for example *'CP=HM.T'*)
- **`sort_and_merge`** – If *True*, the data is sorted and merged into as few subsections as possible (divided by *NaN*)

Returns
Containing the datasets with the quantities as their keys

`get_values_grouped_by_stable_phases_of`(*x_quantity: Union[ThermodynamicQuantity, str]*, *y_quantity: Union[ThermodynamicQuantity, str]*, *sort_and_merge: bool = True*) → Dict[str, *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 Mode syntax strings can be used as an alternative (for example *'T'*), or even a function (for example *'f=T*1.01'*)
- **y_quantity** – The second quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), or even a function (for example *'CP=HM.T'*)
- **sort_and_merge** – If *True*, the data will be sorted and merged into as few subsections as possible (divided by *NaN*)

Returns
Containing the datasets with the quantities as their keys

`get_values_of`(*x_quantity: Union[*ThermodynamicQuantity*, str]*, *y_quantity: Union[*ThermodynamicQuantity*, str]*) → [List[float], 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 Mode syntax strings can be used as an alternative (for example *'T'*) or even a function (for example *'f=T*1.01'*)

- **y_quantity** – The second Thermodynamic quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), or even a function (for example *'CP=HM.T'*)

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

save_to_disk(*path: str*)

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

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

Returns
this *PropertyDiagramResult* object

set_phase_name_style(*phase_name_style_enum:* PhaseNameStyle = *PhaseNameStyle.NONE*)

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.

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

Bases: *AbstractGrid*

The abstract base class for calculated grids.

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

Bases: `object`

The abstract base class for all initial composition profile types.

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

Bases: `object`

The abstract base class for all grids.

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

Bases: `object`

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

`class tc_python.diffusion.`**ActivityFluxFunction**

Bases: *BoundaryCondition*

`get_type()` → str

The type of the boundary condition.

Returns
The type

`set_flux_function`(*element_name: str*, *f: str = '0'*, *g: str = '1'*, *n: float = 1.0*, *to_time: float = 1.7976931348623157e+308*)

The flux for the independent components must be given in the format:

J = f(T,P,TIME) * (ACTIVITY^N - g(T,P,TIME))

where f and g may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer.

f and g must be expressed in DICTRA Console Mode syntax.

Parameters

- **element_name** – The name of the element
- **f** – the function f in the formula above
- **g** – the function g in the formula above
- **n** – the constant N in the formula above
- **to_time** – The max-time for which the flux function is used.

class tc_python.diffusion.**AutomaticSolver**

Bases: *Solver*

Solver using the *homogenization model* if any region has more than one phase, otherwise using the *classic model*.

Note: This is the **default solver** and recommended for most applications.

`get_type()` → str

The type of the solver.

Returns
The type

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

Only valid if the :class:`ClassicSolver` 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 :class:`ClassicSolver` 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 :class:`ClassicSolver` 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: *AbstractBoundaryCondition*

Contains factory methods for the the different boundary conditions available.

`classmethod activity_flux_function()`

Factory method that creates a **new** activity-flux-function boundary condition.

This type of boundary condition is used to take into account the finite rate of a surface reaction.

The flux for the independent components must be given in the format:

J = f(T,P,TIME) * (ACTIVITY^N - g(T,P,TIME))

where f and g may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer.

f and g must be expressed in DICTRA Console Mode syntax.

Note: The activities are those with user-defined reference states. The function mass transfer coefficient is the mass transfer coefficient, activity of the corresponding species in the gas is the activity of the corresponding species in the gas and N is a stoichiometric coefficient.

Note: For more details see L. Sproge and J. Ågren, "Experimental and theoretical studies of gas consumption in the gas carburizing process" J. Heat Treat. 6, 9–19 (1988).

Returns
A new *ActivityFluxFunction* object

`classmethod closed_system()`

Factory method that creates a **new** closed-system boundary condition.

Returns
A new *ClosedSystem* object

`classmethod fix_flux_value()`

Factory method that creates a **new** fix-flux-value boundary condition.

This type of boundary condition makes it possible to enter functions that yield the flux times the molar volume for the independent components. May be a function of time, temperature and pressure: *J(T,P,TIME).*

Returns
A new *FixFluxValue* object

`classmethod fixed_compositions(`*unit_enum: Unit = Unit.MASS_PERCENT*`)`

Factory method that creates a **new** fixed-composition boundary condition.

Parameters
unit_enum – The composition unit

Returns
A new *FixedCompositions* object

classmethod mixed_zero_flux_and_activity()

Factory method that creates a **new** mixed zero-flux and activity boundary condition

Returns
A new *MixedZeroFluxAndActivity* object

class tc_python.diffusion.CalculatedGrid

Bases: `AbstractCalculatedGrid`

Factory class for grids generated by a mathematical series (linear, geometric, . . .). Use `tc_python.diffusion.PointByPointGrid` instead if you want to use an existing grid from experimental data or a previous calculation.

Note: A region must contain a number of grid points. The composition is only known at these grid points and the software assumes that the composition varies linearly between them. The amount and composition of all the phases present at a single grid point in a certain region are those given by thermodynamic equilibrium keeping the over-all composition at the grid point fixed.

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

Factory method that creates a **new** double geometric grid.

Note: Double geometric grids have a high number of grid points in the middle or at both ends of a region. One geometrical factor for the lower (left) and upper (right) half of the region need to specified. In both cases a geometrical factor of larger than one yields a higher density of grid points at the lower end of the half and vice versa for a factor smaller than one.

Parameters

- **no_of_points** – The number of points
- **lower_geometrical_factor** – The geometrical factor for the left half
- **upper_geometrical_factor** – The geometrical factor for the right half

Returns
A new `DoubleGeometricGrid` object

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

Factory method that creates a **new** geometric grid.

Note: A grid that yields a varying density of grid points in the region. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.

Parameters

- **no_of_points** – The number of points
- **geometrical_factor** – The geometrical factor

Returns
A new *GeometricGrid* object

`classmethod linear(no_of_points: int = 50)`

Factory method that creates a **new** equally spaced grid.

Parameters
no_of_points – The number of points

Returns
A new *LinearGrid* object

`class tc_python.diffusion.ClassicSolver`

Bases: *Solver*

Solver using the *Classic model*.

Note: This solver **never switches** to the homogenization model even if it fails to converge. Use the *tc_python.diffusion.AutomaticSolver* if necessary instead.

`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: *BoundaryCondition*

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:* Unit = *Unit.MASS_PERCENT*)

Bases: `object`

Contains initial concentration profiles for the elements.

`add`(*element_name: str*, *profile:* 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: *`ElementProfile`*

Represents a constant initial concentration profile.

`get_type`() → str

The type of the element profile.

Returns

The type

class `tc_python.diffusion.`**`ContinuedDiffusionCalculation`**(*calculation*)

Bases: *`AbstractCalculation`*

Configuration for a diffusion calculation that is a continuation of a previous isothermal or non-isothermal diffusion calculation. It contains a subset of the settings possible in the original calculation.

Use *`set_simulation_time()`* to set a simulation time that is higher than the original calculation.

`calculate`(*timeout_in_minutes: float = 0.0*) → *DiffusionCalculationResult*

Runs the diffusion calculation.

Parameters

`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns

A *`DiffusionCalculationResult`* which later can be used to get specific values from the calculated result

`set_simulation_time`(*simulation_time: float*)

Sets the simulation time.

Parameters

`simulation_time` – The simulation time [s]

Returns

This *`DiffusionIsoThermalCalculation`* object

`with_left_boundary_condition`(*boundary_condition:* BoundaryCondition, *to: float = 1.7976931348623157e+308*)

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

Default: A closed-system boundary condition.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Note: You can specify time-dependent boundary conditions by calling `with_left_boundary_condition()` many times, with different values of the "to" parameter.

Examples:

- *with_left_boundary_condition(BoundaryCondition.closed_system(), to=100)*
- *with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)*
- *with_left_boundary_condition(BoundaryCondition.closed_system())*

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

Parameters

- **`boundary_condition`** – The boundary condition
- **`to`** – The upper time-limit for boundary_condition.

Returns
This `DiffusionIsoThermalCalculation` object

`with_options`(*options: Options*, *to: float = 1.7976931348623157e+308*)

Sets the general simulation conditions.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **`options`** – The general simulation conditions
- **`to`** – The upper time-limit for options.

Returns
This `DiffusionIsoThermalCalculation` object

`with_right_boundary_condition`(*boundary_condition: BoundaryCondition*, *to: float = 1.7976931348623157e+308*)

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

Default: A closed-system boundary condition

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Note: You can specify time-dependent boundary conditions by calling `with_right_boundary_condition()` many times, with different values of the "to" parameter.

Examples:

- *with_right_boundary_condition(BoundaryCondition.closed_system(), to=100)*

- *with_right_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)*
- *with_right_boundary_condition(BoundaryCondition.closed_system())*

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

Parameters

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

Returns
This *DiffusionIsoThermalCalculation* object

with_solver(*solver: Solver*, *to: float = 1.7976931348623157e+308*)

Sets the solver to use (*Classic*, *Homogenization* or *Automatic*). **Default is Automatic**.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **solver** – The solver to use
- **to** – The upper time-limit for solver.

Returns
This *DiffusionIsoThermalCalculation* object

with_timestep_control(*timestep_control: TimestepControl*, *to: float = 1.7976931348623157e+308*)

Sets the timestep control options.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **timestep_control** – The new timestep control options
- **to** – The upper time-limit for timestep_control.

Returns
This *DiffusionIsoThermalCalculation* object

class tc_python.diffusion.**DiffusionCalculationResult**(*result*)

Bases: *AbstractResult*

Result of a diffusion calculation. This can be used to query for specific values. For details of the axis variables, search the Thermo-Calc help.

get_mass_fraction_at_lower_interface(*region: str*, *component: str*) → [List[float], 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*) → [List[float], 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[*SimulationTime*, float]*) → [List[float], 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[*SimulationTime*, float]*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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[*SimulationTime*, float]*) → [List[float], 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[*SimulationTime*, float]*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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_###*) are 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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*) → [List[float], 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[*DiffusionQuantity*, str]*, *y_axis: Union[*DiffusionQuantity*, str]*, *plot_condition: Union[*PlotCondition*, str] = ''*, *independent_variable: Union[*IndependentVariable*, str] = ''*) → [List[float], List[float]]

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

Note: As an alternative, DICTRA Console Mode syntax can be used as well for each quantity and condition.

Warning: This is an advanced mode that is equivalent to the possibilities in the DICTRA Console Mode. Not every combination of settings will return a result.

Parameters

- `x_axis` – The first result quantity
- `y_axis` – The second result quantity
- `plot_condition` – The plot conditions

- **independent_variable** – The independent variable

Returns
A tuple of two lists of floats (the x_axis quantity result, the y_axis quantity result) [units according to the quantities]

get_velocity_of_lower_boundary_of_region(*region: str*) → [List[float], 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*) → [List[float], 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*) → [List[float], List[float]]

Returns the width of region, in dependency of time.

Parameters
region – The name of the region

Returns
A tuple of two lists of floats (time [s], width of the specified region [m])

save_to_disk(*path: str*)

Saves the result to disk. The result can later be loaded using *tc_python.server.SetUp.load_result_from_disk()*.

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

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

Returns
This *DiffusionCalculationResult* object

with_continued_calculation()

Returns a *ContinuedDiffusionCalculation* that is used for continuing a diffusion calculation with altered settings.

Returns
A *ContinuedDiffusionCalculation*

class tc_python.diffusion.**DiffusionIsoThermalCalculation**(*calculation*)

Bases: *AbstractCalculation*

Configuration for an isothermal diffusion calculation.

`add_console_command`(*console_command: str*)

Registers a DICTRA Console Mode command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands are stored and used until explicitly deleted using `tc_python.diffusion.DiffusionIsoThermoCalculation.remove_all_console_commands`.

Parameters
`console_command` – The DICTRA Console Mode command

Returns
This *`DiffusionIsoThermalCalculation`* object

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

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

`add_region`(*region:* Region)

Adds a region to the calculation. Regions are always added in the simulation domain from left to right.

If you want to replace an already added region, call *`remove_all_regions()`*, and add the regions that you want to keep.

Warning: Regions must have unique names.

Parameters
`region` – The region to be added

Returns
This *`DiffusionIsoThermalCalculation`* object

`calculate`(*timeout_in_minutes: float = 0.0*) → *DiffusionCalculationResult*

Runs the diffusion calculation.

Parameters
`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns
A *`DiffusionCalculationResult`* which later can be used to get specific values from the calculated result

`get_system_data`() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *`with_system_modifications()`*.

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

Returns
The system data

remove_all_console_commands()

Removes all previously added Console Mode commands.

Returns
This *DiffusionIsoThermalCalculation* object

remove_all_regions()

Removes all previously added regions.

:return This *DiffusionIsoThermalCalculation* object

set_simulation_time(*simulation_time: float*)

Sets the simulation time.

Parameters
simulation_time – The simulation time [s]

Returns
This *DiffusionIsoThermalCalculation* object

set_temperature(*temperature: float*)

Sets the temperature for the isothermal simulation.

Parameters
temperature – The temperature [K]

Returns
This *DiffusionIsoThermalCalculation* object

with_cylindrical_geometry(*first_interface_position: float = 0.0*)

Sets geometry to *cylindrical*, corresponds to an infinitely long cylinder of a certain radius.

Default: A planar geometry

Note: With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the *first_interface_position*, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

Parameters
first_interface_position – The position of the left-most coordinate along the axis, only necessary for modeling a tube geometry [m]

Returns
This *DiffusionIsoThermalCalculation* object

with_left_boundary_condition(*boundary_condition:* BoundaryCondition, *to: float = 1.7976931348623157e+308*)

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

Default: A closed-system boundary condition.

It is possible specify the upper time-point for which this setting is valid using the parameter “to”.

Default: The end of the simulation.

Note: You can specify time-dependent boundary conditions by calling `with_left_boundary_condition()` many times, with different values of the "to" parameter.

Examples:

- *with_left_boundary_condition(BoundaryCondition.closed_system(), to=100)*
- *with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)*
- *with_left_boundary_condition(BoundaryCondition.closed_system())*

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

Parameters

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

Returns
This `DiffusionIsoThermalCalculation` object

with_options(*options:* Options, *to: float = 1.7976931348623157e+308*)

Sets the general simulation conditions.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **options** – The general simulation conditions
- **to** – The upper time-limit for options.

Returns
This `DiffusionIsoThermalCalculation` object

with_planar_geometry()

Sets geometry to *planar*.

This is default.

Returns
This `DiffusionIsoThermalCalculation` object

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

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

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

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

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

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

Parameters

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

Returns
This *`DiffusionIsoThermalCalculation`* object

`with_right_boundary_condition`(*boundary_condition:* BoundaryCondition, *to: float = 1.7976931348623157e+308*)

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

Default: A closed-system boundary condition

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Note: You can specify time-dependent boundary conditions by calling *`with_right_boundary_condition()`* many times, with different values of the "to" parameter.

Examples:

- *with_right_boundary_condition(BoundaryCondition.closed_system(), to=100)*
- *with_right_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)*
- *with_right_boundary_condition(BoundaryCondition.closed_system())*

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

Parameters

- **`boundary_condition`** – The boundary condition
- **`to`** – The upper time-limit for boundary_condition.

Returns
This *`DiffusionIsoThermalCalculation`* object

with_solver(*solver:* Solver, *to: float = 1.7976931348623157e+308*)

Sets the solver to use (*Classic*, *Homogenization* or *Automatic*). **Default is Automatic**.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **solver** – The solver to use
- **to** – The upper time-limit for solver.

Returns

This *DiffusionIsoThermalCalculation* object

with_spherical_geometry(*first_interface_position: float = 0.0*)

Sets geometry to *spherical*, corresponds to a sphere with a certain radius.

Default: A spherical geometry

Note: With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the *first_interface_position*, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

Parameters

first_interface_position – The position of the left-most coordinate along the axis, only necessary for modeling a hollow sphere geometry [m]

Returns

This *DiffusionIsoThermalCalculation* object

with_system_modifications(*system_modifications:* SystemModifications)

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

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

Parameters

system_modifications – The system modification to be performed

Returns

This *DiffusionIsoThermalCalculation* object

with_timestep_control(*timestep_control:* TimestepControl, *to: float = 1.7976931348623157e+308*)

Sets the timestep control options.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **timestep_control** – The new timestep control options

- **to** – The upper time-limit for timestep_control.

Returns
This *DiffusionIsoThermalCalculation* object

class tc_python.diffusion.**DiffusionNonIsoThermalCalculation**(*calculation*)

Bases: *AbstractCalculation*

Configuration for a non-isothermal diffusion calculation.

add_console_command(*console_command: str*)

Registers a DICTRA Console Mode command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands are stored and used until explicitly deleted using *tc_python.diffusion.DiffusionNonIsoThermalCalculation.remove_all_console_commands*.

Parameters
console_command – The DICTRA Console Mode command

Returns
This *DiffusionNonIsoThermalCalculation* object

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

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

add_region(*region:* Region)

Adds a region to the calculation. Regions are always added in the simulation domain from left to right.

If you want to replace an already added region, call *remove_all_regions()*, and add the regions that you want to keep.

Warning: Regions must have unique names.

Parameters
region – The region to be added

Returns
This *DiffusionNonIsoThermalCalculation* object

calculate(*timeout_in_minutes: float = 0.0*) → *DiffusionCalculationResult*

Runs the diffusion calculation.

Parameters
timeout_in_minutes – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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

`get_system_data()` → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

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

Returns
The system data

`remove_all_console_commands()`

Removes all previously added Console Mode commands.

Returns
This `DiffusionNonIsoThermalCalculation` object

`remove_all_regions()`

Removes all previously added regions.

Returns
This `DiffusionNonIsoThermalCalculation` object

`set_simulation_time`(*simulation_time: float*)

Sets the simulation time.

Parameters
`simulation_time` – The simulation time [s]

Returns
This `DiffusionNonIsoThermalCalculation` object

`with_cylindrical_geometry`(*first_interface_position: float = 0.0*)

Sets geometry to *cylindrical*, corresponds to an infinitely long cylinder of a certain radius.

Default: A planar geometry

Note: With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the *first_interface_position*, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

Parameters
`first_interface_position` – The position of the left-most coordinate along the axis, only necessary for modeling a tube geometry [m]

Returns
This `DiffusionNonIsoThermalCalculation` object

`with_left_boundary_condition`(*boundary_condition:* BoundaryCondition, *to: float = 1.7976931348623157e+308*)

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

Default: A closed-system boundary condition.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Note: You can specify time-dependent boundary conditions by calling `with_left_boundary_condition()` many times, with different values of the "to" parameter.

Examples:

- *with_left_boundary_condition(BoundaryCondition.closed_system(), to=100)*
- *with_left_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)*
- *with_left_boundary_condition(BoundaryCondition.closed_system())*

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

Parameters

- **`boundary_condition`** – The boundary condition
- **`to`** – The upper time-limit for boundary_condition.

Returns
This `DiffusionNonIsoThermalCalculation` object

`with_options`(*options: Options*, *to: float = 1.7976931348623157e+308*)

Sets the general simulation conditions.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **`options`** – The general simulation conditions
- **`to`** – The upper time-limit for options.

Returns
This `DiffusionNonIsoThermalCalculation` object

`with_planar_geometry`()

Sets geometry to *planar*.

This is default.

Returns
This `DiffusionNonIsoThermalCalculation` object

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

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

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

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

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

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

Parameters

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

Returns

This *`DiffusionNonIsoThermalCalculation`* object

`with_right_boundary_condition`(*boundary_condition:* BoundaryCondition, *to: float = 1.7976931348623157e+308*)

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

Default: A closed-system boundary condition

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Note: You can specify time-dependent boundary conditions by calling *`with_right_boundary_condition()`* many times, with different values of the "to" parameter.

Examples:

- *with_right_boundary_condition(BoundaryCondition.closed_system(), to=100)*
- *with_right_boundary_condition(BoundaryCondition.mixed_zero_flux_and_activity().set_activity_for_element("C", surface_activity), to=500)*
- *with_right_boundary_condition(BoundaryCondition.closed_system())*

This example sets an closed-system-boundary-condition from start up to 100s and a activity-boundary-condition from 100s to 500s and finally a closed-system-boundary-condition from 500s to the end of simulation.

Parameters

- `boundary_condition` – The boundary condition
- `to` – The upper time-limit for boundary_condition.

Returns

This *`DiffusionNonIsoThermalCalculation`* object

with_solver(*solver:* Solver, *to: float = 1.7976931348623157e+308*)

Sets the solver to use (*Classic*, *Homogenization* or *Automatic*). **Default is Automatic**.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **solver** – The solver to use
- **to** – The upper time-limit for solver.

Returns
This *DiffusionNonIsoThermalCalculation* object

with_spherical_geometry(*first_interface_position: float = 0.0*)

Sets geometry to *spherical*, corresponds to a sphere with a certain radius.

Default: A spherical geometry

Note: With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere by default. By specifying the *first_interface_position*, a different left-most coordinate can be defined. This allows to model a tube or a hollow sphere geometry. The highest coordinate (right boundary) is defined by the cylinder or sphere radius (i.e. by the width of all regions).

Parameters
first_interface_position – The position of the left-most coordinate along the axis, only necessary for modeling a hollow sphere geometry [m]

Returns
This *DiffusionNonIsoThermalCalculation* object

with_system_modifications(*system_modifications:* SystemModifications)

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

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

Parameters
system_modifications – The system modification to be performed

Returns
This *DiffusionNonIsoThermalCalculation* object

with_temperature_profile(*temperature_profile:* 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: TimestepControl*, *to: float = 1.7976931348623157e+308*)

Sets the timestep control options.

It is possible specify the upper time-point for which this setting is valid using the parameter "to".

Default: The end of the simulation.

Parameters

- **timestep_control** – The new timestep control options
- **to** – The upper time-limit for timestep_control.

Returns

This *DiffusionNonIsoThermalCalculation* object

class tc_python.diffusion.**DoubleGeometricGrid**(*no_of_points: int = 50*, *lower_geometrical_factor: float = 1.1*, *upper_geometrical_factor: float = 0.9*)

Bases: *CalculatedGrid*

Represents a double geometric grid.

get_lower_geometrical_factor() → float

Returns the lower geometrical factor (for the left half).

Returns

The lower geometrical factor

get_no_of_points() → int

Returns number of grid points.

Returns

The number of grid points

get_type() → str

Type of the grid.

Returns

The type of the grid

get_upper_geometrical_factor()

Returns the upper geometrical factor (for the right half).

Returns

The upper geometrical factor

set_lower_geometrical_factor(*geometrical_factor: float = 1.1*)

Sets the lower (left half) geometrical factor.

Note: A geometrical factor of larger than one yields a higher density of grid points at the lower end of the half and vice versa for a factor smaller than one.

Parameters

geometrical_factor – The geometrical factor for the left half

Returns

This *DoubleGeometricGrid* object

set_no_of_points(*no_of_points: int = 50*)

Sets the number of grid points.

Parameters
no_of_points – The number of points

Returns
This *DoubleGeometricGrid* object

set_upper_geometrical_factor(*geometrical_factor: float = 0.9*)

Sets the upper (right half) geometrical factor.

Note: A geometrical factor of larger than one yields a higher density of grid points at the lower end of the half and vice versa for a factor smaller than one.

Parameters
geometrical_factor – The geometrical factor for the right half

Returns
This *DoubleGeometricGrid* object

class tc_python.diffusion.**ElementProfile**

Bases: *AbstractElementProfile*

Factory class providing objects for configuring a step, function or linear initial concentration profile.

classmethod constant(*value: float*)

Factory method that creates a **new** constant initial concentration profile.

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

Returns
A new *ConstantProfile* object

classmethod funct(*dictra_console_mode_function: str*)

Factory method that creates a **new** initial concentration profile defined by a function in DICTRA Console Mode syntax.

Parameters
dictra_console_mode_function – The function, expressed in DICTRA Console Mode syntax.

Returns
A new *FunctionProfile* object

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

classmethod linear(*start_value: float*, *end_value: float*)

Factory method that creates a **new** linear initial concentration profile.

Parameters

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

- **end_value** – 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*)

Factory method that creates a **new** initial concentration profile with a step at the specified distance, otherwise the composition is constant at the specified values.

Parameters

- **lower_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.**FixFluxValue**

Bases: `BoundaryCondition`

get_type() → str

The type of the boundary condition.

Returns
The type

set_flux(*element_name: str*, *J: str = '0'*, *to_time: float = 1.7976931348623157e+308*)

Enter functions that yield the flux times the molar volume for the specified element. May be a function of time, temperature and pressure: *J(T,P,TIME)*.

Parameters

- **element_name** – The name of the element
- **J** – the function *J(T,P,TIME)*
- **to_time** – The max-time for which the flux function is used.

class tc_python.diffusion.**FixedCompositions**(*unit_enum:* Unit = *Unit.MASS_PERCENT*)

Bases: `BoundaryCondition`

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: *ElementProfile*

Creates an initial concentration profile defined by a function in DICTRA Console Mode syntax.

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

get_type() → str

The type of the element profile.

Returns
The type

class tc_python.diffusion.**GeneralLowerHashinShtrikman**

Bases: *HomogenizationFunctions*

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

class tc_python.diffusion.**GeneralLowerHashinShtrikmanExcludedPhase**(*excluded_phases: List[str] = []*)

Bases: *HomogenizationFunctions*

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

class tc_python.diffusion.**GeneralUpperHashinShtrikman**

Bases: *HomogenizationFunctions*

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

class tc_python.diffusion.**GeneralUpperHashinShtrikmanExcludedPhase**(*excluded_phases: List[str] = []*)

Bases: *HomogenizationFunctions*

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

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

Bases: `CalculatedGrid`

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.`**`HashinShtrikmanBoundMajority`**

Bases: `HomogenizationFunctions`

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

class `tc_python.diffusion.`**`HashinShtrikmanBoundMajorityExcludedPhase`**(*excluded_phases: List[str] = []*)

Bases: `HomogenizationFunctions`

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

class `tc_python.diffusion.`**`HashinShtrikmanBoundPrescribed`**(*matrix_phase: str*)

Bases: `HomogenizationFunctions`

Hashin-Shtrikman bounds with prescribed phase as matrix phase: the outermost shell consists of the prescribed phase.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

class `tc_python.diffusion.`**`HashinShtrikmanBoundPrescribedExcludedPhase`**(*matrix_phase: str, excluded_phases: List[str] = []*)

Bases: `HomogenizationFunctions`

class `tc_python.diffusion.`**`HomogenizationFunction`**(*value*)

Bases: `Enum`

Homogenization function used for the *homogenization solver*. Many homogenization functions are based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. **Default**: *RULE_OF_MIXTURES* (i.e. upper Wiener bounds)

`GENERAL_LOWER_HASHIN_SHTRIKMAN = 0`

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

`GENERAL_UPPER_HASHIN_SHTRIKMAN = 1`

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

`HASHIN_SHTRIKMAN_BOUND_MAJORITY = 2`

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

`INVERSE_RULE_OF_MIXTURES = 4`

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion

`RULE_OF_MIXTURES = 3`

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion

`class tc_python.diffusion.HomogenizationFunctions`

Bases: `object`

`classmethod general_lower_hashin_shtrikman()`

Factory method that creates a **new** homogenization function of the type *GeneralLowerHashinShtrikman*.

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

Returns
A new *GeneralLowerHashinShtrikman* object

`classmethod general_lower_hashin_shtrikman_excluded_phase(excluded_phases: List[str] = [])`

Factory method that creates a **new** homogenization function of the type *GeneralLowerHashinShtrikmanExcludedPhase*.

General lower Hashin-Shtrikman bounds: the outermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Parameters
excluded_phases – The excluded phases

Returns
A new *GeneralLowerHashinShtrikmanExcludedPhase* object

`classmethod general_upper_hashin_shtrikman()`

Factory method that creates a **new** homogenization function of the type *GeneralUpperHashinShtrikman*.

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

Returns
A new *GeneralUpperHashinShtrikman* object

`classmethod general_upper_hashin_shtrikman_excluded_phase(excluded_phases: List[str] = [])`

Factory method that creates a **new** homogenization function of the type *GeneralUpperHashinShtrikmanExcludedPhase*.

General upper Hashin-Shtrikman bounds: the innermost shell consists of the phase with the most sluggish kinetics.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Parameters
`excluded_phases` – The excluded phases

Returns
A new *GeneralUpperHashinShtrikmanExcludedPhase* object

classmethod hashin_shtrikman_bound_majority()

Factory method that creates a **new** homogenization function of the type *HashinShtrikmanBoundMajority*.

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

Returns
A new *HashinShtrikmanBoundMajority* object

classmethod hashin_shtrikman_bound_majority_excluded_phase(*excluded_phases: List[str] = []*)

Factory method that creates a **new** homogenization function of the type *HashinShtrikmanBoundMajorityExcludedPhase*.

Hashin-Shtrikman bounds with majority phase as matrix phase: the outermost shell consists of the phase with the highest local volume fraction. Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Parameters
`excluded_phases` – The excluded phases

Returns
A new *HashinShtrikmanBoundMajorityExcludedPhase* object

classmethod hashin_shtrikman_bound_prescribed(*matrix_phase: str*)

Factory method that creates a **new** homogenization function of the type *HashinShtrikmanBoundPrescribed*.

Hashin-Shtrikman bounds with prescribed phase as matrix phase: the outermost shell consists of the prescribed phase.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase.

Parameters
`matrix_phase` – The matrix phase

Returns
A new *HashinShtrikmanBoundPrescribed* object

classmethod hashin_shtrikman_bound_prescribed_excluded_phase(*matrix_phase: str, excluded_phases: List[str] = []*)

Factory method that creates a **new** homogenization function of the type *HashinShtrikmanBoundPrescribedExcludedPhase*.

Hashin-Shtrikman bounds with prescribed phase as matrix phase: the outermost shell consists of the prescribed phase.

Based on a variant of the Hashin-Shtrikman bounds, their geometrical interpretation are concentric spherical shells of each phase. The excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Parameters

- **matrix_phase** – The matrix phase
- **excluded_phases** – The excluded phases

Returns
A new *HashinShtrikmanBoundPrescribedExcludedPhase* object

classmethod inverse_rule_of_mixtures()

Factory method that creates a **new** homogenization function of the type *InverseRuleOfMixtures*.

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion.

Returns
A new *InverseRuleOfMixtures* object

classmethod inverse_rule_of_mixtures_excluded_phase(*excluded_phases: List[str] = []*)

Factory method that creates a **new** homogenization function of the type *InverseRuleOfMixturesExcludedPhase*.

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion. Excluded phases are not considered in the diffusion calculations.

Parameters
excluded_phases – The excluded phases

Returns
A new *InverseRuleOfMixturesExcludedPhase* object

classmethod labyrinth_factor_f(*matrix_phase: str*)

Factory method that creates a **new** homogenization function of the type *LabyrinthFactorF*.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase.

Parameters
matrix_phase – The matrix phase

Returns
A new *LabyrinthFactorF* object

classmethod labyrinth_factor_f2(*matrix_phase: str*)

Factory method that creates a **new** homogenization function of the type *LabyrinthFactorF2*.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase squared.

Parameters
matrix_phase – The matrix phase

Returns
A new *LabyrinthFactorF2* object

classmethod rule_of_mixtures()

Factory method that creates a **new** homogenization function of the type *RuleOfMixtures*.

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion.

Returns
A new `RuleOfMixtures` object

classmethod rule_of_mixtures_excluded_phase(*excluded_phases: List[str] = []*)

Factory method that creates a **new** homogenization function of the type `RuleOfMixturesExcludedPhase`.

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion. Excluded phases are not considered in the diffusion calculations.

Parameters
excluded_phases – The excluded phases

Returns
A new `RuleOfMixturesExcludedPhase` object

class tc_python.diffusion.**HomogenizationSolver**

Bases: `Solver`

Solver using the *Homogenization model*.

Note: This solver always uses the homogenization model, even if all regions have only one phase. The solver is **significantly slower than the Classic model**. Use the `tc_python.diffusion.AutomaticSolver` instead if you do not need that behavior.

disable_global_minimization()

Disables global minimization to be used in equilibrium calculations. **Default**: Disabled

Note: In general, using global minimization **significantly increases the simulation time**, but there is also a significantly reduced risk for non-converged equilibrium calculations.

Returns
A new `HomogenizationSolver` object

disable_interpolation_scheme()

Configures the simulation not use *any interpolation scheme*. **Default**: To use the *logarithmic interpolation scheme* with 10000 discretization steps

Note: The homogenization scheme can be switched on by using *with_linear_interpolation_scheme* or *with_logarithmic_interpolation_scheme*.

enable_global_minimization()

Enables global minimization to be used in equilibrium calculations. **Default**: Disabled

Note: In general, using global minimization **significantly increases the simulation time**, but there is also a significantly reduced risk for non-converged equilibrium calculations.

Returns
A new `HomogenizationSolver` object

get_type() → str

The type of solver.

Returns
The type

set_fraction_of_free_memory_to_use(*fraction: float*)

Sets the maximum fraction of free physical memory to be used by the interpolation scheme. **Default**: 1 / 10 of the free physical memory

Parameters
fraction – The maximum free physical memory fraction to be used

Returns
A new *HomogenizationSolver* object

set_memory_to_use(*memory_in_megabytes: float*)

Sets the maximum physical memory in megabytes to be used by the interpolation scheme. **Default**: 1000 MBytes of the free physical memory

Parameters
memory_in_megabytes – The maximum physical memory to be used

Returns
A new *HomogenizationSolver* object

with_function(*homogenization_function:* HomogenizationFunctions)

Sets the *homogenization function* used by the *homogenization model*.

Parameters
homogenization_function – The homogenization function used by the homogenization model

Returns
A new *HomogenizationSolver* object

with_linear_interpolation_scheme(*steps: int = 10000*)

Configures the simulation to use the *linear interpolation scheme*. **Default**: To use the *logarithmic interpolation scheme* with 10000 discretization steps

Parameters
steps – The number of discretization steps in each dimension

Returns
A new *HomogenizationSolver* object

with_logarithmic_interpolation_scheme(*steps: int = 10000*)

Configures the simulation to use the *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.**InverseRuleOfMixtures**

Bases: *HomogenizationFunctions*

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion.

class tc_python.diffusion.**InverseRuleOfMixturesExcludedPhase**(*excluded_phases: List[str] = []*)

Bases: *HomogenizationFunctions*

Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion.

Excluded phases are not considered in the diffusion calculations.

class tc_python.diffusion.**LabyrinthFactorF**(*matrix_phase: str*)

Bases: *HomogenizationFunctions*

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase.

class tc_python.diffusion.**LabyrinthFactorF2**(*matrix_phase: str*)

Bases: *HomogenizationFunctions*

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with the volume fraction of the matrix phase squared.

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

Bases: *CalculatedGrid*

Represents an equally spaced grid.

get_no_of_points() → int

Returns the number of grid points.

Returns
The number of grid points

get_type() → str

Type of the grid.

Returns
The type

set_no_of_points(*no_of_points: int = 50*)

Sets the number of grid points.

Parameters
no_of_points – The number of points

Returns
This *LinearGrid* object

class tc_python.diffusion.**LinearProfile**(*start_value: float*, *end_value: float*)

Bases: *ElementProfile*

Represents a linear initial concentration profile.

get_type() → str

The type of the element profile.

Returns
The type

class tc_python.diffusion.**MixedZeroFluxAndActivity**

Bases: *BoundaryCondition*

Represents a boundary having zero-flux as well as fixed-activity conditions.

Default: On that boundary for every element without an explicitly defined condition, a zero-flux boundary condition is used.

get_type() → str

The type of the boundary condition.

Returns
The type

set_activity_for_element(*element_name: str*, *activity: str*, *to_time: float = 1.7976931348623157e+308*)

Sets an activity expression for an element at the boundary. Enter a formula that the software evaluates during the calculation.

The formula can be:

- a function of the variable *TIME*
- a constant

The formula must be written with these rules:

- a number must begin with a number (not a .)
- a number must have a dot or an exponent (*E*)

The operators +, -, *, /, ** (exponentiation) can be used and with any level of parenthesis. As shown, the following operators must be followed by open and closed parentheses *()*

- *SQRT(X)* is the square root
- *EXP(X)* is the exponential
- *LOG(X)* is the natural logarithm
- *LOG10(X)* is the base 10 logarithm
- *SIN(X)*, *COS(X)*, *TAN(X)*, *ASIN(X)*, *ACOS(X)*, *ATAN(X)*
- *SINH(X)*, *COSH(X)*, *TANH(X)*, *ASINH(X)*, *ACOSH(X)*, *ATANH(X)*
- *SIGN(X)*
- *ERF(X)* is the error function

Default: the expression entered is used for the entire simulation.

Parameters

- **element_name** – The name of the element
- **activity** – The activity
- **to_time** – The max-time for which the activity is used.

set_zero_flux_for_element(*element_name: str*)

Sets a zero-flux condition for an element at the boundary. **Default for all elements at the boundary without an explicitly defined condition**

Parameters
element_name – The name of the element

class `tc_python.diffusion.`**`Options`**

Bases: `object`

General simulation conditions for the diffusion calculations.

`disable_forced_starting_values_in_equilibrium_calculations()`

Disables forced starting values for the equilibrium calculations. **The default is 'enable_automatic_forced_starting_values_in_equilibrium_calculations'**.

Returns
This *`Options`* object

`disable_save_results_to_file()`

Disables the saving of results to file during the simulation. **Default**: Saving of the results at every timestep

Returns
This *`Options`* object

`enable_automatic_forced_starting_values_in_eq_calculations()`

Lets calculation engine decide if forced start values for the equilibrium calculations should be used. **This is the default setting**.

Returns
This *`Options`* object

`enable_forced_starting_values_in_equilibrium_calculations()`

Enables forced start values for the equilibrium calculations. **The default is 'enable_automatic_forced_starting_values_in_equilibrium_calculations'**.

Returns
This *`Options`* object

`enable_save_results_to_file`(*every_nth_step: int = -1*)

Enables and configures saving of results to file during the simulation. They can be saved for every n-th or optionally for every timestep (*-1*). **Default**: Saving of the results at every timestep

Parameters
`every_nth_step` – *-1* or a value ranging from 0 to 99

Returns
This *`Options`* object

`enable_time_integration_method_automatic()`

Enables automatic selection of integration method. **This is the default method**.

Returns
This *`Options`* object

`enable_time_integration_method_euler_backwards()`

Enables *Euler backwards* integration. **The default method is enable_time_integration_method_automatic**.

Note: This method is more stable but less accurate and may be necessary if large fluctuations occur in the profiles.

Returns
This *`Options`* object

`enable_time_integration_method_trapezoidal()`

Enables *trapezoidal* integration.

Note: If large fluctuations occur in the profiles, it may be necessary to use the more stable but less accurate *Euler backwards method*.

Returns
This `Options` object

`set_default_driving_force_for_phases_allowed_to_form_at_interf`(*driving_force: float = 1e-05*)

Sets the default required driving force for phases allowed to form at the interfaces. **Default**: 1.0e-5

Note: The required driving force (evaluated as *DGM(ph)*) is used for determining whether an inactive phase is stable, i.e. actually formed. *DGM* represents the driving force normalized by *RT* and is dimensionless.

Parameters
driving_force – The driving force (*DGM(ph)*) [-]

Returns
This `Options` object

class `tc_python.diffusion.PointByPointGrid`(*unit_enum:* Unit *= Unit.MASS_PERCENT*)

Bases: `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:* 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: bool = False*)

Adds a phase to the region, each region must contain at least one phase.

Note: Normally the *matrix phase* and the *precipitate phases* are automatically chosen based on the presence of all profile elements in the phase and if it has diffusion data. If multiple phases have equal properties, the phase that was added first is chosen. The matrix phase can be explicitly set by using *is_matrix_phase=True*.

Note: If multiple phases are added to a region, the *homogenization model* is applied. That means that average properties of the local phase mixture are used.

Parameters

- `phase_name` – The phase name
- `is_matrix_phase` – If set to *True* this phase is explicitly set as matrix phase for the region, if no phase is set to *True*, the matrix phase is chosen automatically

Returns
This `Region` object

`add_phase_allowed_to_form_at_left_interface`(*phase_name: str*, *driving_force: float = 1e-05*)

Adds a phase allowed to form at the left boundary of the region (an *inactive phase*). The phase will only appear at the interface as a new automatic region if the driving force to form it is sufficiently high.

Parameters

- `phase_name` – The phase name
- `driving_force` – The driving force for the phase to form (*DGM(ph)*)

Returns
This `Region` object

`add_phase_allowed_to_form_at_right_interface`(*phase_name: str*, *driving_force: float = 1e-05*)

Adds a phase allowed to form at the right boundary of the region (an *inactive phase*). The phase will only appear at the interface as a new automatic region if the driving force to form it is sufficiently high.

Parameters

- `phase_name` – The phase name
- `driving_force` – The driving force for the phase to form (*DGM(ph)*)

Returns
This `Region` object

`remove_all_phases`()

Removes all previously added phases from the region.

Returns
This `Region` object

set_width(*width: float*)

Defined the width of the region.

Note: This method needs only to be used if a calculated grid has been defined (using *with_grid()*).

Parameters
width – The width [m]

Returns
This *Region* object

with_composition_profile(*initial_compositions:* 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:* 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:* 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.`**`RuleOfMixtures`**

Bases: *`HomogenizationFunctions`*

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion.

`class tc_python.diffusion.`**`RuleOfMixturesExcludedPhase`**`(`*excluded_phases: List[str] = []*`)`

Bases: *`HomogenizationFunctions`*

Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion.

Excluded phases are not considered in the diffusion calculations.

`class tc_python.diffusion.`**`SimulationTime`**`(`*value*`)`

Bases: `Enum`

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: *`AbstractSolver`*

Factory class providing objects representing a solver.

`classmethod` **`automatic()`**

Factory method that creates a **new** *automatic solver*. **This is the default solver and recommended for most applications**.

Note: This solver uses the homogenization model if any region has more than one phase, otherwise it uses the classic model.

Returns
A new *`AutomaticSolver`* object

`classmethod` **`classic()`**

Factory method that creates a **new** *classic solver*.

Note: This solver never switches to the homogenization model even if the solver fails to converge. Use the *`tc_python.diffusion.AutomaticSolver`* if necessary instead.

Returns
A new *`ClassicSolver`* object

classmethod homogenization()

Factory method that creates a **new** *homogenization solver*.

Note: This solver always uses the homogenization model, even if all regions have only one phase. The solver is **significantly slower than the Classic model**. Use the `tc_python.diffusion.AutomaticSolver` instead if you do not need that behavior.

Returns
A new *HomogenizationSolver* object

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

Bases: *ElementProfile*

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 :func:`enable_automatic_check_interface_position`**.

Returns
This *TimestepControl* object

enable_automatic_check_interface_position()

Lets calculation engine decide if checking of the interface position should be used. **This is the default setting**.

Returns
This *TimestepControl* object

enable_check_interface_position()

Enables checking of the interface position, i.e. the timesteps are controlled by the phase interface displacement during the simulation. **The default setting is :func:`enable_automatic_check_interface_position`**.

Returns
This *TimestepControl* object

set_initial_time_step(*initial_time_step: float = 1e-07*)

Sets the initial timestep. **Default**: 1.0e-7 s

Parameters
initial_time_step – The initial timestep [s]

Returns
This *TimestepControl* object

set_max_absolute_error(*absolute_error: float = 1e-05*)

Sets the maximum absolute error. **Default**: 1.0e-5

Parameters
absolute_error – The maximum absolute error

Returns
This *TimestepControl* object

set_max_relative_error(*relative_error: float = 0.05*)

Sets the maximum relative error. **Default**: 0.05

Parameters
relative_error – The maximum relative error

Returns
This *TimestepControl* object

set_max_timestep_allowed_as_percent_of_simulation_time(*max_timestep_allowed_as_percent_of_simulation_time: float = 10.0*)

The maximum timestep allowed during the simulation, specified in percent of the simulation time. **Default**: 10.0%

Parameters
max_timestep_allowed_as_percent_of_simulation_time – The maximum timestep allowed [%]

Returns
This *TimestepControl* object

set_max_timestep_increase_factor(*max_timestep_increase_factor: float = 2.0*)

Sets the maximum timestep increase factor. **Default**: 2

Note: For example, if 2 is entered the maximum time step is twice as long as the previous time step taken.

Parameters
max_timestep_increase_factor – The maximum timestep increase factor

Returns
This *TimestepControl* object

set_smallest_time_step_allowed(*smallest_time_step_allowed: float = 1e-07*)

Sets the smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step. **Default**: 1.0e-7 s

Parameters
smallest_time_step_allowed – The smalles timestep allowed [s]

Returns
This *TimestepControl* object

class tc_python.diffusion.**Unit**(*value*)

Bases: 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: `AbstractCalculation`

Configuration for a Property Model calculation.

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

add_poly_command(*poly_command: str*)

This function has no effect and will be removed in 2024b. If you use it, please remove from your code.

Parameters
poly_command –

Returns
This `PropertyModelCalculation` object

calculate(*timeout_in_minutes: float = 0.0*) → *PropertyModelResult*

Runs the Property Model calculation.

Parameters
timeout_in_minutes – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a CalculationEngineException will be thrown.

Returns
A `PropertyModelResult` which later can be used to get specific values from the simulation.

get_argument_default(*argument_id: str*) → object

Returns the default value for the specified argument. The argument id can be obtained with `get_arguments()`.

Parameters
argument_id – The argument id

Returns
The default value (the type depends on the argument)

get_argument_description(*argument_id: str*) → str

Returns the detailed description of the argument. The id can be obtained with `get_arguments()`.

Parameters
argument_id – The argument id

Returns
The detailed description

`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.

Returns
The ids of the available arguments

`get_dynamic_arguments()` → Set[str]

Returns a list of the dynamic arguments of the Property Model.

Note: Dynamic arguments are "extra" arguments created by pressing the "plus" button that can occur next to the UI-panel for some models, when running the Property Model from within Thermo-Calc. You can use them also from the API by *`invoke_dynamic_argument()`*.

Returns
The ids of the available dynamic arguments

`get_model_description()` → str

Returns the description text of the current model.

Returns
the description

`get_model_parameter_value`(*model_parameter_id: str*) → float

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

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

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

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

Returns
The system data

invoke_dynamic_argument(*argument_id: str*)

Increases the number of instances of this dynamic argument by one, the argument will have an id such as *argument_1*, *argument_2*, … if the dynamic argument is called *argument*.

Note: You can obtain all available dynamic arguments by using `get_dynamic_arguments()`.

Parameters
argument_id – argument_id: The argument id

Returns
This `PropertyModelCalculation` object

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()

This function has no effect and will be removed in 2024b. If you use it, please remove from your code.

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:* CompositionUnit = *CompositionUnit.MOLE_PERCENT*)

Sets the composition unit.

Default: Mole percent (`CompositionUnit.MOLE_PERCENT`).

Parameters
unit_enum – The new composition unit

Returns
This *PropertyModelCalculation* object

`set_condition`(*classic_condition: str*, *value: float*)

Adds a classic POLY condition. If that method is used, all conditions need to be specified in such a way. If this method is used, it is necessary to set the dependent element manually using *set_dependent_element()*.

Default if not specified: pressure P = 1e5 Pa, system size N = 1, Temperature T = 1000 K

Warning: It is not possible to mix POLY-commands and compositions using *set_composition()*.

Note: It should not be necessary for most users to use this method, try to use *set_composition()* instead.

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

Parameters

- **classic_condition** – The classic POLY condition (for example: *X(CR)*)
- **value** – The value of the condition

Returns
This *PropertyModelCalculation* object

`set_dependent_element`(*dependent_element_name: str*)

Sets the dependent element manually.

Note: It should not be necessary for most users to use this method. Setting the dependent element manually is only necessary and allowed if `set_condition()` is used.

Parameters
`dependent_element_name` – The name of the dependent element

Returns
This `PropertyModelCalculation` object

`set_model_parameter`(*model_parameter_id: str*, *value*)

Resets an optimizable model parameter. The id can be obtained with `get_model_parameters()`.

Parameters

- `model_parameter_id` – The model parameter id
- `value` – The new value of the parameter

Returns
This `PropertyModelCalculation` object

`set_temperature`(*temperature: float = 1000*)

Sets the temperature.

Default: 1000 K

Parameters
`temperature` – The temperature [K]

Returns
This `PropertyModelCalculation` object

`with_system_modifications`(*system_modifications:* SystemModifications)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This `PropertyModelCalculation` object

`class tc_python.propertymodel.`**`PropertyModelResult`**(*result*)

Bases: `AbstractResult`

The result of a Property Model calculation.

`get_result_quantities`() → Set[str]

Returns a list of the available result quantities defined in the Property Model.

Returns
The ids of the defined result quantities

get_result_quantity_description(*result_quantity_id*) → str

Returns the detailed description of the result quantity. The id can be obtained by *get_result_quantities()*.

Parameters
result_quantity_id – The result quantity id

Returns
The detailed description

get_single_equilibrium_result(*result_quantity_id: str = ''*) → *SingleEquilibriumResult*

Returns a result quantity value. The available result quantities can be obtained by *get_result_quantities()*.

Parameters
result_quantity_id – The id of the result quantity.

Returns
The requested value [unit depending on the quantity], if the result is a SingleEquilibriumResult, is returned.

get_value_of(*result_quantity_id: str*) → Union[float, Dict[str, float]]

Returns a result quantity value. The available result quantities can be obtained by *get_result_quantities()*.

Parameters
result_quantity_id – The id of the result quantity

Returns
The requested value [unit depending on the quantity]. If the result is parameterized, parameter-value pairs are returned.

save_to_disk(*path: str*)

Saves the result to disk. The result can later be loaded using *tc_python.server.SetUp.load_result_from_disk()*.

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

5.1.8 Module "material_to_material"

class tc_python.material_to_material.**AbstractConstantCondition**

Bases: `object`

The abstract base class for all constant conditions.

class tc_python.material_to_material.**AbstractMaterialToMaterialCalculationAxis**

Bases: `object`

The abstract base class of all calculation axis.

class `tc_python.material_to_material.`**`ConstantCondition`**

Bases: *`AbstractConstantCondition`*

A constant condition.

classmethod **`fraction_of_material_b`**(*fraction_of_material_b: float = 0.5*)

Creates a constant fraction of material B condition object.

Note: The unit depends on the composition unit setting in the calculator object.

Parameters

`fraction_of_material_b` – The fraction of material B [weight-fraction or mole-fraction]

Returns

The condition object

classmethod **`temperature`**(*temperature: float = 1000*)

Creates a constant temperature condition object.

Parameters

`temperature` – The temperature [K]

Returns

The condition object

class `tc_python.material_to_material.`**`FractionOfMaterialBAxis`**(*from_fraction: float = 0.0, to_fraction: float = 1.0, start_fraction: float = 0.5*)

Bases: *`MaterialToMaterialCalculationAxis`*

A fraction of material B axis.

class `tc_python.material_to_material.`**`FractionOfMaterialBCondition`**(*fraction_of_material_b: float = 0.5*)

Bases: *`ConstantCondition`*

A constant fraction of material B condition.

class `tc_python.material_to_material.`**`MaterialToMaterialCalculationAxis`**

Bases: *`AbstractMaterialToMaterialCalculationAxis`*

A calculation axis.

classmethod **`fraction_of_material_b`**(*from_fraction: float = 0.0, to_fraction: float = 1.0, start_fraction: float = 0.5*)

Creates a fraction of material B axis object.

Note: The unit depends on the composition unit setting in the calculator.

Parameters

- **`from_fraction`** – The left axis limit [weight-fraction or mole-fraction]
- **`to_fraction`** – The right axis limit [weight-fraction or mole-fraction]
- **`start_fraction`** – The start fraction of the calculation [weight-fraction or mole-fraction]

Returns
A new `FractionOfMaterialBAxis` axis object

classmethod temperature(*from_temperature: float = 1000*, *to_temperature: float = 3000*, *start_temperature: float = 2000*)

Creates a temperature calculation axis object.

Parameters

- **from_temperature** – The left axis limit [K]
- **to_temperature** – The right axis limit [K]
- **start_temperature** – The start temperature of the calculation [K]

Returns
A new `TemperatureAxis` condition object

class tc_python.material_to_material.**MaterialToMaterialCalculationContainer**(*instance*)

Bases: `object`

Provides access to the calculation objects for all Material to Material calculations.

These are specialised calculations for mixtures of two materials A and B. Otherwise they behave identical to the corresponding regular single equilibrium, property diagram and phase diagram calculations.

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

Creates a Material to Material phase diagram (map) calculation.

Parameters

- **default_conditions** – If *True*, automatically sets the conditions *N=1* and *P=100000*
- **components** – Specify here the components of the system (for example: *[AL2O3, …]*), *only necessary if they differ from the elements*. If this option is used, **all elements** of the system need to be replaced by a component.

Returns
A new `MaterialToMaterialPhaseDiagramCalculation` object

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

Creates a Material to Material property diagram (step) calculation.

Parameters

- **default_conditions** – If *True*, automatically sets the conditions *N=1* and *P=100000*
- **components** – Specify here the components of the system (for example: *[AL2O3, …]*), *only necessary if they differ from the elements*. If this option is used, **all elements** of the system need to be replaced by a component.

Returns
A new `MaterialToMaterialPropertyDiagramCalculation` object

with_single_equilibrium_calculation(*default_conditions: bool = True*, *components: List[str] = []*) → *MaterialToMaterialSingleEquilibriumCalculation*

Creates a Material to Material single equilibrium calculation.

Parameters

- **default_conditions** – If *True*, automatically sets the conditions *N=1* and *P=100000*

- **components** – Specify here the components of the system (for example: *[AL2O3, ...]*), *only necessary if they differ from the elements*. If this option is used, **all elements** of the system need to be replaced by a component.

Returns
A new `MaterialToMaterialSingleEquilibriumCalculation` object

class `tc_python.material_to_material.`**`MaterialToMaterialPhaseDiagramCalculation`**(*calculator*)

Bases: `AbstractPhaseDiagramCalculation`

Configuration for a Material to Material phase diagram calculation.

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

`add_initial_equilibrium`(*initial_equilibrium:* InitialEquilibrium)

Add initial equilibrium start points from which a phase diagram is calculated.

Scans along the axis variables and generates start points when the scan procedure crosses a phase boundary.

It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the core remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria.

Parameters
initial_equilibrium – The initial equilibrium

Returns
This `MaterialToMaterialPhaseDiagramCalculation` object

`calculate`(*keep_previous_results: bool = False*, *timeout_in_minutes: float = 0.0*) → *MaterialToMaterialPhaseDiagramResult*

Performs the phase diagram calculation.

Warning: If you use *keep_previous_results=True*, you must not use another calculator or even get results in between the calculations using *calculate()*. Then the previous results will actually be lost.

Parameters

- **keep_previous_results** – If *True*, results from any previous call to this method are appended. This can be used to combine calculations with multiple start points if the mapping fails at a certain condition.
- **timeout_in_minutes** – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns
A new `MaterialToMaterialPhaseDiagramResult` object which later can be used to get specific values from the calculated result.

`disable_global_minimization`()

Disables global minimization.

Default: Enabled

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

dont_keep_default_equilibria()

Do not keep the initial equilibria added by default.

This is only relevant in combination with *add_initial_equilibrium()*.

This is the default behavior.

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

enable_global_minimization()

Enables global minimization.

Default: Enabled

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

get_components() → List[str]

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

Returns
The component names

get_gibbs_energy_addition_for(*phase: str*) → float

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

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

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

Returns
Gibbs energy addition to G per mole formula unit.

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

keep_default_equilibria()

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

Default behavior is to not keep default equilibria.

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

`remove_all_initial_equilibria()`

Removes all previously added initial equilibria.

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

`run_poly_command`(*command: str*)

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

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

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

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

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

`set_activities`(*activities: Dict[str, float]*)

Sets the constant activity conditions.

Note: The activity conditions are identical for both materials.

Parameters
`activities` – The constant activities

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

`set_composition_unit`(*unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*)

Sets the composition unit of **both materials A and B**.

Default: Weight percent

Parameters
`unit` – The composition unit of both materials A and B

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

`set_gibbs_energy_addition_for`(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

set_material_a(*composition: Dict[str, float]*, *dependent_component: Optional[str] = None*)

Sets the composition of the material A.

The unit is set with *set_composition_unit()*.

Tip: The material can also have constant activity conditions, they are set in *set_activities()*.

Parameters

- **composition** – The composition of the material A
- **dependent_component** – The dependent component of the material A

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

set_material_b(*composition: Dict[str, float]*, *dependent_component: Optional[str] = None*)

Sets the composition of the material B.

The unit is set with *set_composition_unit()*.

Tip: The material can also have constant activity conditions, they are set in *set_activities()*.

Parameters

- **composition** – The composition of the material B
- **dependent_component** – The dependent component of the material B

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

set_phase_to_dormant(*phase: str*)

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

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

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

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

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

Parameters

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

Returns
This *MaterialToMaterialPhaseDiagramCalculation* object

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

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

Parameters

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

Returns

This *MaterialToMaterialPhaseDiagramCalculation* object

set_phase_to_suspended(*phase: str*)

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

Parameters

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

Returns

This *MaterialToMaterialPhaseDiagramCalculation* object

set_pressure(*pressure: float*)

Sets the pressure (i.e. the condition *P*).

Note: If the flag *default_conditions=True* has been set during the creation of the calculator, the pressure is set to 1000 hPa by default.

Parameters

pressure – The pressure [Pa]

Returns

This *MaterialToMaterialPhaseDiagramCalculation* object

set_system_size(*system_size: float*)

Sets the system size (i.e. the condition 'N', the number of moles).

Note: If the flag *default_conditions=True* has been set during the creation of the calculator, the system size is set to 1.0 moles by default.

Parameters

system_size – The system size [mole]

Returns

This *MaterialToMaterialPhaseDiagramCalculation* object

with_first_axis(*axis:* MaterialToMaterialCalculationAxis)

Sets the first axis (either temperature of fraction of material B). This calculation type requires that both temperature and fraction of material B axis are set.

Parameters

axis – The axis

Returns

This *MaterialToMaterialPhaseDiagramCalculation* object

with_options(*options:* PhaseDiagramOptions)

Sets the simulation options.

Parameters
`options` – The simulation options

Returns
This `PhaseDiagramCalculation` object

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

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

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

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

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

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

Parameters

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

Returns
This *`MaterialToMaterialPhaseDiagramCalculation`* object

with_second_axis(*axis:* MaterialToMaterialCalculationAxis)

Sets the second axis (either temperature of fraction of material B). This calculation type requires that both temperature and fraction of material B axis are set.

Parameters
`axis` – The axis

Returns
This *`MaterialToMaterialPhaseDiagramCalculation`* object

with_system_modifications(*system_modifications:* SystemModifications)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This `MaterialToMaterialPhaseDiagramCalculation` object

`class tc_python.material_to_material.MaterialToMaterialPhaseDiagramResult(`*result*`)`

Bases: `PhaseDiagramResult`

Result of a Material to Material 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 `MaterialToMaterialPhaseDiagramResult` object

`get_values_grouped_by_quantity_of(`*x_quantity: Union[ThermodynamicQuantity, str]*, *y_quantity: Union[ThermodynamicQuantity, str]*`)` → *PhaseDiagramResultValues*

Returns x-y-line data grouped by the multiple datasets of the specified quantities (for example in dependency of components). The available quantities can be found in the documentation of the factory class `ThermodynamicQuantity`. Usually the result data represents the phase diagram.

Note: The different datasets will contain *NaN*-values between different subsections and are not sorted (because they are unsortable due to their nature).

Note: Its possible to use functions as axis variables, either by using `ThermodynamicQuantity.user_defined_function`, or by using an expression that contains '='.

Example *get_values_grouped_by_quantity_of('T', ThermodynamicQuantity.user_defined_function('HM.T'))*

Example *get_values_grouped_by_quantity_of('T', 'CP=HM.T')*

Parameters

- **`x_quantity`** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example *‘T’*), *MATERIAL_B_FRACTION*, or even a function (for example *‘f=T*1.01’*)
- **`y_quantity`** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example *‘NV’*), *MATERIAL_B_FRACTION*, or even a function (for example *‘CP=HM.T’*)

Returns
The phase diagram data

`get_values_grouped_by_stable_phases_of`(*x_quantity: Union[*ThermodynamicQuantity*, str]*, *y_quantity: Union[*ThermodynamicQuantity*, str]*) → *PhaseDiagramResultValues*

Returns x-y-line data grouped by the sets of “stable phases” (for example “LIQUID” or “LIQUID + FCC_A1”). The available quantities can be found in the documentation of the factory class `ThermodynamicQuantity`. Usually the result data represents the phase diagram.

Note: The different datasets will contain *NaN*-values between different subsections and are not sorted (because they are unsortable due to their nature).

Note: Its possible to use functions as axis variables, either by using `ThermodynamicQuantity.user_defined_function`, or by using an expression that contains ‘=’.

Example *get_values_grouped_by_quantity_of(‘T’, ThermodynamicQuantity.user_defined_function(‘HM.T’))*

Example *get_values_grouped_by_quantity_of(‘T’, ‘CP=HM.T’)*

Parameters

- **`x_quantity`** – The first quantity (“x-axis”), Console Mode syntax strings can be used as an alternative (for example *‘T’*), *MATERIAL_B_FRACTION*, or even a function (for example *‘f=T*1.01’*)
- **`y_quantity`** – The second quantity (“y-axis”), Console Mode syntax strings can be used as an alternative (for example *‘NV’*), *MATERIAL_B_FRACTION*, or even a function (for example *‘CP=HM.T’*)

Returns
The phase diagram data

`remove_phase_labels`()

Erases all added coordinates for phase labels.

Returns
This *`MaterialToMaterialPhaseDiagramResult`* object

`save_to_disk`(*path: str*)

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

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

Returns
this `MaterialToMaterialPhaseDiagramResult` object

`set_phase_name_style`(*phase_name_style_enum: PhaseNameStyle = PhaseNameStyle.NONE*)

Sets the style of the phase name labels that will be used in the result data object (constitution description, ordering description, . . .).

Default: PhaseNameStyle.NONE

Parameters
`phase_name_style_enum` – The phase name style

Returns
This `MaterialToMaterialPhaseDiagramResult` object

class `tc_python.material_to_material.`**`MaterialToMaterialPropertyDiagramCalculation`**(*calculator*)

Bases: `AbstractPropertyDiagramCalculation`

Configuration for a Material to Material property diagram calculation.

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

`calculate`(*keep_previous_results: bool = False*, *timeout_in_minutes: float = 0.0*) → *MaterialToMaterialPropertyDiagramResult*

Performs the Material to Material property diagram calculation.

Warning: If you use *keep_previous_results=True*, you must not use another calculator or even get results in between the calculations using `calculate()`. Then the previous results will actually be lost.

Parameters

- **`keep_previous_results`** – If *True*, results from any previous call to this method are appended. This can be used to combine calculations with multiple start points if the stepping fails at a certain condition.
- **`timeout_in_minutes`** – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns
A new `MaterialToMaterialPropertyDiagramResult` object which later can be used to get specific values from the calculated result

`disable_global_minimization`()

Disables global minimization.

Default: Enabled

Returns
This `MaterialToMaterialPropertyDiagramCalculation` object

`disable_step_separate_phases`()

Disables *step separate phases*. This is the **default** setting.

Returns
This `MaterialToMaterialPropertyDiagramCalculation` object

enable_global_minimization()

Enables global minimization.

Default: Enabled

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

enable_step_separate_phases()

Enables *step separate phases*.

Default: By default separate phase stepping is *disabled*

Note: This is an advanced option, it is used mostly to calculate how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIGMA-phase, G-phase, MU-phase, etc.).

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

get_components() → List[str]

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

Returns
The component names

get_gibbs_energy_addition_for(*phase: str*) → float

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

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

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

Returns
Gibbs energy addition to G per mole formula unit.

get_system_data() → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *with_system_modifications()*.

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

Returns
The system data

run_poly_command(*command: str*)

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

Parameters
command – The Thermo-Calc Console Mode command

Returns
This `MaterialToMaterialPropertyDiagramCalculation` object

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

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

set_activities(*activities: Dict[str, float]*)

Sets the constant activity conditions.

Note: The activity conditions are identical for both materials.

Parameters
activities – The constant activities

Returns
This `MaterialToMaterialPropertyDiagramCalculation` object

set_composition_unit(*unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*)

Sets the composition unit of **both materials A and B**.

Default: Weight percent

Parameters
unit – The composition unit of both materials A and B

Returns
This `MaterialToMaterialPropertyDiagramCalculation` object

set_gibbs_energy_addition_for(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This `MaterialToMaterialPropertyDiagramCalculation` object

set_material_a(*composition: Dict[str, float]*, *dependent_component: Optional[str] = None*)

Sets the composition of the material A.

The unit is set with `set_composition_unit()`.

Tip: The material can also have constant activity conditions, they are set in `set_activities()`.

Parameters

- **composition** – The composition of the material A
- **dependent_component** – The dependent component of the material A

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

set_material_b(*composition: Dict[str, float], dependent_component: Optional[str] = None*)

Sets the composition of the material B.

The unit is set with *set_composition_unit()*.

Tip: The material can also have constant activity conditions, they are set in *set_activities()*.

Parameters

- **composition** – The composition of the material B
- **dependent_component** – The dependent component of the material B

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

set_phase_to_dormant(*phase: str*)

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

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

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

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

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

Parameters

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

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

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

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

Parameters

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

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

`set_phase_to_suspended`(*phase: str*)

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

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

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

`set_pressure`(*pressure: float*)

Sets the pressure (i.e. the condition *P*).

Note: If the flag *default_conditions=True* has been set during the creation of the calculator, the pressure is set to 1000 hPa by default.

Parameters
`pressure` – The pressure [Pa]

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

`set_system_size`(*system_size: float*)

Sets the system size (i.e. the condition 'N', the number of moles).

Note: If the flag *default_conditions=True* has been set during the creation of the calculator, the system size is set to 1.0 moles by default.

Parameters
`system_size` – The system size [mole]

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

`with_axis`(*axis:* MaterialToMaterialCalculationAxis)

Sets the axis (either temperature of fraction of material B). This calculation type requires that either temperature or fraction of material B is set as a constant condition - the other one is set as an axis.

Parameters
`axis` – The axis

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

`with_constant_condition`(*condition:* ConstantCondition)

Sets the constant condition (either temperature of fraction of material B). This calculation type requires that either temperature or fraction of material B is set as a constant condition - the other one is set as an axis.

Parameters
`condition` – The condition

Returns
This *MaterialToMaterialPropertyDiagramCalculation* object

with_options(*options:* PropertyDiagramOptions)

Sets the simulation options.

Parameters

options – The simulation options

Returns

This *MaterialToMaterialPropertyDiagramCalculation* object

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

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

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

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

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

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

Parameters

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

Returns

This *MaterialToMaterialPropertyDiagramCalculation* object

with_system_modifications(*system_modifications:* SystemModifications)

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

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

Parameters

system_modifications – The system modification to be performed

Returns
This `MaterialToMaterialPropertyDiagramCalculation` object

`class tc_python.material_to_material.`**`MaterialToMaterialPropertyDiagramResult`**`(`*result*`)`

Bases: `PropertyDiagramResult`

Result of a Material to Material property diagram. It can be used to query for specific values.

`get_values_grouped_by_quantity_of``(`*x_quantity: Union[*ThermodynamicQuantity*, str], y_quantity: Union[*ThermodynamicQuantity*, str], sort_and_merge: bool = True*`)` → Dict[str, *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 Mode syntax strings can be used as an alternative (for example *'T'*), *MATERIAL_B_FRACTION*, or even a function (for example *'f=T*1.01'*)
- **`y_quantity`** – The second quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), *MATERIAL_B_FRACTION*, or even a function (for example *'CP=HM.T'*)
- **`sort_and_merge`** – If *True*, the data is sorted and merged into as few subsections as possible (divided by *NaN*)

Returns
Containing the datasets with the quantities as their keys

`get_values_grouped_by_stable_phases_of``(`*x_quantity: Union[*ThermodynamicQuantity*, str], y_quantity: Union[*ThermodynamicQuantity*, str], sort_and_merge: bool = True*`)` → Dict[str, *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 Mode syntax strings can be used as an alternative (for example *'T'*), *MATERIAL_B_FRACTION*, or even a function (for example *'f=T*1.01'*)
- **`y_quantity`** – The second quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), *MATERIAL_B_FRACTION*, or even a function (for example *'CP=HM.T'*)
- **`sort_and_merge`** – If *True*, the data will be sorted and merged into as few subsections as possible (divided by *NaN*)

Returns
Containing the datasets with the quantities as their keys

`get_values_of`(*x_quantity: Union[*ThermodynamicQuantity*, str], y_quantity: Union[*ThermodynamicQuantity*, str]*) → [List[float], 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 Mode syntax strings can be used as an alternative (for example *'T'*, *MATERIAL_B_FRACTION*, or even a function (for example *'f=T*1.01'*).
- **`y_quantity`** – The second thermodynamic quantity ("y-axis"), Console Mode syntax strings can be used as an alternative (for example *'NV'*), *MATERIAL_B_FRACTION*, or even a function (for example *'CP=HM.T'*)

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

`save_to_disk`(*path: str*)

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

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

Returns
this *`MaterialToMaterialPropertyDiagramResult`* object

`set_phase_name_style`(*phase_name_style_enum:* PhaseNameStyle *= PhaseNameStyle.NONE*)

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 *`MaterialToMaterialPropertyDiagramResult`* object

class `tc_python.material_to_material.`**`MaterialToMaterialSingleEquilibriumCalculation`**(*calculator*)

Bases: *`AbstractSingleEquilibriumCalculation`*

Configuration for a Material to Material single fraction of B calculation.

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

`calculate`(*timeout_in_minutes: float = 0.0*) → *MaterialToMaterialSingleEquilibriumResult*

Performs the material to material calculation.

Note: The calculation result is **no** temporary result object.

Parameters
`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a UnrecoverableCalculationException will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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

`disable_global_minimization`()

Turns the global minimization completely off.

Returns
This *`MaterialToMaterialSingleEquilibriumCalculation`* object

`enable_global_minimization()`

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

Returns
This `MaterialToMaterialSingleEquilibriumCalculation` object

`get_components()` → List[str]

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

Returns
The components

`get_gibbs_energy_addition_for(`*phase: str*`)` → float

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

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

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

Returns
Gibbs energy addition to G per mole formula unit.

`get_system_data()` → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

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

Returns
The system data

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

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

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

Returns
This `MaterialToMaterialSingleEquilibriumCalculation` object

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

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

`set_activities(`*activities: Dict[str, float]*`)`

Sets the constant activity conditions.

Note: The activity conditions are identical for both materials.

Parameters
`activities` – The constant activities

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`set_component_to_entered`(*component: str*)

Sets the specified component to the status ENTERED, that is the default state.

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

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`set_component_to_suspended`(*component: str*, *reset_conditions: bool = False*)

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

Parameters

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

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`set_composition_unit`(*unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*)

Sets the composition unit of **both materials A and B**.

Default: Weight percent

Parameters
`unit` – The composition unit of both materials A and B

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`set_gibbs_energy_addition_for`(*phase: str*, *gibbs_energy: float*)

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

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

Parameters

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

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

set_material_a(*composition: Dict[str, float]*, *dependent_component: Optional[str] = None*)

Sets the composition of the material A.

The unit is set with *set_composition_unit()*.

Tip: The material can also have constant activity conditions, they are set in *set_activities()*.

Parameters

- **composition** – The composition of the material A
- **dependent_component** – The dependent component of the material A

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

set_material_b(*composition: Dict[str, float]*, *dependent_component: Optional[str] = None*)

Sets the composition of the material B.

The unit is set with *set_composition_unit()*.

Tip: The material can also have constant activity conditions, they are set in *set_activities()*.

Parameters

- **composition** – The composition of the material B
- **dependent_component** – The dependent component of the material B

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

set_phase_to_dormant(*phase: str*)

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

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

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

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

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

Parameters

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

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

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

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

Parameters

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

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`set_phase_to_suspended`(*phase: str*)

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

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

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`set_pressure`(*pressure: float*)

Sets the pressure (i.e. the condition *P*).

Note: If the flag *default_conditions=True* has been set during the creation of the calculator, the pressure is set to 1000 hPa by default.

Parameters
`pressure` – The pressure [Pa]

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`set_system_size`(*system_size: float*)

Sets the system size (i.e. the condition 'N', the number of moles).

Note: If the flag *default_conditions=True* has been set during the creation of the calculator, the system size is set to 1.0 moles by default.

Parameters
`system_size` – The system size [mole]

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`with_first_constant_condition`(*condition:* ConstantCondition)

Sets the first constant condition (either temperature of fraction of material B).

Parameters
`condition` – The condition

Returns
This *MaterialToMaterialSingleEquilibriumCalculation* object

`with_options`(*options:* SingleEquilibriumOptions)

Sets the simulation options.

Parameters
`options` – The simulation options

Returns
This `SingleEquilibriumCalculation` object

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

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

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

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

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

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

Parameters

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

Returns
This *`MaterialToMaterialSingleEquilibriumCalculation`* object

`with_second_constant_condition`(*condition:* ConstantCondition)

Sets the second constant condition (either temperature of fraction of material B).

Parameters
`condition` – The condition

Returns
This *`MaterialToMaterialSingleEquilibriumCalculation`* object

`with_system_modifications`(*system_modifications:* SystemModifications)

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

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

Parameters
`system_modifications` – The system modification to be performed

Returns
This *`MaterialToMaterialSingleEquilibriumCalculation`* object

class `tc_python.material_to_material.`**`MaterialToMaterialSingleEquilibriumResult`**(*result*)

Bases: *`SingleEquilibriumResult`*

Result of a Material To Material calculation for a single fraction of material B, it can be evaluated using a quantity or Console Mode syntax.

`change_pressure`(*pressure: float*)

Change the pressure and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with higher performance. The properties are calculated at the new pressure using the phase amount, temperature and composition of phases from the initial equilibrium. Use *`get_value_of()`* to obtain them.

Parameters
`pressure` – The pressure [Pa]

Returns
This *`MaterialToMaterialSingleEquilibriumResult`* object

`change_temperature`(*temperature: float*)

Change the temperature and re-evaluate the results from the equilibrium without minimizing Gibbs energy, i.e. with high performance. The properties are calculated at the new temperature using the phase amount, pressure and composition of phases from the initial equilibrium. Use *`get_value_of()`* to obtain them.

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

Parameters
`temperature` – The temperature [K]

Returns
This *`MaterialToMaterialSingleEquilibriumResult`* object

`get_components`() → List[str]

Returns the names of the components selected in the system (including any components auto-selected by the database(s)).

Returns
The names of the selected components

`get_conditions`() → List[str]

Returns the conditions.

Returns
The selected conditions

`get_phases`() → List[str]

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

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

get_stable_phases() → List[str]

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

Returns
The names of the stable phases

get_value_of(*quantity: Union[*ThermodynamicQuantity*, str]*) → float

Returns a value from a single equilibrium calculation.

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

Returns
The requested value

run_poly_command(*command: str*)

Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine. This affects only the state of the result object.

Parameters
command – The Thermo-Calc Console Mode command

Returns
This *MaterialToMaterialSingleEquilibriumResult* object

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

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

save_to_disk(*path: str*)

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

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

Returns
this *MaterialToMaterialSingleEquilibriumResult* object

class tc_python.material_to_material.**TemperatureAxis**(*from_temperature: float = 1000*, *to_temperature: float = 3000*, *start_temperature: float = 2000*)

Bases: *MaterialToMaterialCalculationAxis*

A temperature calculation axis.

class tc_python.material_to_material.**TemperatureCondition**(*temperature: float = 1000.0*)

Bases: *ConstantCondition*

A constant temperature condition.

5.1.9 Package “process_metallurgy”

5.1.9.1 Module “base”

`class tc_python.process_metallurgy.base.AbstractAddition`

Bases: `object`

The base class for representing an addition to an equilibrium calculation or process simulation.

`get_composition()` → Dict[str, float]

Returns the composition of the addition - without containing a dependent component.

Returns
The composition [in the unit provided by `getCompositionUnit()`]

`abstract get_composition_unit()`

Returns the composition unit used in this addition.

Returns
The composition unit

`get_dependent_component()` → str

Returns the dependent component.

Returns
The dependent component or an empty string if no dependent component is defined

`get_elements()` → Set[str]

Returns all elements of the addition.

Returns
The elements

`get_id()` → str

Returns the unique ID of the addition.

Returns
The unique ID of the addition

`get_temperature()` → float

Returns the temperature of the addition. This refers to the temperature before it is added to the process.

Returns
The temperature [K]

`is_do_scale()` → bool

Returns if the composition of the addition is being scaled to 100% / 1 or not.

Returns
If the composition is scaled

`is_empty()` → bool

Returns if the addition is “empty”, i.e., has zero amount.

Returns
If the addition is empty

class tc_python.process_metallurgy.base.**ActivityReference**(*value*)

Bases: `Enum`

The reference for a slag activity calculation. The actual reference phase depends on the component for which the activity is request and can be obtained by using these methods on the result object: *tc_python.process_metallurgy.process.ProcessSimulationResult.get_formula_for_activity_of_slag()* or *tc_python.process_metallurgy.equilibrium.EquilibriumResult.get_formula_for_activity_of_slag()*.

LIQUID = 1

The reference is liquid slag.

SOLID = 0

The reference is solid slag.

class tc_python.process_metallurgy.base.**PhaseGroup**(*value*)

Bases: `Enum`

The phase group, such a group is collecting all phases that belong to a certain type.

ALL_METAL = 2

All metal phases.

ALL_SLAG = 5

All slag phases.

GAS = 6

All gas phases.

LIQUID_METAL = 0

All liquid metal phases.

LIQUID_SLAG = 4

All liquid slag phases.

SOLID_METAL = 1

All solid metal phases.

SOLID_SLAG = 3

All solid slag phases.

class tc_python.process_metallurgy.base.**ProcessDatabase**(*value*)

Bases: `Enum`

The database used for a Process Metallurgy calculation.

LATEST = 0

The latest database available.

OXDEMO = 1

The database OXDEMO.

TCOX10 = 4

The database TCOX10.

TCOX11 = 5

The database TCOX11.

`TCOX12 = 6`

The database TCOX12.

`TCOX13 = 7`

The database TCOX13.

`TCOX8 = 2`

The database TCOX8.

`TCOX9 = 3`

The database TCOX9.

`get_name()` → str

Returns the name of the actually used database.

Tip: This is especially useful if *LATEST* is used.

Returns

The name of the database

`class tc_python.process_metallurgy.base.`**`ProcessMetallurgyOptions`**

Bases: *`SingleEquilibriumOptions`*

The options for a process metallurgy calculation.

`disable_approximate_driving_force_for_metastable_phases()`

Disables the approximation of the driving force for metastable phases.

Default: Enabled

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

If it is important that these driving forces are correct, use *`disable_approximate_driving_force_for_metastable_pha`* to force the calculation to converge for the metastable phases.

Returns

This *`ProcessMetallurgyOptions`* object

`disable_control_step_size_during_minimization()`

Disables step size control during minimization (non-global).

Default: Enabled

Returns

This *`ProcessMetallurgyOptions`* object

`disable_force_positive_definite_phase_hessian()`

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

Default: Enabled

Returns
This *ProcessMetallurgyOptions* object

`enable_approximate_driving_force_for_metastable_phases()`

Enables the approximation of the driving force for metastable phases.

Default: Enabled

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

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

Returns
This *ProcessMetallurgyOptions* object

`enable_control_step_size_during_minimization()`

Enables step size control during normal minimization (non-global).

Default: Enabled

Returns
This *ProcessMetallurgyOptions* object

`enable_force_positive_definite_phase_hessian()`

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

Default: Enabled

Returns
This *ProcessMetallurgyOptions* 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 *ProcessMetallurgyOptions* object

`set_max_no_of_iterations`(*max_no_of_iterations: int = 2000*)

Sets the maximum number of iterations for the CALPHAD minimizer.

Default: max. 2000 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 *ProcessMetallurgyOptions* object

set_process_minimization_policy(*minimization_policy: ProcessMinimizationPolicy*)

Sets the minimization policy for the process metallurgy calculation. It is possible to choose policies that try different methods if one method fails.

Parameters
minimization_policy – The minimization policy to be used

Returns
This *ProcessMetallurgyOptions* 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 *ProcessMetallurgyOptions* object

set_smallest_fraction(*smallest_fraction: float = 1e-16*)

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-16 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 *ProcessMetallurgyOptions* object

class tc_python.process_metallurgy.base.**ProcessMinimizationPolicy**(*value*)

Bases: `Enum`

The policy for the CALPHAD minimization routine used in a calculation.

Note: This affects the runtime and stability of a calculation. Global minimization is more stable but more time-consuming. Local minimization is much faster but can miss new phases coming up. Global test is a compromise between both approaches.

GLOBAL = 0

Always use global minimization.

`GLOBAL_TEST = 1`

Always use global test.

`GLOBAL_TEST__GLOBAL = 5`

First try global test, if that fails use global minimization.

`LOCAL = 2`

Always use local minimization.

`LOCAL__GLOBAL_TEST = 3`

First try local minimization, if that fails use global test.

`LOCAL__GLOBAL_TEST__GLOBAL = 4`

First try local minimization, if that fails try global test and if that fails use global minimization.

`class tc_python.process_metallurgy.base.SlagProperty(`*value*`)`

Bases: `Enum`

The slag property, different definitions are available. The actual definition of a certain slag property for the current system can be obtained using these methods on the result object: `tc_python.process_metallurgy.process.ProcessSimulationResult.getFormulaForSlagProperty()` or `tc_python.process_metallurgy.equilibrium.EquilibriumResult.getFormulaForSlagProperty()`.

Note: If not all components required by the definition of slag property are available in a given system, the slag property will return *NaN*.

`B2 = 0`

Basicity *B2* (based on: *CaO / SiO2*).

`B3 = 1`

Basicity *B3* (based on: *CaO / MgO / SiO2*).

`B4 = 3`

Basicity *B4* (based on: *CaO / MgO / SiO2 / Al2O3*).

`BAS2 = 2`

Basicity *Bas2* (based on: *CaO / MgO / SiO2 / Al2O3 / TiO2*).

`BELLS_RATIO = 4`

Basicity *Bell's ratio* (based on: *CaO / MgO / SiO2 / Al2O3*).

`LOG_10_SULPHUR_CAPACITY = 5`

Logarithmic sulphur capacity of the slag.

`LS = 6`

Sulphur capacity *Ls* of the slag.

`class tc_python.process_metallurgy.base.SlagType(`*value*`)`

Bases: `Enum`

The type of slag considered for a slag property calculation.

`ALL = 2`

The slag property is calculated for all slag, i.e. for both the liquid and solid slag.

`LIQUID = 1`

The slag property is calculated for all liquid slag.

`SOLID = 0`

The slag property is calculated for all solid slag.

5.1.9.2 Module "equilibrium"

`class tc_python.process_metallurgy.equilibrium.`**`AbstractEquilibriumAddition`**

Bases: *`AbstractAddition`*

The base class for representing an addition to an equilibrium calculation.

`set_amount``(`*amount: float*`)`

Change the amount of the addition.

Parameters

`amount` – The new amount [in the amount unit of this addition]

Returns

This *`AbstractEquilibriumAddition`* object

`set_component_composition``(`*component: str*, *content: float*`)`

Change the composition of a component of the addition.

Parameters

- **`component`** – The component to be changed
- **`content`** – The new content of the component [in the composition unit defined for this addition]

Returns

This *`AbstractEquilibriumAddition`* object

`class tc_python.process_metallurgy.equilibrium.`**`AdiabaticEquilibriumCalculation`**`(`*calculator*`)`

Bases: *`EquilibriumCalculation`*

An *adiabatic* Process Metallurgy equilibrium calculation. Such calculations can for example be used to determine the global equilibrium state of a process.

`add_addition``(`*addition:* AbstractEquilibriumAddition`)`

Adds an addition to the calculation.

Parameters

`addition` – A *`EquilibriumAddition`* or *`EquilibriumGasAddition`*

Returns

This *`AdiabaticEquilibriumCalculation`* object

`add_poly_command``(`*command: str*`)`

Adds a Thermo-Calc Console syntax POLY module command which will be executed when performing the calculation using the *`calculate()`* method.

If multiple commands are added, they will be executed in the order of addition. Each command will only be executed one.

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).

Parameters
`command` – The POLY module command in Thermo-Calc console syntax

Returns
This `AdiabaticEquilibriumCalculation` object

`calculate`(*timeout_in_minutes: float = 0.0*) → *EquilibriumResult*

Runs the Process Metallurgy equilibrium calculation.

Parameters
`timeout_in_minutes` – The calculation will be aborted after that time, **default: no timeout**

Returns
A new `EquilibriumResult` object

`remove_addition`(*addition:* AbstractEquilibriumAddition)

Removes an addition from the calculation.

Parameters
`addition` – The addition to be removed

Returns
This `AdiabaticEquilibriumCalculation` object

`remove_all_additions`()

Removes all additions from the calculation.

Returns
This `AdiabaticEquilibriumCalculation` object

`set_pressure`(*pressure: float = 100000.0*)

Sets the pressure.

Parameters
`pressure` – The pressure [Pa]

Returns
This `AdiabaticEquilibriumCalculation` object

`with_options`(*options:* ProcessMetallurgyOptions)

Sets the options for the calculation.

Parameters
`options` – The options

Returns
This `AdiabaticEquilibriumCalculation` object

`class tc_python.process_metallurgy.equilibrium.EquilibriumAddition`(*composition: Dict[str, float], amount: float, temperature: float = 293.15, composition_unit:* CompositionUnit *= CompositionUnit.MASS_PERCENT, do_scale: bool = False*)

Bases: *AbstractEquilibriumAddition*

An addition to an equilibrium calculation.

Tip: By setting *do_scale=True*, the composition will be scaled to 100% / fraction of 1. This is useful if the composition provided is not summing to 100% / 1. An example could be a slag addition which is provided like this: *90 wt-% CaO - 5 wt-% Al2O3 - 4 wt-% SiO2*.

Parameters

- **composition** – The composition
- **amount** – The amount [kg]
- **temperature** – The initial addition temperature (**default: 20 °C**) [K]
- **composition_unit** – The composition unit
- **do_scale** – If the composition is scaled to 100% / fraction of 1

get_amount() → float

Returns the amount of this addition.

Returns
The amount [kg]

get_composition_unit() → *CompositionUnit*

Returns the composition unit used in this addition.

Returns
The composition unit

class tc_python.process_metallurgy.equilibrium.**EquilibriumCalculation**(*metallurgical_reaction*)

Bases: object

A Process Metallurgy equilibrium calculation. Such calculations can for example be used to determine the global equilibrium state of a process.

abstract **add_addition**(*addition: AbstractEquilibriumAddition*)

Adds an addition to the calculation.

Parameters
addition – The addition

Returns
This *EquilibriumCalculation* object

abstract **add_poly_command**(*command: str*)

Adds a Thermo-Calc Console syntax POLY module command which will be executed when performing the calculation using the *calculate()* method.

If multiple commands are added, they will be executed in the order of addition. Each command will only be executed one.

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).

Parameters
`command` – The POLY module command in Thermo-Calc console syntax

Returns
This *`EquilibriumCalculation`* object

`abstract calculate`(*timeout_in_minutes: float = 0.0*) → *EquilibriumResult*

Runs the Process Metallurgy equilibrium calculation.

Parameters
`timeout_in_minutes` – The calculation will be aborted after that time, **default: no timeout**

Returns
A new *`EquilibriumResult`* object

`abstract remove_addition`(*addition:* AbstractEquilibriumAddition)

Removes an addition from the calculation.

Parameters
`addition` – The addition to be removed

Returns
This *`EquilibriumCalculation`* object

`abstract remove_all_additions`()

Removes all additions from the calculation.

Returns
This *`EquilibriumCalculation`* object

`abstract set_pressure`(*pressure: float = 100000.0*)

Sets the pressure.

Parameters
`pressure` – The pressure [Pa]

Returns
This *`EquilibriumCalculation`* object

`update_addition`(*addition:* AbstractEquilibriumAddition)

Replaces an already added addition with an updated one. This is usually used to change the composition or amount of an addition while iterating over them. Typically, this is done for stepping or mapping calculations.

Note: The calculation must already contain the addition object to be updated.

Parameters
`addition` – The new addition containing updated values

Returns
This `IsoThermalMetallurgyCalculation` object

abstract with_options(*options: ProcessMetallurgyOptions*)

Sets the options for the calculation.

Parameters

`options` – The options

Returns

This `EquilibriumCalculation` object

class `tc_python.process_metallurgy.equilibrium.`**EquilibriumGasAddition**(*composition: Dict[str, float], amount: float, temperature: float = 293.15, amount_unit: GasAmountUnit = GasAmountUnit.NORM_CUBIC_METER, composition_unit: GasCompositionUnit = GasCompositionUnit.VOLUME_PERCENT, do_scale: bool = False*)

Bases: `AbstractEquilibriumAddition`

A gas addition to an equilibrium calculation.

Tip: By setting *do_scale=True*, the composition will be scaled to 100% / fraction of 1. This is useful if the composition provided is not summing to 100% / 1. An example could be a gas addition which is provided like this: *90 vol–% Ar - 10 vol-% O2*.

get_amount() → float

Returns the amount of this addition.

Note: The amount unit can be obtained using `get_amount_unit()`.

Returns

The amount [in the amount unit]

get_amount_unit() → *GasAmountUnit*

Returns the amount unit used in this addition.

Returns

The amount unit

get_composition_unit() → *GasCompositionUnit*

Returns the composition unit used in this addition.

Returns

The composition unit

class `tc_python.process_metallurgy.equilibrium.`**EquilibriumResult**(*result*)

Bases: `AbstractResult`

The result of a Process Metallurgy equilibrium calculation.

get_activity_of_slag(*component: str*, *reference:* ActivityReference = *ActivityReference.LIQUID*) → float

Returns the activity of a component in the slag.

Parameters

- **component** – The component
- **reference** – The reference for the activity, can be liquid or solid slag, **default: liquid slag**

Returns
The activity of the component [-]

get_amount() → float

Returns the total amount.

Returns
The total amount [kg]

get_amount_of_elements() → Dict[str, float]

Returns the amount of each element.

Returns
The amount of the elements [kg]

get_amount_of_phase_groups() → Dict[*PhaseGroup*, float]

Returns the amount of each phase group (e.g., for example all liquid slag).

Returns
The amount of the phase groups [kg]

get_amount_of_phases() → Dict[str, float]

Returns the amount of each phase.

Returns
The amount of the phases [kg]

get_components() → Set[str]

Returns all components defined for the elements present in this result.

Returns
The components present in this result

get_composition(*composition_unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*) → Dict[str, float]

Returns the composition of the result.

Parameters
composition_unit – The composition unit, **default: mass percent**

Returns
The composition

get_composition_of_phase(*phase: str*, *composition_unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*, *composition_type:* CompositionType = *CompositionType.COMPONENT*) → Dict[str, float]

Returns the composition of a phase in the result.

Parameters

- **phase** – The phase name

- **`composition_unit`** – The composition unit, **default: mass percent**
- **`composition_type`** – Defines if the composition is given by element (e.g., *75 wt-% Fe - 25 wt-% Cr*) or by component (e.g. *65 wt-% Al2O3 - 35 wt-% CaO*). In case of a metallic phase, the composition is given by element even if *component* is selected. **Default: by component**.

Returns
The composition

`get_composition_of_phase_group`(*phase_group:* PhaseGroup, *composition_unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*, *composition_type:* CompositionType = *CompositionType.COMPONENT*) → Dict[str, float]

Returns the composition of a phase group (e.g., all liquid slag) in the result.

Parameters

- **`phase_group`** – The phase group
- **`composition_unit`** – The composition unit, **default: mass percent**
- **`composition_type`** – Defines if the composition is given by element (e.g., *75 wt-% Fe - 25 wt-% Cr*) or by component (e.g. *65 wt-% Al2O3 - 35 wt-% CaO*). In case of a metallic phase, the composition is given by element even if *component* is selected. **Default: by component**.

Returns
The composition

`get_elements`() → Set[str]

Returns all elements defined for the result.

Returns
All elements present in this result

`get_formula_for_activity_of_slag`(*component: str*, *reference:* ActivityReference = *ActivityReference.LIQUID*) → str

Returns the Thermo-Calc Console syntax formula used for calculating the activity of a component in the slag (e.g. *AC(AL2O3, IONIC_LIQ)*. The actual activity can be obtained using `get_activity_of_slag()`.

Parameters

- **`component`** – The component
- **`reference`** – The reference for the activity, can be liquid or solid slag, **default: liquid slag**

Returns
The formula for calculating the activity

`get_formula_for_slag_property`(*slag_property:* SlagProperty, *slag_type:* SlagType = *SlagType.ALL*) → str

Returns the Thermo-Calc Console syntax formula used for calculating a property of the slag (e.g. *B(CAO)/B(SIO2)*. The actual slag property can be obtained using `get_slag_property()`.

Parameters

- **`slag_property`** – The slag property
- **`slag_type`** – The part of the slag for which the property will be calculated. Can be all slag, the liquid or the solid slag. **Default: all slag**

Returns
The formula for calculating the slag property

get_fraction_of_phase_groups(*unit:* PhaseUnit = *PhaseUnit.MASS_FRACTION*) → Dict[*PhaseGroup*, float]

Returns the fraction of the phase groups (e.g., all liquid slag) in the result.

Parameters
`unit` – The unit of the fraction, **default: volume fraction**

Returns
The phase fractions

get_fraction_of_phases(*unit:* PhaseUnit = *PhaseUnit.MASS_FRACTION*) → Dict[str, float]

Returns the fraction of the stable phases in the result.

Parameters
`unit` – The unit of the fraction, **default: volume fraction**

Returns
The phase fractions

get_gas_components() → Set[str]

Returns all components of the gas phase defined for the elements present in this result.

Returns
The components of the gas phase present in this result

get_oxygen_partial_pressure() → float

Returns the partial pressure of oxygen in the result.

Returns
The partial pressure [Pa]

get_pressure() → float

Returns the pressure in the result.

Returns
The pressure [Pa]

get_slag_property(*slag_property:* SlagProperty, *slag_type:* SlagType = *SlagType.ALL*) → float

Returns a property of the slag. These properties are mostly used to describe the property of a slag to pick up sulfur.

Parameters

- `slag_property` – The slag property
- `slag_type` – The part of the slag for which the property will be calculated. Can be all slag, the liquid or the solid slag. **Default: all slag**

Returns
The slag property [unit depending on the property]

get_stable_phases() → Set[str]

Returns the stable phases in the result.

Returns
The stable phases

get_stable_phases_in_phase_group(*phase_group: PhaseGroup*) → Set[str]

Returns the stable phases of a phase group (e.g., all liquid slag) in the result.

Parameters
phase_group – The phase group

Returns
The stable phases

get_temperature() → float

Returns the temperature in the result.

Returns
The temperature [K]

get_value_of(*classic_expression: str*) → float

Returns a value for a thermodynamic quantity.

> **Warning:** It should normally not be required to use this method, use the appropriate method available in the API instead.

Parameters
classic_expression – The thermodynamic quantity to get the value of in Thermo-Calc Console Mode syntax (for example "NPM(FCC_A1)")

Returns
The requested value

get_viscosity_dynamic_of_phase(*phase: str*) → float

Returns the dynamic viscosity of a phase in the result.

Parameters
phase – The phase name

Returns
The dynamic viscosity [Pa*s]

get_viscosity_kinematic_of_phase(*phase: str*) → float

Returns the kinematic viscosity of a phase in the result.

Parameters
phase – The phase name

Returns
The kinematic viscosity [m**2/s]

class tc_python.process_metallurgy.equilibrium.**IsoThermalEquilibriumCalculation**(*calculation*)

Bases: *EquilibriumCalculation*

An *isothermal* Process Metallurgy equilibrium calculation. Such calculations can for example be used to determine the global equilibrium state of a process.

add_addition(*addition: AbstractEquilibriumAddition*)

Adds an addition to the calculation.

Parameters
addition – A *EquilibriumAddition* or *EquilibriumGasAddition*

Returns
This *IsoThermalEquilibriumCalculation* object

add_poly_command(*command: str*)

Adds a Thermo-Calc Console syntax POLY module command which will be executed when performing the calculation using the `calculate()` method.

If multiple commands are added, they will be executed in the order of addition. Each command will only be executed one.

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).

Parameters
command – The POLY module command in Thermo-Calc console syntax

Returns
This *IsoThermalEquilibriumCalculation* object

calculate(*timeout_in_minutes: float = 0.0*) → *EquilibriumResult*

Runs the Process Metallurgy equilibrium calculation.

Parameters
timeout_in_minutes – The calculation will be aborted after that time, **default: no timeout**

Returns
A new *EquilibriumResult* object

remove_addition(*addition:* AbstractEquilibriumAddition)

Removes an addition from the calculation.

Parameters
addition – The addition to be removed

Returns
This *IsoThermalEquilibriumCalculation* object

remove_all_additions()

Removes all additions from the calculation.

Returns
This *IsoThermalEquilibriumCalculation* object

set_pressure(*pressure: float = 100000.0*)

Sets the pressure.

Parameters
pressure – The pressure [Pa]

Returns
This *IsoThermalEquilibriumCalculation* object

set_temperature(*temperature: float*)

Sets the temperature.

Parameters
temperature – The temperature [K]

Returns
This *IsoThermalEquilibriumCalculation* object

update_addition(*addition:* AbstractEquilibriumAddition)

Replaces an already added addition with an updated one.

Tip: This is usually used to change the composition or amount of an addition while iterating over multiple values. Typically, this is done for stepping or mapping calculations.

Note: The calculation must already contain the addition object to be updated.

Parameters
addition – A previously added addition object with the updated values

Returns
This *IsoThermalEquilibriumCalculation* object

with_options(*options:* ProcessMetallurgyOptions)

Sets the options for the calculation.

Parameters
options – The options

Returns
This *IsoThermalEquilibriumCalculation* object

5.1.9.3 Module "process"

class tc_python.process_metallurgy.process.**AbstractContinuousAddition**

Bases: *AbstractProcessAddition*

The base class representing an addition in a process simulation that is added continuously over a period of time.

class tc_python.process_metallurgy.process.**AbstractProcessAddition**

Bases: *AbstractAddition*

The base class for representing an addition in a process simulation.

class tc_python.process_metallurgy.process.**AbstractSingleTimeAddition**

Bases: *AbstractProcessAddition*

The base class representing an addition in a process simulation that is added at a distinct time point.

class tc_python.process_metallurgy.process.**BulkZone**(*density: float*, *phase_group_to_transfer:* PhaseGroup, *name: str*)

Bases: *Zone*

A bulk zone in a process simulation, this is representing a large volume in the process, for example the steel melt or the top slag. A zone is a volume in a process that has identical temperature and composition. It has well-defined boundaries to other zones.

Tip: This is a generic class and seldom used directly. Use instead *MetalBulkZone* or *SlagBulkZone*.

add_addition(*addition: AbstractSingleTimeAddition*, *time: float = 0.0*)

Adds a single-time addition at the specified time point to the zone. The addition will be dissolved immediately.

Parameters

- **addition** – A *SingleTimeAddition* or *SingleTimeGasAddition*
- **time** – The time point [s]

Returns

This *BulkZone* object

add_continuous_addition(*addition: AbstractContinuousAddition*, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant addition continuously during the specified time period to the zone. All added material will be dissolved immediately.

Parameters

- **addition** – A *ContinuousAddition* or *ContinuousGasAddition*
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns

This *BulkZone* object

add_power(*power: float*, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant power during a specified time period to the zone (for example heating or cooling).

Parameters

- **power** – The power [W]
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns

This *BulkZone* object

disable_degassing()

Disables degassing for this zone, i.e. all gas formed at any time step will be staying in this zone.

Returns

This *BulkZone* object

enable_degassing()

Enables degassing for this zone, i.e. any gas formed at any time step will be removed after that time step. This gas will be transferred into the *exhaust gas zone*. **This is the default**.

Returns

This *BulkZone* object

`get_density()` → float

Returns the density of the zone

Returns
The density [kg/m**3]

`get_elements()` → Set[str]

Returns the elements present in the zone. The elements are determined by the additions.

Returns
The elements

`get_id()` → str

Returns the unique id of the zone. :return: The zone id

`get_phase_group_to_transfer()` → *PhaseGroup*

Returns the phase group that is transferred from the attached reaction zones back to this zone after each time step.

Returns
The phase group

`is_degassing_enabled()` → bool

Returns if degassing is enabled in the zone.

Returns
If degassing is enabled

class `tc_python.process_metallurgy.process.ContinuousAddition`(*composition: Dict[str, float], rate: float, temperature: float = 293.15, composition_unit:* CompositionUnit *= CompositionUnit.MASS_PERCENT, do_scale: bool = False*)

Bases: *AbstractContinuousAddition*

An addition in a process simulation that is added continuously during a period of time.

It is assumed that the material added during that period is dissolved instantaneously.

Tip: By setting *do_scale=True*, the composition will be scaled to 100% / fraction of 1. This is useful if the composition provided is not scaling to 100% / 1. An example could be a slag addition which is provided like this: *90 wt-% CaO - 5 wt-% Al2O3 - 4 wt-% SiO2*.

Parameters

- **composition** – The composition
- **rate** – The rate of addition [kg/s]
- **temperature** – The initial addition temperature (**default: 20 °C**) [K]
- **composition_unit** – The composition unit
- **do_scale** – If the composition is scaled to 100% / fraction of 1

`get_composition_unit()` → *CompositionUnit*

Returns the composition unit used in this addition.

Returns
The composition unit

`get_rate()` → float

Returns the rate of addition.

Returns
The addition rate [kg/s]

`class tc_python.process_metallurgy.process.ContinuousGasAddition`(*composition: Dict[str, float], rate: float, temperature: float = 293.15, rate_unit:* GasRateUnit *= GasRateUnit.NORM_CUBIC_METER_PER_SEC, composition_unit:* GasCompositionUnit *= GasCompositionUnit.VOLUME_PERCENT, do_scale: bool = False*)

Bases: `AbstractContinuousAddition`

A gas addition in a process simulation that is added continuously during a period of time.

It is assumed that the gas added during that period is dissolved instantaneously.

Tip: By setting *do_scale=True*, the composition will be scaled to 100% / fraction of 1. This is useful if the composition provided is not scaling to 100% / 1. An example could be a gas addition which is provided like this: *90 vol–% Ar - 10 vol-% O2*.

`get_composition_unit()` → *GasCompositionUnit*

Returns the composition unit used in this addition.

Returns
The composition unit

`get_rate()` → float

Returns the rate of addition.

Note: The rate unit can be obtained using `get_rate_unit()`.

Returns
The addition rate [in the rate unit]

`get_rate_unit()` → *GasRateUnit*

Returns the rate unit used in this addition.

Returns
The rate unit

class `tc_python.process_metallurgy.process.`**`ExhaustGasResult`**(*result*)

Bases: `object`

A result representing the exhaust gas zone, here all exhaust gas generated during the process is accumulated.

The data is returned for each time point of the process simulation. These time points can be obtained from this method: *`ProcessSimulationResult.get_time_points()`*.

`get_amount``()` → List[float]

Returns the amount of exhaust gas present at each time point.

This is the amount of gas accumulated since the beginning of the process.

Returns
The accumulated amount of gas at each time point [kg]

`get_amount_of_components``()` → Dict[str, List[float]]

Returns the amount of each exhaust gas component present at each time point.

This is the amount of gas accumulated since the beginning of the process. This is different from the **current composition at each time point** obtained using *`get_composition()`*.

Returns
The accumulated amount of each gas component at each time point [kg]

`get_composition`(*composition_type:* CompositionType = *CompositionType.COMPONENT*, *unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*) → Dict[str, List[float]]

Returns the current composition of the exhaust gas zone at each time point. This is the composition **at each time point**. This is different from the **accumulated amount** obtained using *`get_amount_of_components()`*.

Parameters

- **`composition_type`** – The type of the composition, can be by gas component or by element, **default: by gas component**
- **`unit`** – The composition unit, **default: mass percent**

Returns
The current composition of the gas components at each time point

`get_pressure``()` → List[float]

Returns the pressure of the exhaust gas zone at each time point.

Returns
The pressure [Pa]

`get_stable_phases``()` → Set[str]

Returns the stable phases within the exhaust gas zone at each time point.

Returns
The stable phases

`get_temperature``()` → List[float]

Returns the temperature of the exhaust gas at each time point.

Returns
The temperature at each time point [K]

class `tc_python.process_metallurgy.process.`**`MassTransferCoefficients`**

Bases: `object`

The mass transfer coefficients between a reaction zone and a bulk zone vs. time.

add(*mass_transfer_coefficient: float*, *time: float = 0.0*)

Adds the mass transfer coefficient valid beginning at a time point.

This value is valid until another value is defined for a later time point.

Parameters

- **mass_transfer_coefficient** – The mass transfer coefficient [m/s]
- **time** – The time-point where the mass transfer coefficient begins to be valid [s]

Returns

This *MassTransferCoefficients* object

class tc_python.process_metallurgy.process.**MetalBulkZone**(*density: float*)

Bases: *Zone*

A metallic bulk zone in a process simulation.

This is representing a large volume in the process, for example the steel melt. A zone is a volume in a process that has identical temperature and composition. It has well-defined boundaries to other zones.

The name of this zone is automatically defined and unique.

add_addition(*addition:* AbstractSingleTimeAddition, *time: float = 0.0*)

Adds a single-time addition at the specified time point to the zone. The addition will be dissolved immediately.

Parameters

- **addition** – A *SingleTimeAddition* or *SingleTimeGasAddition*
- **time** – The time point [s]

Returns

This *MetalBulkZone* object

add_continuous_addition(*addition:* AbstractContinuousAddition, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant addition continuously during the specified time period to the zone. All added material will be dissolved immediately.

Parameters

- **addition** – A *ContinuousAddition* or *ContinuousGasAddition*
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns

This *MetalBulkZone* object

add_power(*power: float*, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant power during a specified time period to the zone (for example heating or cooling).

Parameters

- **power** – The power [W]
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns

This *MetalBulkZone* object

disable_degassing()

Disables degassing for this zone, i.e. all gas formed at any time step will be staying in this zone.

Returns
This *MetalBulkZone* object

enable_degassing()

Enables degassing for this zone, i.e. any gas formed at any time step will be removed after that time step. This gas will be transferred into the *exhaust gas zone*. **This is the default**.

Returns
This *MetalBulkZone* object

get_density() → float

Returns the density of the zone

Returns
The density [kg/m**3]

get_elements() → Set[str]

Returns the elements present in the zone. The elements are determined by the additions.

Returns
The elements

get_id() → str

Returns the unique name / id of the zone.

Returns
The zone name / id

get_phase_group_to_transfer() → *PhaseGroup*

Returns the phase group that is transferred from the attached reaction zones back to this zone after each time step.

Returns
The phase group

is_degassing_enabled() → bool

Returns if degassing is enabled in the zone.

Returns
If degassing is enabled

class tc_python.process_metallurgy.process.**ProcessSimulationCalculation**(*calculation*)

Bases: `object`

A Process Metallurgy process simulation. Such calculations represent complete metallurgical processes with several zones and simulate their evolution over time.

calculate(*timeout_in_minutes: float = 0.0*) → *ProcessSimulationResult*

Runs the Process Metallurgy process simulation.

Parameters
timeout_in_minutes – The calculation will be aborted after that time, **default: no timeout**

Returns
A new *ProcessSimulationResult* object

set_end_time(*end_time: float*)

Sets the end time of a process.

Parameters
`end_time` – The end time point [s]

Returns
This *ProcessSimulationCalculation* object

set_initial_time_step(*initial_time_step: float = 1.0*)

Sets the initial time step used in the process simulation.

Note: All later time steps are automatically determined to limit the expected temperature change during that step, this is controlled by *set_max_allowed_temp_change_per_step()*.

Parameters
`initial_time_step` – The initial time step [s]

Returns
This *ProcessSimulationCalculation* object

set_max_allowed_temp_change_per_step(*max_allowed_temp_change: float = 10.0*)

The maximum allowed temperature change per time step. This is implicitly also limiting the composition change during a time step and required for numerical stability.

Parameters
`max_allowed_temp_change` – The maximum allowed temperature change [K]

Returns
This *ProcessSimulationCalculation* object

set_max_time_step(*max_time_step: float = 180.0*)

The maximum time step chosen by the automatic time step control.

Note: All time steps are automatically determined to limit the expected temperature change during that step, this is controlled by *set_max_allowed_temp_change_per_step()*.

Parameters
`max_time_step` – The maximum time step [s]

Returns
This *ProcessSimulationCalculation* object

set_min_time_step(*min_time_step: float = 1.0*)

The minimum time step chosen by the automatic time step control.

Note: All time steps are automatically determined to limit the expected temperature change during that step, this is controlled by *set_max_allowed_temp_change_per_step()*.

Parameters
`min_time_step` – The minimum time step [s]

Returns
This *ProcessSimulationCalculation* object

`set_pressure`(*pressure: float = 100000.0*)

Sets a constant pressure during the complete process.

Parameters
pressure – The pressure [Pa]

Returns
This *ProcessSimulationCalculation* object

`set_pressure_in_time_period`(*pressure_in_pa: float*, *from_time: float = 0.0*, *to_time: float = nan*)

Sets a constant pressure during a time period.

Default: 1.0e5 Pa.

Parameters

- **pressure_in_pa** – The pressure [Pa]
- **from_time** – The start time [s]
- **to_time** – The end time [s]

Returns
This *ProcessSimulationCalculation* object

`with_options`(*options:* ProcessMetallurgyOptions)

Sets the options for the process simulation.

Parameters
options – The options

Returns
This *ProcessSimulationCalculation* object

`with_reaction_zone`(*reaction_zone:* ReactionZone)

Sets the reaction zone of the process simulation. The bulk zones attached to this reaction zone are configured in the reaction zone object.

Note: In the present release, **only one** reaction zone is supported.

Parameters
reaction_zone – The reaction zone object

Returns
This *ProcessSimulationCalculation* object

`class tc_python.process_metallurgy.process.ProcessSimulationResult`(*result*)

Bases: *AbstractResult*

The result of a Process Metallurgy process simulation.

`get_activity_of_slag`(*zone: Union[*Zone*, str]*, *component: str*, *reference:* ActivityReference = *ActivityReference.LIQUID*) → List[float]

Returns the activity of a component in the slag in a zone at each time point.

Parameters

- **zone** – The zone object or the zone name
- **component** – The component
- **reference** – The reference for the activity, can be liquid or solid slag, **default: liquid slag**

Returns
The activity of the component at each time point [-]

`get_amount`(*zone: Union[Zone, str]*) → List[float]

Returns the amount of a zone at each time point.

Parameters
zone – The zone object or the zone name

Returns
The amount at each time point [kg]

`get_amount_of_elements`() → Dict[str, List[float]]

Returns the total amount of each element in the simulation at each time point.

Returns
The total amount of the elements at each time point [kg]

`get_amount_of_phase_groups`(*zone: Union[Zone, str]*) → Dict[*PhaseGroup*, List[float]]

Returns the amount of each phase group (e.g., for example all liquid slag) in a zone at each time point.

Parameters
zone – The zone object or the zone name

Returns
The amount of the phase groups at each time point [kg]

`get_amount_of_phases`(*zone: Union[Zone, str]*) → Dict[str, List[float]]

Returns the amount of each phase in a zone at each time point.

Parameters
zone – The zone object or the zone name

Returns
The amount of the phases at each time point [kg]

`get_components`() → Set[str]

Returns all components defined in the simulation.

Returns
The components

`get_composition`(*zone: Union[Zone, str]*, *composition_unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*) → Dict[str, List[float]]

Returns the composition of a zone per element at each time point.

Parameters

- **zone** – The zone object or the zone name
- **composition_unit** – The composition unit, **default: mass percent**

Returns
The composition at each time point

`get_composition_of_phase`(*zone: Union[*Zone*, str]*, *phase: str*, *composition_unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*, *composition_type:* CompositionType = *CompositionType.COMPONENT*) → Dict[str, List[float]]

Returns the composition of a phase in a zone at each time point.

Parameters

- **`zone`** – The zone object or the zone name
- **`phase`** – The phase name
- **`composition_unit`** – The composition unit, **default: mass percent**
- **`composition_type`** – Defines if the composition is given by element (e.g., *75 wt-% Fe - 25 wt-% Cr*) or by component (e.g. *65 wt-% Al2O3 - 35 wt-% CaO*). In case of a metallic phase, the composition is given by element even if *component* is selected. **Default: by component**.

Returns
The composition at each time point

`get_composition_of_phase_group`(*zone: Union[*Zone*, str]*, *phase_group:* PhaseGroup, *composition_unit:* CompositionUnit = *CompositionUnit.MASS_PERCENT*, *composition_type:* CompositionType = *CompositionType.COMPONENT*) → Dict[str, List[float]]

Returns the composition of a phase group (e.g., all liquid slag) in a zone at each time point.

Parameters

- **`zone`** – The zone object or the zone name
- **`phase_group`** – The phase group
- **`composition_unit`** – The composition unit, **default: mass percent**
- **`composition_type`** – Defines if the composition is given by element (e.g., *75 wt-% Fe - 25 wt-% Cr*) or by component (e.g. *65 wt-% Al2O3 - 35 wt-% CaO*). In case of a metallic phase, the composition is given by element even if *component* is selected. **Default: by component**.

Returns
The composition at each time point

`get_elements`() → Set[str]

Returns all elements present in the simulation.

Returns
The elements

`get_enthalpy`() → List[float]

Returns the total enthalpy of the process at each time point.

Returns
The enthalpy at each time point [J]

`get_exhaust_gas`() → *ExhaustGasResult*

Returns the result for the exhaust gas zone.

This result object can be used to evaluate the exhaust gas zone at each time point.

Returns
The exhaust gas zone result object.

get_formula_for_activity_of_slag(*zone: Union[Zone, str]*, *component: str*, *reference: ActivityReference = ActivityReference.LIQUID*) → List[str]

Returns the Thermo-Calc Console syntax formula used for calculating the activity of a component in the slag (e.g. *AC(AL2O3, IONIC_LIQ)* in a zone at each time point. The actual activity can be obtained using `get_activity_of_slag()`.

Parameters

- **zone** – The zone object or the zone name
- **component** – The component
- **reference** – The reference for the activity, can be liquid or solid slag, **default: liquid slag**

Returns
The formula for calculating the activity at each time point

get_formula_for_slag_property(*zone: Union[Zone, str]*, *slag_property: SlagProperty*, *slag_type: SlagType = SlagType.ALL*) → List[str]

Returns the Thermo-Calc Console syntax formula used for calculating a property of the slag (e.g. *B(CAO)/B(SIO2)* in a zone at each time point. The actual slag property can be obtained using `get_slag_property()`.

Parameters

- **zone** – The zone object or the zone name
- **slag_property** – The slag property
- **slag_type** – The part of the slag for which the property will be calculated. Can be all slag, the liquid or the solid slag. **Default: all slag**

Returns
The formula for calculating the slag property at each time point

get_fraction_of_phase_groups(*zone: Union[Zone, str]*, *unit: PhaseUnit = PhaseUnit.MASS_FRACTION*) → Dict[*PhaseGroup*, List[float]]

Returns the fractions of the phase groups (e.g., all liquid slag) in a zone at each time point.

Parameters

- **zone** – The zone object or the zone name
- **unit** – The unit of the fraction

Returns
The phase fractions at each time point

get_fraction_of_phases(*zone: Union[Zone, str]*, *unit: PhaseUnit = PhaseUnit.MASS_FRACTION*) → Dict[str, List[float]]

Returns the fractions of all stable phases in a zone at each time point.

Parameters

- **zone** – The zone object or the zone name
- **unit** – The unit of the fraction

Returns
The phase fractions at each time point

`get_gas_components()` → Set[str]

Returns all components of the gas phase defined for the elements present in the simulation.

Returns
The components of the gas phase

`get_num_of_performed_steps()` → List[int]

Returns the accumulated number of performed time steps at each time point.

Note: The number of performed time steps can differ from the index of the time step in the result list because time steps might have been repeated with smaller step size during a process simulation.

Returns
The accumulated number of performed time steps

`get_oxygen_partial_pressure`(*zone: Union[Zone, str]*) → List[float]

Returns the partial pressure of oxygen in the zone at each time point.

Parameters
`zone` – The zone object or the zone name

Returns
The partial pressure [Pa]

`get_pressure`(*zone: Union[Zone, str]*) → List[float]

Returns the pressure in a zone at each time point.

Parameters
`zone` – The zone object or the zone name

Returns
The pressure at each time point [Pa]

`get_slag_property`(*zone: Union[Zone, str]*, *slag_property: SlagProperty*, *slag_type: SlagType = SlagType.ALL*) → List[float]

Returns a property of the slag in a zone at each time point. These properties are mostly used to describe the property of a slag to pick up sulfur.

Parameters

- **`zone`** – The zone object or the zone name
- **`slag_property`** – The slag property
- **`slag_type`** – The part of the slag for which the property will be calculated. Can be all slag, the liquid or the solid slag. **Default: all slag**

Returns
The slag property at each time point [unit depending on the property]

`get_stable_phases`(*zone: Union[Zone, str]*) → Set[str]

Returns the stable phases in a zone.

Parameters
`zone` – The zone object or the zone name

Returns
The stable phases

get_stable_phases_in_phase_group(*zone: Union[Zone, str]*, *phase_group: PhaseGroup*) → Set[str]

Returns the stable phases of a phase group (e.g., all solid slag) in a zone.

Parameters

- **zone** – The zone object or the zone name
- **phase_group** – The phase group

Returns

The stable phases of the phase group

get_temperature(*zone: Union[Zone, str]*) → List[float]

Returns the temperature of a zone at each time point.

Parameters

zone – The zone object or the zone name

Returns

The temperature at each time point [K]

get_time_points() → List[float]

Returns the time points of the process simulation. All result quantities are returned for exactly these time points.

Returns

The time points [s]

get_value_of(*zone: Union[Zone, str]*, *classic_expression: str*) → List[float]

Returns a value for a thermodynamic quantity in a zone at each time point.

Warning: It should normally not be required to use this method, use the appropriate method available in the API instead.

Parameters

- **zone** – The zone object or the zone name
- **classic_expression** – The thermodynamic quantity to get the value of in Thermo-Calc Console Mode syntax (for example "NPM(FCC_A1)")

Returns

The requested value at each time point

get_viscosity_dynamic_of_phase(*zone: Union[Zone, str]*, *phase: str*) → List[float]

Returns the dynamic viscosity of a phase in a zone at each time point.

Parameters

- **zone** – The zone object or the zone name
- **phase** – The phase name

Returns

The dynamic viscosity at each time point [Pa*s]

get_viscosity_kinematic_of_phase(*zone: Union[Zone, str]*, *phase: str*) → List[float]

Returns the kinematic viscosity of a phase in a zone at each time point.

Parameters

- **zone** – The zone object or the zone name
- **phase** – The phase name

Returns
The kinematic viscosity at each time point [m**2/s]

class tc_python.process_metallurgy.process.**ReactionZone**(*area: float*, *left_zone:* Zone, *mass_transfer_coefficient_left: Union[float,* MassTransferCoefficients*]*, *right_zone:* Zone, *mass_transfer_coefficient_right: Union[float,* MassTransferCoefficients*]*)

Bases: *Zone*

A reaction zone in a process simulation, this is representing the interface layer between two bulk zones that are in contact and can react with each other, for example the steel melt and the top slag. The size of the reaction zone is dynamic and determined by the mass transfer coefficient. A zone is a volume in a process that has identical temperature and composition. It has well-defined boundaries to other zones.

add_addition(*addition:* AbstractSingleTimeAddition, *time: float = 0.0*)

Adds a single-time addition at the specified time point to the zone. The addition will be dissolved immediately.

Parameters

- **addition** – A *SingleTimeAddition* or *SingleTimeGasAddition*
- **time** – The time point [s]

Returns
This *ReactionZone* object

add_continuous_addition(*addition:* AbstractContinuousAddition, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant addition continuously during the specified time period to the zone. All added material will be dissolved immediately.

Parameters

- **addition** – A *ContinuousAddition* or *ContinuousGasAddition*
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns
This *ReactionZone* object

add_heat_transfer(*heat_transfer_coefficient: float*)

Adds heat transfer through the reaction zone, i.e., between the two attached bulk zones.

Parameters
heat_transfer_coefficient – The heat transfer coefficient [W/(K*m**2)]

Returns
This *ReactionZone* object

add_power(*power: float*, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant power during a specified time period to the zone (for example heating or cooling).

Parameters

- **power** – The power [W]

- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns
This *ReactionZone* object

add_transfer_of_phase_group(*transfer_of_phase_group: TransferOfPhaseGroup*)

Adds transfer of a certain phase group through the reaction zone during each time step, i.e. from one of the attached bulk zones to the other. This is for example used to model inclusion flotation from the steel melt to the slag.

Parameters
transfer_of_phase_group – The transfer of phase group configuration, can be time-dependent.

Returns
This *ReactionZone* object

disable_degassing()

Disables degassing for this zone, i.e. all gas formed at any time step will be staying in this zone.

Returns
This *ReactionZone* object

enable_degassing()

Enables degassing for this zone, i.e. any gas formed at any time step will be removed after that time step. This gas will be transferred into the *exhaust gas zone*. **This is the default**.

Returns
This *ReactionZone* object

get_elements() → Set[str]

Returns the elements present in the zone. The elements are determined by the additions.

Returns
The elements

get_id() → str

Returns the unique id of the zone. :return: The zone id

is_degassing_enabled() → bool

Returns if degassing is enabled in the zone.

Returns
If degassing is enabled

class tc_python.process_metallurgy.process.**SingleTimeAddition**(*composition: Dict[str, float], amount: float, temperature: float = 293.15, composition_unit: CompositionUnit = CompositionUnit.MASS_PERCENT, do_scale: bool = False*)

Bases: *AbstractSingleTimeAddition*

An addition in a process simulation that is added at a distinct time point.

It is assumed that the addition is dissolved instantaneously.

Tip: By setting *do_scale=True*, the composition will be scaled to 100% / fraction of 1. This is useful if the composition provided is not summing to 100% / 1. An example could be a slag addition which is provided like this: *90 wt-% CaO - 5 wt-% Al2O3 - 4 wt-% SiO2*.

Parameters

- `composition` – The composition
- `amount` – The amount [kg]
- `temperature` – The initial addition temperature (**default: 20 °C**) [K]
- `composition_unit` – The composition unit
- `do_scale` – If the composition is scaled to 100% / fraction of 1

`get_amount()` → float

Returns the amount of this addition.

Returns
The amount [kg]

`get_composition_unit()` → *CompositionUnit*

Returns the composition unit used in this addition.

Returns
The composition unit

`class tc_python.process_metallurgy.process.SingleTimeGasAddition`(*composition: Dict[str, float]*, *amount: float*, *temperature: float = 293.15*, *amount_unit: GasAmountUnit = GasAmountUnit.NORM_CUBIC_METER*, *composition_unit: GasCompositionUnit = GasCompositionUnit.VOLUME_PERCENT*, *do_scale: bool = False*)

Bases: `AbstractSingleTimeAddition`

A gas addition in a process simulation that is added at a distinct time point.

It is assumed that the addition is dissolved instantaneously.

Tip: By setting *do_scale=True*, the composition will be scaled to 100% / fraction of 1. This is useful if the composition provided is not scaling to 100% / 1. An example could be a gas addition which is provided like this: *90 vol–% Ar - 10 vol-% O2*.

Parameters

- `composition` – The composition
- `amount` – The amount
- `temperature` – The initial addition temperature (**default: 20 °C**) [K]
- `amount_unit` – The amount unit

- **composition_unit** – The composition unit
- **do_scale** – If the composition is scaled to 100% / fraction of 1

get_amount() → float

Returns the amount of this addition.

Note: The amount unit can be obtained using *get_amount_unit()*.

Returns
The amount [in the amount unit]

get_amount_unit() → *GasAmountUnit*

Returns the amount unit used in this addition.

Returns
The amount unit

get_composition_unit() → *GasCompositionUnit*

Returns the composition unit used in this addition.

Returns
The composition unit

class tc_python.process_metallurgy.process.**SlagBulkZone**(*density: float*)

Bases: *Zone*

A slag bulk zone in a process simulation.

This is representing a large volume in the process, for example the top slag. A zone is a volume in a process that has identical temperature and composition. It has well-defined boundaries to other zones.

The name of this zone is automatically defined and unique.

add_addition(*addition:* AbstractSingleTimeAddition, *time: float = 0.0*)

Adds a single-time addition at the specified time point to the zone. The addition will be dissolved immediately.

Parameters

- **addition** – A *SingleTimeAddition* or *SingleTimeGasAddition*
- **time** – The time point [s]

Returns
This *SlagBulkZone* object

add_continuous_addition(*addition:* AbstractContinuousAddition, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant addition continuously during the specified time period to the zone. All added material will be dissolved immediately.

Parameters

- **addition** – A *ContinuousAddition* or *ContinuousGasAddition*
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns
This *SlagBulkZone* object

add_power(*power: float*, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant power during a specified time period to the zone (for example heating or cooling).

Parameters

- **power** – The power [W]
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns
This *SlagBulkZone* object

disable_degassing()

Disables degassing for this zone, i.e. all gas formed at any time step will be staying in this zone.

Returns
This *SlagBulkZone* object

enable_degassing()

Enables degassing for this zone, i.e. any gas formed at any time step will be removed after that time step. This gas will be transferred into the *exhaust gas zone*. **This is the default**.

Returns
This *SlagBulkZone* object

get_density() → float

Returns the density of the zone

Returns
The density [kg/m**3]

get_elements() → Set[str]

Returns the elements present in the zone. The elements are determined by the additions.

Returns
The elements

get_id() → str

Returns the unique id of the zone. :return: The zone id

get_phase_group_to_transfer() → *PhaseGroup*

Returns the phase group that is transferred from the attached reaction zones back to this zone after each time step.

Returns
The phase group

is_degassing_enabled() → bool

Returns if degassing is enabled in the zone.

Returns
If degassing is enabled

class tc_python.process_metallurgy.process.**TransferOfPhaseGroup**(*phase_group_to_transfer:* PhaseGroup, *source_zone:* Zone)

Bases: `object`

The transfer of a percentage of a certain phase group (.e.g., solid slag) between zones during each time step. This is for example used to model inclusion flotation from the steel melt to the slag.

add(*transfer_rate: float*, *time: float = 0*)

Adds the transfer rate valid beginning at a time point.

This value is valid until another value is defined for a later time point.

Parameters

- **transfer_rate** – The transfer rate [% of phase group amount/s]
- **time** – The time point where the transfer of a phase group begins to be valid [s]

Returns

This *TransferOfPhaseGroup* object

get_phase_group_to_transfer() → *PhaseGroup*

Returns the phase group to be transferred

Returns

The phase group

get_transfer_source_zone_id() → str

The id of the source zone of the transfer

Returns

This source zone id

class `tc_python.process_metallurgy.process.`**Zone**

Bases: `object`

The base class of a zone in a process simulation. A zone is a volume in a process that has identical temperature and composition. It has well-defined boundaries to other zones.

add_addition(*addition:* AbstractSingleTimeAddition, *time: float = 0.0*)

Adds a single-time addition at the specified time point to the zone. The addition will be dissolved immediately.

Parameters

- **addition** – A *SingleTimeAddition* or *SingleTimeGasAddition*
- **time** – The time point [s]

Returns

This *Zone* object

add_continuous_addition(*addition:* AbstractContinuousAddition, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant addition continuously during the specified time period to the zone. All added material will be dissolved immediately.

Parameters

- **addition** – A *ContinuousAddition* or *ContinuousGasAddition*
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns
This *Zone* object

`add_power`(*power: float*, *from_time: float = 0.0*, *to_time: float = nan*)

Adds a constant power during a specified time period to the zone (for example heating or cooling).

Parameters

- **power** – The power [W]
- **from_time** – The start time point [s]
- **to_time** – The end time point [s]

Returns
This *Zone* object

`disable_degassing`()

Disables degassing for this zone, i.e. all gas formed at any time step will be staying in this zone.

Returns
This *Zone* object

`enable_degassing`()

Enables degassing for this zone, i.e. any gas formed at any time step will be removed after that time step. This gas will be transferred into the *exhaust gas zone*. **This is the default**.

Returns
This *Zone* object

`get_elements`() → Set[str]

Returns the elements present in the zone. The elements are determined by the additions.

Returns
The elements

`get_id`() → str

Returns the unique id of the zone. :return: The zone id

`is_degassing_enabled`() → bool

Returns if degassing is enabled in the zone.

Returns
If degassing is enabled

5.1.10 Module "additive_manufacturing"

class `tc_python.am.AdditiveManufacturingCalculation`(*calculation*)

Bases: `object`

Abstract base class for an Additive Manufacturing calculation.

`disable_fluid_flow_marangoni`()

Disables the fluid flow modelling of the Marangoni effect.

Default: Enabled

Returns
This *AdditiveManufacturingCalculation* object

`disable_separate_materials()`

Disables separate material properties for powder and solid material.

Default: Disabled

Returns
This *AdditiveManufacturingCalculation* object

`enable_fluid_flow_marangoni()`

Enables the fluid flow modelling of the Marangoni effect.

Default: Enabled

Note: This option is not possible to use in conjunction with the option *separate material*, which is therefore automatically disabled.

Returns
This *AdditiveManufacturingCalculation* object

`enable_separate_materials()`

Enables separate material properties for powder and solid material.

Default: Disabled

Note: This option is not possible to use in conjunction with the option *Marangoni fluid flow*, which is therefore automatically disabled.

Returns
This *AdditiveManufacturingCalculation* object

`get_configuration_as_string()` → str

Returns detailed information about the current state of the calculation object.

Warning: The structure of the calculation 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 afterward.

`set_ambient_temperature`(*temperature: float = 296.15*)

Sets the ambient temperature.

Default: 23 degree Celsius

Parameters
`temperature` – The ambient temperature [K]

Returns
This *AdditiveManufacturingCalculation* object

`set_base_plate_temperature`(*temperature: float = 303.15*)

Sets the baseplate temperature.

Default: 30 degree Celsius

Parameters
: `temperature` – The baseplate temperature [K]

Returns
: This *AdditiveManufacturingCalculation* object

`set_gas_pressure`(*pressure: float = 100000.0*)

Sets the gas pressure.

Default: 1.0e5 Pa

Parameters
: `pressure` – The pressure [Pa]

Returns
: This *AdditiveManufacturingCalculation* object

`set_height`(*height: float = 0.002*)

Sets the height of the simulation domain.

Default: 2.0e-3 m

Parameters
: `height` – The height [m]

Returns
: This *AdditiveManufacturingCalculation* object

`set_layer_thickness`(*layer_thickness: float = 4e-05*)

Sets the layer thickness.

Default: 40.0e-6 m

Parameters
: `layer_thickness` – The layer thickness [m]

Returns
: This *AdditiveManufacturingCalculation* object

`set_powder_density`(*powder_density: float = 80.0*)

Sets the powder density.

Default: 80.0%

Parameters
: `powder_density` – The powder density [%]

Returns
: This *AdditiveManufacturingCalculation* object

`with_heat_source`(*heat_source:* HeatSource)

Sets the heat source.

Parameters
: `heat_source` – The heat source

Returns
: This *AdditiveManufacturingCalculation* object

with_material_properties(*material_properties:* MaterialProperties)

Sets the material properties.

Tip: Material properties can be defined like this: `MaterialProperties.from_library("IN718")` or `MaterialProperties.from_scheil_result(scheil_result)`.

Parameters
material_properties – The material properties

Returns
This *AdditiveManufacturingCalculation* object

with_mesh(*mesh:* Mesh)

Sets the mesh.

Parameters
mesh – The mesh

Returns
This *AdditiveManufacturingCalculation* object

with_numerical_options(*numerical_options:* NumericalOptions)

Sets the numerical options.

Parameters
numerical_options – The numerical options

Returns
This *AdditiveManufacturingCalculation* object

with_top_boundary_conditions(*boundary_conditions:* TopBoundaryConditions)

Sets the boundary conditions.

Parameters
boundary_conditions – The boundary conditions

Returns
This *AdditiveManufacturingCalculation* object

class tc_python.am.**AdditiveManufacturingResult**(*result*)

Bases: *AbstractResult*

Base class for additive manufacturing results.

get_pyvista_mesh(*scalar:* Scalar = *Scalar.TEMPERATURE*, *material_type:* MaterialType = *MaterialType.SHOW_ALL*)

Returns a *pyvista* mesh object that can be added to a *pyvista* plotter.

More details about *pyvista* meshes can be found in their documentation: https://docs.pyvista.org/version/stable/api/plotting/_autosummary/pyvista.Plotter.add_mesh.html

Tip: This method is typically used to obtain additional meshes with other settings if the plot object has already been retrieved with *get_pyvista_plotter()*.

Parameters

- **scalar** – The quantity to be visualized in the plot
- **material_type** – The material type to be visualized in the plot

Returns

A `pyvista.DataSet` object

get_pyvista_plotter(*scalar: Scalar = Scalar.TEMPERATURE, material_type: MaterialType = MaterialType.SHOW_ALL, camera: Optional[Dict[str, List[float]]] = None, anti_aliasing: str = 'msaa', multi_samples: int = 16, color_map: str = 'jet', enable_camera_orientation_widget: bool = False, render_lines_as_tubes: bool = True, background: str = 'LightSteelBlue', shape: Optional[bool] = None, view_buttons: bool = True, update_plot_callback: Optional[Callable] = None*)

Returns a *pyvista* plotter and a mesh object containing the data from this result. They can be used to create 3D-plots visualizing the results of the AM calculation. More details about the *pyvista* settings can be found in their documentation: https://docs.pyvista.org/version/stable/api/plotting/_autosummary/pyvista.Plotter.html

The most simple usage of this method is:

```
plotter, mesh = result.get_pyvista_plotter()
plotter.add_mesh(mesh)
plotter.show()
```

Parameters

- **scalar** – The quantity to be visualized in the plot
- **material_type** – The material type to be visualized in the plot, only available if *AdditiveManufacturingCalculation.enable_separate_materials()* has been used
- **camera** – Defining the camera position, view-up vector and focus point, the default is `DEFAULT_CAMERA`, for example: *{'position': [-2, -2, 1], 'viewup': [0, 0, 1], 'focal_point': [0.0, 0.0, 0.0]}*. More details can be found here: https://docs.pyvista.org/version/stable/api/core/camera.html
- **anti_aliasing** – The *pyvista* antialiasing setting, can be one of: *"msaa"* - Multi-Sample Anti-Aliasing, *"fxaa"* - Fast Approximate Anti-Aliasing or *"ssaa"* - Super-Sample Anti-Aliasing. More details can be found here: https://docs.pyvista.org/version/stable/examples/02-plot/anti-aliasing.html
- **multi_samples** – The number of samples used for antialiasing
- **color_map** – The *pyvista* colormap. Can be any colormap provided by Matplotlib and some other plotting libraries. More details can be found here: https://docs.pyvista.org/version/stable/examples/02-plot/cmap.html
- **enable_camera_orientation_widget** – Enables the *pyvista* camera orientation widget in the plotter
- **render_lines_as_tubes** – Controls if lines are rendered as tubes
- **background** – The *pyvista* background color, either a string, rgb list or hex color string. https://docs.pyvista.org/version/stable/api/plotting/_autosummary/pyvista.Plotter.background_color.html
- **shape** – The shape of the plot, i.e. how many subplots will be created - a tuple (y, x), for example *(2, 2)*. They are accessed using `pyvista.Plotter.subplot`.

- **`view_buttons`** – If buttons for quick navigation between camera and x-, y-, or z-direction view should be added to the plot
- **`update_plot_callback`** – A plot update function that will be called every time the slider with simulation time is dragged in the plot windows, this can be used to dynamically apply changes to the plot, required syntax: `def update_plot(plotter:  pv.Plotter, mesh:  pv.DataSet)`

Returns
Tuple containing the `pyvista.Plotter` and the `pyvista.DataSet` mesh object

`get_result_file_path``()` → str

Returns the path to the main result file (for example a ParaView `*.pvd` file) on disk containing the complete result data set. Its directory contains also further result data that can be useful.

Tip: The Python API of ParaView can be used to extract any kind of data from the result in a programmatic way. See here for more details: https://kitware.github.io/paraview-docs/latest/python/

Returns
The path to the main result file

`class tc_python.am.`**`Automatic`**

Bases: *`FileSavingStrategy`*

An automatic saving strategy.

`get_type``()` → str

Returns the type of the file saving strategy.

Returns
The type

`set_max_number_of_files_stored``(`*max_number: int = 1000000*`)`

Sets the maximum number of files that are stored.

Default: unlimited

Parameters
`max_number` – The maximum number of files that is stored

Returns
This *`FileSavingStrategy`* object

`set_saving_interval_strategy``(`*saving_interval_strategy=AutomaticSavingIntervalStrategy.LINEAR*`)`

Sets the saving interval strategy.

Default: A linear saving interval strategy.

Parameters
`saving_interval_strategy` – The saving interval strategy

Returns
This *`FileSavingStrategy`* object

`store_unlimited_number_of_files``()`

Sets the maximum number of files that are stored to unlimited.

Returns
This *`FileSavingStrategy`* object

`class tc_python.am.`**`AutomaticSavingIntervalStrategy`**`(`*value*`)`

Bases: `Enum`

The strategy for choosing the time interval for saving files in *automatic* mode.

`EXPONENTIALLY_INCREASING = 2`

An exponentially increasing time interval

`LINEAR = 1`

A linear time interval

`class tc_python.am.`**`BiDirectionalScanningStrategy`**

Bases: *`ScanningStrategy`*

A bidirectional scanning strategy (flipping scanning direction of the heat source between alternate tracks).

`get_type``()` → str

Returns the type of scanning strategy.

Returns

The type

`set_angle``(`*angle: float = 0.0*`)`

Sets the rotation of the scanning direction between two consecutive layers.

Note: The scanning direction of the first layer is always aligned parallel to the x-axis.

Default: 0 degree

Parameters

`angle` – The angle [degree]

Returns

This *`BiDirectionalScanningStrategy`* object

`set_hatch_spacing``(`*hatch_spacing: float = 0.0*`)`

Sets the horizontal separation between two consecutive tracks.

Default: 0 m

Parameters

`hatch_spacing` – The hatch spacing [m]

Returns

This *`BiDirectionalScanningStrategy`* object

`set_lift_time``(`*lift_time: float = 0.0*`)`

Sets the lift time, i.e. the time between two tracks where the heat source is inactive.

Default: 0 s

Parameters

`lift_time` – The lift time [s]

Returns

This *`BiDirectionalScanningStrategy`* object `set_margin`(*margin: float = 0.001*)

Sets the margin.

This is the offset of the scanning path from the sides of the computational domain.

Default: 1.0e-3 [m]

Parameters
`margin` – The margin [m]

Returns
This *BiDirectionalScanningStrategy* object

`set_number_of_layers`(*number_of_layers: int = 1*)

Sets the number of layers.

Default: 1

Parameters
`number_of_layers` – The number of layers

Returns
This *BiDirectionalScanningStrategy* object

`set_powder_fill_time`(*powder_fill_time: float = 0.0*)

Sets the powder fill time.

Default: 0 s

Parameters
`powder_fill_time` – The powder fill time [s]

Returns
This *BiDirectionalScanningStrategy* object

`class tc_python.am.CoarseMesh`

Bases: *Mesh*

An initially coarse mesh.

Note: It is adaptive and will be automatically refined as required.

`class tc_python.am.ConicalHeatSource`

Bases: *HeatSource*

A conical heat source.

`get_type`() → str

Returns the type of heat source.

Returns
The type

`set_absorptivity`(*absorptivity: float = 60.0*)

Sets the absorptivity.

Default: 60%

Parameters
`absorptivity` – The absorptivity [%]

Returns
This `ConicalHeatSource` object

`set_hi`(*hi_dim: float = 0.0001*)

Sets the parameter Hi that defines the dimensions of the heat source.

Tip: See Thermo-Calc Online Help for details about this heat source model.

Default: 100.0e-6 m

Parameters
`hi_dim` – The Hi parameter [m]

Returns
This `ConicalHeatSource` object

`set_power`(*power: float = 120.0*)

Sets the power of the heat source.

Default: 120 W

Parameters
`power` – The power [W]

Returns
This `ConicalHeatSource` object

`set_re`(*re_dim: float = 0.0001*)

Sets the parameter Re that defines the dimensions of the heat source.

Tip: See Thermo-Calc Online Help for details about this heat source model.

Default: 100.0e-6 m

Parameters
`re_dim` – The Re parameter [m]

Returns
This `ConicalHeatSource` object

`set_ri`(*ri_dim: float = 6e-05*)

Sets the parameter Ri that defines the dimensions of the heat source.

Tip: See Thermo-Calc Online Help for details about this heat source model.

Default: 60.0e-6 m

Parameters
`ri_dim` – The Ri parameter [m]

Returns
This `ConicalHeatSource` object

`set_scanning_speed`(*beam_speed: float = 0.5*)

Sets the moving velocity of the heat source.

Default: 500.0e-3 m/s

Parameters
`beam_speed` – The beam speed [m/s]

Returns
This `ConicalHeatSource` object

`class tc_python.am.CustomMesh`(*minimum_element_size: float = 1e-05*, *maximum_element_size: float = 0.0001*)

Bases: `Mesh`

An initial mesh with explicitly defined dimensions.

Note: It is adaptive and will be automatically refined as required.

Parameters

- `minimum_element_size` – The minimum element size [m]
- `maximum_element_size` – The maximum element size [m]

`tc_python.am.DEFAULT_CAMERA = {'focal_point': [0.0, 0.0, 0.0], 'position': [-2, -2, 1], 'viewup': [0, 0, 1]}`

The default *pyvista* camera view.

`class tc_python.am.DoubleEllipsoidalHeatSource`

Bases: `HeatSource`

A double ellipsoidal heat source.

`get_type`() → str

Returns the type of heat source.

Returns
The type

`set_absorptivity`(*absorptivity: float = 60.0*)

Sets the absorptivity.

Default: 60%

Parameters
`absorptivity` – The absorptivity [%]

Returns
This `DoubleEllipsoidalHeatSource` object

`set_af`(*af: float = 7e-05*)

Sets the parameter Af that defines the dimensions of the heat source.

Tip: See Thermo-Calc Online Help for details about this heat source model.

Default: 70.0e-6 m

Parameters
`af` – The Af parameter [m]

Returns
This `DoubleEllipsoidalHeatSource` object

`set_ar`(*ar: float = 70.0*)

Sets the parameter Ar that defines the dimensions of the heat source.

Tip: See Thermo-Calc Online Help for details about this heat source model.

Default: 70.0e-6 m

Parameters
`ar` – The Ar parameter [m]

Returns
This *DoubleEllipsoidalHeatSource* object

`set_b`(*b: float = 8.5e-05*)

Sets the parameter B that defines the dimensions of the heat source.

Tip: See Thermo-Calc Online Help for details about this heat source model.

Default: 85.0e-6 m

Parameters
`b` – The B parameter [m]

Returns
This *DoubleEllipsoidalHeatSource* object

`set_c`(*c: float = 0.0002*)

Sets the parameter C that defines the dimensions of the heat source.

Tip: See Thermo-Calc Online Help for details about this heat source model.

Default: 200.0e-6 m

Parameters
`c` – The C parameter [m]

Returns
This *DoubleEllipsoidalHeatSource* object

`set_power`(*power: float = 120.0*)

Sets the power of the heat source.

Default: 120 W

Parameters
`power` – The power [W]

Returns
This *DoubleEllipsoidalHeatSource* object

`set_scanning_speed`(*beam_speed: float = 0.5*)

Sets the moving velocity of the heat source.

Default: 500.0e-3 m/s

Parameters
`beam_speed` – The beam speed [m/s]

Returns
This *DoubleEllipsoidalHeatSource* object

class `tc_python.am.`**`EveryNthTimeStep`**

Bases: *FileSavingStrategy*

Saving at every n-th time step.

`get_type``()` → str

Returns the type of the file saving strategy.

Returns
The type

`set_n``(`*n: int = 1*`)`

Sets at which n-th time step files are saved.

Default: 1

Parameters
n – The n-th time step where files are saved

Returns
This *FileSavingStrategy* object

class `tc_python.am.`**`EveryTimeInterval`**

Bases: *FileSavingStrategy*

Saving after regular time intervals.

`get_type``()` → str

Returns the type of the file saving strategy.

Returns
The type

`set_time_interval``(`*time_interval: float = 0.01*`)`

Sets the time interval at which files are saved.

Default: 0.01 s

Parameters
time_interval – The time interval [s]

Returns
This *FileSavingStrategy* object

class `tc_python.am.`**`FileSavingStrategy`**

Bases: `object`

The strategy for how result files are saved on disk. Both the number and time point of saving can be controlled.

classmethod automatic`()`

An automatic saving strategy. **This is the default.**

classmethod every_n_th_time_step`()`

Saving at every n-th time step.

classmethod every_time_interval`()`

Saving after regular time intervals.

class tc_python.am.**FineMesh**

Bases: *Mesh*

An initially fine mesh.

Note: It is adaptive and will be automatically refined as required.

class tc_python.am.**GaussianHeatSource**

Bases: *HeatSource*

A Gaussian heat source.

disable_keyhole_model()

Disables using a keyhole model in the simulation.

Returns
This *GaussianHeatSource* object

get_type() → str

Returns the type of heat source.

Returns
The type

set_absorptivity(*absorptivity: float = 60.0*)

Sets the absorptivity.

Default: 60%

Parameters
absorptivity – The absorptivity [%]

Returns
This *GaussianHeatSource* object

set_beam_radius(*beam_radius: float = 0.00011*)

Sets the beam radius.

Default: 110.0e-6 m

Parameters
beam_radius – The beam radius [m]

Returns
This *GaussianHeatSource* object

set_power(*power: float = 120.0*)

Sets the power of the heat source.

Default: 120 W

Parameters
power – The power [W]

Returns
This *GaussianHeatSource* object

set_scanning_speed(*beam_speed: float = 0.5*)

Sets the moving velocity of the heat source.

Default: 500.0e-3 m/s

Parameters
`beam_speed` – The beam speed [m/s]

Returns
This *GaussianHeatSource* object

`with_keyhole_model`(*config:* KeyholeModel)

Sets the keyhole model applied in the simulation.

Default: None

Parameters
`config` – The keyhole model

Returns
This *GaussianHeatSource* object

`class tc_python.am.HeatSource`

Bases: `object`

The heat source.

The heat source model has either a *Gaussian*, *double ellipsoidal* or *conical* distribution.

Default: A Gaussian heat source.

`classmethod conical()`

A conical heat source.

The default is a Gaussian heat source.

Returns
A new *ConicalHeatSource* object

`classmethod double_ellipsoidal()`

A double ellipsoidal heat source.

The default is a Gaussian heat source.

Returns
A new *DoubleEllipsoidalHeatSource* object

`classmethod gaussian()`

A Gaussian heat source.

This is the default.

Returns
A new *GaussianHeatSource* object

`classmethod get_calibrated_heatsource_names()` → List[str]

Returns a list of the names of the available calibrated heat sources.

The name can then be used with the function *get_path_of_calibrated_heatsource()*.

Returns
The list of names

`classmethod get_path_of_calibrated_heatsource`(*optimized_heatsource_name: str*) → str

Returns the file path of the calibrated heat source.

Parameters
`optimized_heatsource_name` – The name of the calibrated heat source

Returns
The file path

`class tc_python.am.`**`KeyholeModel`**

Bases: `object`

A model for an "analytic" keyhole in the AM calculation.

`set_rayleigh_length`(*rayleigh_length: float = 0.0025*)

Sets the Rayleigh length.

Default: 2.5e-3 m

Parameters
`rayleigh_length` – The Rayleigh length [m]

Returns
This *`KeyholeModel`* object

`class tc_python.am.`**`LibraryMaterialProperties`**(*library_name: str*)

Bases: *`MaterialProperties`*

Material properties previously saved on disk using the specified library name.

`class tc_python.am.`**`MaterialProperties`**

Bases: `object`

The material properties used in the AM calculation, can be either from a Scheil calculation or from a previously stored library.

`delete_library`()

Deletes the material library from disk.

`classmethod` **`from_library`**(*library_name: str*)

Uses material properties previously saved on disk using a library name.

Parameters
`library_name` – The library name

Returns
A new *`LibraryMaterialProperties`* object

`classmethod` **`from_scheil_result`**(*result:* ScheilCalculationResult)

Creates material properties from the result of a Scheil calculation.

Parameters
`result` – The Scheil result to create material properties from

Returns
A new *`ScheilMaterialProperties`* object

`classmethod` **`get_all_library_names`**() → List[str]

Returns a list with the names of all material libraries available on disk.

Returns
A list with the names of all material libraries

`get_average_material_property_in_range`(*material_property_enum:* MaterialProperty, *from_zone:* Zone, *to_zone:* Zone) → float

Returns average values for the specified material property in the specified zone interval.

Parameters

- **material_property_enum** – The material property
- **from_zone** – The lower zone boundary
- **to_zone** – The upper zone boundary

Returns
The average value for the specified material property in the specified zone interval

get_evaporation_temperature() → float

Returns the evaporation temperature for the material.

Returns
The evaporation temperature [K]

get_liquidus_temperature() → float

Returns the liquidus temperature for the material.

Returns
The liquidus temperature [K]

get_name() → str

Returns the name of the library.

Returns
The name of the library

get_smoothed_values_for_material_property(*material_property_enum:* MaterialProperty) → [List[float], List[float]]

Returns smoothed values for the specified material property.

Parameters
material_property_enum – The material property

Returns
The temperature [K] and the values of the specified material property

get_smoothing_for(*material_property_enum:* MaterialProperty) → *Smoothing*

Returns the smoothing level for the specified material property.

Parameters
material_property_enum – The material property to get smoothing level for

Returns
The smoothing level for the specified material property

get_solidification_temperature() → float

Returns the solidification temperature for the material.

Returns
The solidification temperature [K]

rename_as_library(*name: str*)

Renames the material library.

Parameters
name – The new name of the library

Returns
This `MaterialProperties` object

save_as_library(*name: str = ''*)

Saves the material library with the specified name to disk.

Default: Re-save the current object with the previously chosen name

Parameters
`name` – The new name of the library

Returns
This `MaterialProperties` object

save_library()

Saves the material library to disk.

Returns
This `MaterialProperties` object

set_smoothing_for_all_properties(*smoothing_enum: Smoothing*)

Sets the smoothing level for all material properties.

Parameters
`smoothing_enum` – The smoothing level

Returns
This `MaterialProperties` object

set_smoothing_for_property(*material_property_enum: MaterialProperty, smoothing_enum: Smoothing*)

Sets the smoothing level for the specified material property.

Parameters

- `material_property_enum` – The specified material property
- `smoothing_enum` – The smoothing level

Returns
This `MaterialProperties` object

class tc_python.am.**MaterialProperty**(*value*)

Bases: `Enum`

A single material property used in the class `MaterialProperties`.

CP = 0

Apparent heat capacity [J/(kg K)]

DENSITY = 1

Density [kg/m3]

DRIVING_FORCE_EVAPORATION = 8

Driving force for evaporation [J/mol]

DYNAMIC_VISCOSITY = 4

Dynamic viscosity [Pa s]

ENTHALPY_PER_KG = 10

Enthalpy [J/kg]

ENTHALPY_PER_MOLE = 2

Enthalpy [J/mol]

EVAPORATION_ENTHALPY = 9
: Evaporation enthalpy [J/mol]

MOLAR_MASS_OF_GAS = 7
: Molar mass of Gas [kg/mol]

MOLAR_VOLUME = 6
: Molar volume [m3/mol]

SURFACE_TENSION = 5
: Surface tension [J/m2]

THERMAL_CONDUCTIVITY = 3
: Thermal conductivity [W/(m K)]

class tc_python.am.**MaterialType**(*value*)

Bases: `Enum`

The material (solid, liquid, powder) to be plotted in a *pyvista* visualization plot.

LIQUID = 'Liquid'
: Onl liquid material

POWDER = 'Powder'
: Only powder

SHOW_ALL = 'All'
: All material

SOLID = 'Solid'
: Only solid material

SOLID_AND_LIQUID = 'Solid and liquid'
: Only solid and liquid material

SOLID_AND_POWDER = 'Solid and powder'
: Only solid material and powder

class tc_python.am.**MediumMesh**

Bases: *Mesh*

An initially medium mesh.

Note: It is adaptive and will be automatically refined as required.

class tc_python.am.**Mesh**

Bases: `object`

The initial mesh size in the simulation.

Can be coarse, medium, fine, or custom.

Note: It is adaptive and will be automatically refined as required.

classmethod coarse()

Selecting the mesh to be initially coarse.

Note: It is adaptive and will be automatically refined as required.

Returns
A new *CoarseMesh* object

classmethod custom(*minimum_element_size: float = 1e-05*, *maximum_element_size: float = 0.0001*)

Selecting explicitly the initial mesh.

Default: Minimum element size: 10 um, maximum element size: 100 um

Note: It is adaptive and will be automatically refined as required.

Parameters

- **minimum_element_size** – The minimum element size [m]
- **maximum_element_size** – The maximum element size [m]

Returns
A new *CustomMesh* object

classmethod fine()

Selecting the mesh to be initially fine.

Note: It is adaptive and will be automatically refined as required.

Returns
A new *FineMesh* object

classmethod medium()

Selecting the mesh to be initially medium.

Note: It is adaptive and will be automatically refined as required.

Returns
A new *MediumMesh* object

class tc_python.am.**NumericalOptions**

Bases: `object`

The numerical options for an AM simulation.

disable_damping()

Disable numerical damping.

Default: disabled

Returns
This *NumericalOptions* object

disable_petrov_galerkin()

Disables Streamline upwind Petrov-Galerkin (SUPG) for the numerical solver.

Default: enabled

Returns
This *NumericalOptions* object

enable_petrov_galerkin()

Enables Streamline upwind Petrov-Galerkin (SUPG) for the numerical solver.

Default: enabled

Returns
This *NumericalOptions* object

set_damping_factor(*damping_factor: float = 0.0*)

Sets the numerical damping factor.

Default: numerical damping is disabled

Parameters
damping_factor – The numerical damping factor

Returns
This *NumericalOptions* object

set_number_of_cores(*num_cores: int*)

Sets the number of used processor cores.

Default: Half of the available cores on the CPU, 2 cores on a 2-core CPU, and 1 core on a 1-core CPU.

Parameters
num_cores – The number of used cores

Returns
This *NumericalOptions* object

with_file_saving_strategy(*file_saving_strategy:* FileSavingStrategy)

Sets the strategy how result files are saved on disk. Both the number and time point of saving can be controlled.

Default: an automatic file saving strategy

Parameters
file_saving_strategy – The file saving strategy

Returns
This *NumericalOptions* object

class tc_python.am.**ProbeCoordinate**(*x: float*, *y: float*, *z: float*)

Bases: `object`

The coordinates of a probe. This is a point in the simulation domain whose properties can be obtained from the result object after the calculation using *TransientResult.get_temperatures_at_probe()*.

class tc_python.am.**Scalar**(*value*)

Bases: `Enum`

A quantity to be plotted in a *pyvista* visualization plot.

MATERIAL_TYPE = 'subdomain_id'
Material type

MOLAR_VOLUME = 'molar_volume'
Molar volume

SURFACE_TENSION = 'gamma'
Surface tension

TEMPERATURE = 'temperature'
Temperature

THERMAL_CONDUCTIVITY = 'k'
Thermal conductivity

VOLUME_FRACTION_LIQUID = 'liquid_vfrac'
Volume fraction of liquid

class `tc_python.am.`**ScanningStrategy**

Bases: `object`

The scanning pattern of the heat source.

Single track, bidirectional (flipping scanning direction of the heat source between alternate tracks), or unidirectional (same scanning direction of the heat source for all tracks) are available.

classmethod bi_directional()

A bidirectional scanning strategy (flipping scanning direction of the heat source between alternate tracks).

Returns
A new *BiDirectionalScanningStrategy* object

classmethod single_track()

A single track scanning strategy.

Returns
A new *SingleTrackScanningStrategy* object

classmethod uni_directional()

A unidirectional scanning strategy (same scanning direction of the heat source for all tracks).

Returns
A new *UniDirectionalScanningStrategy* object

class `tc_python.am.`**ScheilMaterialProperties**(*scheil_result:* ScheilCalculationResult)

Bases: *MaterialProperties*

Material properties created from the result of a Scheil calculation.

class `tc_python.am.`**SingleTrackScanningStrategy**

Bases: *ScanningStrategy*

A single track scanning strategy.

get_type() → str

Returns the type of scanning strategy.

Returns
The type

set_margin(*margin: float = 0.001*)

Sets the margin.

This is the offset of the scanning path from the sides of the computational domain. In case of single tracks, offset is placed from the sides transverse to the scanning direction.

Default: 1.0e-3 [m]

Parameters
margin – The margin [m]

Returns
This *SingleTrackScanningStrategy* object

set_number_of_layers(*number_of_layers: int = 1*)

Sets the number of layers.

Default: 1

Parameters
number_of_layers – The number of layers

Returns
This *SingleTrackScanningStrategy* object

set_powder_fill_time(*powder_fill_time: float = 0.0*)

Sets the powder fill time.

Default: 0 [s]

Parameters
powder_fill_time – [s]

Returns
This *SingleTrackScanningStrategy* object

class tc_python.am.**Smoothing**(*value*)

Bases: Enum

The smoothing level used in the class *MaterialProperties*.

CONSTANT = -200

Constant smoothing

LARGE = 600

Large smoothing

LINEAR = -100

Linear smoothing

LITTLE = 60

Little smoothing

MEDIUM = 150

Medium smoothing

NONE = 0

No smoothing

class `tc_python.am.`**`SteadyStateCalculation`**(*calculation*)

Bases: *`AdditiveManufacturingCalculation`*

A steady-state Additive Manufacturing calculation.

Note: This computes the temperature distribution in a steady-state environment, either on a bare metal substrate or with a powder layer on the top, with the possibility to add fluid flow inside the melt pool.

`calculate`(*timeout_in_minutes: float = 0.0*) → *SteadyStateResult*

Runs the calculation.

Parameters

`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a :class`UnrecoverableCalculationException` will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns

A *`SteadyStateResult`* which later can be used to get specific values from the calculated result

class `tc_python.am.`**`SteadyStateResult`**(*result*)

Bases: *`AdditiveManufacturingResult`*

A result for a steady-state calculation.

`get_heat_affected_zone_depth`() → float

Returns the depth of the heat affected zone.

Returns

The depth of the heat affected zone [m]

`get_heat_affected_zone_length`() → float

Returns the length of the heat affected zone.

Returns

The heat affected zone length [m]

`get_heat_affected_zone_width`() → float

Returns the width of the heat affected zone.

Returns

The width of the heat affected zone [m]

`get_keyhole_depth`() → float

The depth of the keyhole.

Returns

The depth of the keyhole [m]

`get_keyhole_length`() → float

The length of the keyhole.

Returns

The length of the keyhole [m]

`get_keyhole_width`() → float

The width of the keyhole.

Returns
The width of the keyhole [m]

`get_meltpool_depth()` → float

Returns the meltpool depth.

Returns
The meltpool depth [m]

`get_meltpool_length()` → float

Returns the meltpool length.

Returns
The meltpool length [m]

`get_meltpool_width()` → float

Returns the meltpool width.

Returns
The meltpool width [m]

`has_keyhole()` → bool

Returns if the result contains a keyhole.

Returns
True if the result has a keyhole

`class tc_python.am.TopBoundaryConditions`

Bases: `object`

The top boundary conditions of the simulation.

`disable_evaporation()`

Disables the evaporation heat loss due to heating of the powder layer or the metallic surface when being close to the evaporation temperature.

Default: enabled

Returns
This *TopBoundaryConditions* object

`enable_evaporation()`

Enables the evaporation heat loss due to heating of the powder layer or the metallic surface when being close to the evaporation temperature.

Default: enabled

Returns
This *TopBoundaryConditions* object

`set_convective_heat_coefficient`(*convective_heat_coefficient: float = 20.0*)

Sets the convective heat transfer coefficient for the top surface to the surrounding gas.

Enter 0 to disable convective heat transfer.

Default: 20.0 W/m**2

Parameters
`convective_heat_coefficient` – The convective heat transfer coefficient [W/m**2]

Returns
This *TopBoundaryConditions* object

`set_radiation_emissivity`(*radiation_emissivity: float = 0.8*)

Sets the radiation from the top surface to the surrounding gas.

Enter 0 to disable radiation.

Default: 0.8

Parameters
`radiation_emissivity` – The radiation emissivity, range: [0 - 1] [-]

Returns
This *`TopBoundaryConditions`* object

`class tc_python.am.`**`TransientCalculation`**(*calculation*)

Bases: *`AdditiveManufacturingCalculation`*

A transient Additive Manufacturing calculation.

Note: This computes the temperature distribution in a transient case with the given scanning strategy including multiple paths and layers and the possibility to add fluid flow inside the melt pool.

`add_probe`(*coordinate:* ProbeCoordinate)

Adds a probe, this a point in the simulation domain whose properties can be obtained from the result after the calculation using *`TransientResult.get_temperatures_at_probe()`*.

Parameters
`coordinate` – The probe to be added

Returns
This *`TransientCalculation`* object

`calculate`(*timeout_in_minutes: float = 0.0*) → *TransientResult*

Runs the calculation.

Parameters
`timeout_in_minutes` – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a `UnrecoverableCalculationException` will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

Returns
A *`TransientResult`* which later can be used to get specific values from the calculated result

`remove_all_probes`()

Removes all probes.

Returns
This *`TransientCalculation`* object

`remove_probe`(*coordinate:* ProbeCoordinate)

Removes a probe.

Parameters
`coordinate` – The coordinates of the probe to be removed

Returns
This *`TransientCalculation`* object

set_length(*length: float = 0.005*)

Sets the length of the simulation domain.

Default: 5.0e-3 m :param length: The length [m] :return: This *TransientCalculation* object

set_width(*width: float = 0.004*)

Sets the width of the simulation domain.

Default: 4.0e-3 m

Parameters
width – The width [m]

Returns
This *TransientCalculation* object

with_scanning_strategy(*scanning_strategy:* ScanningStrategy)

Sets the scanning strategy of the heat source, i.e. beam.

Parameters
scanning_strategy – The scanning strategy

Returns
This *TransientCalculation* object

class tc_python.am.**TransientResult**(*result*)

Bases: *AdditiveManufacturingResult*

A result for transient calculations (also with steady-state heat source).

get_temperatures_at_probe(*coordinate:* ProbeCoordinate) → Tuple[List[float], List[float]]

Obtains the temperature at a probe (i.e., a point in the simulation domain) that had previously been defined for the calculation using *TransientCalculation.add_probe()* or *TransientWithSteadyStateCalculation.add_probe()*.

Parameters
coordinate – The coordinates of the probe - must have been defined in the calculator previously

Returns
A tuple (time points [s], temperatures [K])

class tc_python.am.**TransientWithSteadyStateCalculation**(*transient_with_ss_calculation*, *ss_calculation*)

Bases: *AdditiveManufacturingCalculation*

A transient Additive Manufacturing calculation using a heat source from steady-state.

Note: This computes the temperature distribution in a transient case with the given scanning strategy including multiple paths and layers.

1. A steady-state simulation runs with the configured heat source and with the possibility to add fluid flow in the melt pool.
2. A volume heat source (based on the solution of steady-state calculation) is used in the transient simulation.

Tip: This type of calculation is significantly faster than fully transient calculations using *TransientCalculation*.

add_probe(*coordinate: ProbeCoordinate*)

Adds a probe, this a point in the simulation domain whose properties can be obtained from the result after the calculation using `TransientResult.get_temperatures_at_probe()`.

Parameters
coordinate – The probe to be added

Returns
This `TransientWithSteadyStateCalculation` object

calculate(*timeout_in_minutes: float = 0.0*) → *TransientResult*

Runs the calculation.

Parameters
timeout_in_minutes – Used to prevent the calculation from running longer than what is wanted, or from hanging. If the calculation runs longer than timeout_in_minutes, a `UnrecoverableCalculationException` will be thrown, the current TCPython-block will be unusable and a new TCPython block must be created for further calculations.

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

disable_fluid_flow_marangoni()

Disables the fluid flow modelling of the Marangoni effect.

Default: Enabled

Returns
This `TransientWithSteadyStateCalculation` object

disable_separate_materials()

Disables separate material properties for powder and solid material.

Default: Disabled

Returns
This `TransientWithSteadyStateCalculation` object

enable_fluid_flow_marangoni()

Enables the fluid flow modelling of the Marangoni effect.

Default: Enabled

Note: This option is not possible to use in conjunction with the option *separate material*, which is therefore automatically disabled.

Returns
This `TransientWithSteadyStateCalculation` object

enable_separate_materials()

Enables separate material properties for powder and solid material.

Default: Disabled

Note: This option is not possible to use in conjunction with the option *Marangoni fluid flow*, which is therefore automatically disabled.

Returns
This *TransientWithSteadyStateCalculation* object

remove_all_probes()

Removes all probes.

Returns
This *TransientWithSteadyStateCalculation* object

remove_probe(*coordinate:* ProbeCoordinate)

Removes a probe.

Parameters
coordinate – The coordinates of the probe to be removed

Returns
This *TransientWithSteadyStateCalculation* object

set_ambient_temperature(*temperature: float = 296.15*)

Sets the ambient temperature.

Default: 23 degree Celsius

Parameters
temperature – The ambient temperature [K]

Returns
This *TransientWithSteadyStateCalculation* object

set_base_plate_temperature(*temperature: float = 303.15*)

Sets the baseplate temperature.

Default: 30 degree Celsius

Parameters
temperature – The baseplate temperature [K]

Returns
This *TransientWithSteadyStateCalculation* object

set_gas_pressure(*pressure: float = 100000.0*)

Sets the gas pressure.

Default: 1.0e5 Pa

Parameters
pressure – The pressure [Pa]

Returns
This *TransientWithSteadyStateCalculation* object

set_height(*height: float = 0.002*)

Sets the height of the simulation domain.

Default: 2.0e-3 m

Parameters
height – The height [m]

Returns
This *TransientWithSteadyStateCalculation* object

set_layer_thickness(*layer_thickness: float = 4e-05*)

Sets the layer thickness.

Default: 40.0e-6 m

Parameters
`layer_thickness` – The layer thickness [m]

Returns
This *TransientWithSteadyStateCalculation* object

set_length(*length: float = 0.005*)

Sets the length of the simulation domain.

Default: 5.0e-3 m :param length: The length [m] :return: This *TransientWithSteadyStateCalculation* object

set_powder_density(*powder_density: float = 80.0*)

Sets the powder density.

Default: 80.0%

Parameters
`powder_density` – The powder density [%]

Returns
This *TransientWithSteadyStateCalculation* object

set_width(*width: float = 0.004*)

Sets the width of the simulation domain.

Default: 4.0e-3 m

Parameters
`width` – The width [m]

Returns
This *TransientWithSteadyStateCalculation* object

with_heat_source(*heat_source:* HeatSource)

Sets the heat source.

Parameters
`heat_source` – The heat source

Returns
This *TransientWithSteadyStateCalculation* object

with_material_properties(*material_properties:* MaterialProperties)

Sets the material properties.

Tip: Material properties can be defined like this: `MaterialProperties.from_library("IN718")` or `MaterialProperties.from_scheil_result(scheil_result)`.

Parameters
`material_properties` – The material properties

Returns
This *TransientWithSteadyStateCalculation* object

with_mesh(*mesh:* Mesh)

Sets the mesh.

Parameters
`mesh` – The mesh

Returns
This *TransientWithSteadyStateCalculation* object

with_numerical_options(*numerical_options:* NumericalOptions)

Sets the numerical options.

Parameters
`numerical_options` – The numerical options

Returns
This *TransientWithSteadyStateCalculation* object

with_scanning_strategy(*scanning_strategy:* ScanningStrategy)

Sets the scanning strategy of the heat source, i.e. beam.

Parameters
`scanning_strategy` – The scanning strategy

Returns
This *TransientWithSteadyStateCalculation* object

with_top_boundary_conditions(*boundary_conditions:* TopBoundaryConditions)

Sets the boundary conditions.

Parameters
`boundary_conditions` – The boundary conditions

Returns
This *TransientWithSteadyStateCalculation* object

class tc_python.am.**UniDirectionalScanningStrategy**

Bases: *ScanningStrategy*

A unidirectional scanning strategy (same scanning direction of the heat source for all tracks).

get_type() → str

Returns the type of scanning strategy.

Returns
The type

set_angle(*angle: float = 0.0*)

Sets the rotation of the scanning direction between two consecutive layers.

Note: The scanning direction of the first layer is always aligned parallel to the x-axis.

Default: 0 degree

Parameters
`angle` – The angle [degree]

Returns
This *UniDirectionalScanningStrategy* object

`set_hatch_spacing`(*hatch_spacing: float = 0.0*)

Sets the horizontal separation between two consecutive tracks.

Default: 0 m

Parameters
`hatch_spacing` – The hatch spacing [m]

Returns
This *UniDirectionalScanningStrategy* object

`set_lift_time`(*lift_time: float = 0.0*)

Sets the lift time, i.e. the time between two tracks where the heat source is inactive.

Default: 0 s

Parameters
`lift_time` – The lift time [s]

Returns
This *UniDirectionalScanningStrategy* object

`set_margin`(*margin: float = 0.001*)

Sets the margin.

This is the offset of the scanning path from the sides of the computational domain.

Default: 1.0e-3 [m]

Parameters
`margin` – The margin [m]

Returns
This *UniDirectionalScanningStrategy* object

`set_number_of_layers`(*number_of_layers: int = 1*)

Sets the number of layers.

Default: 1

Parameters
`number_of_layers` – The number of layers

Returns
This *UniDirectionalScanningStrategy* object

`set_powder_fill_time`(*powder_fill_time: float = 0.0*)

Sets the powder fill time.

Default: 0 s

Parameters
`powder_fill_time` – The powder fill time [s]

Returns
This *UniDirectionalScanningStrategy* object

`class tc_python.am.Zone`(*value*)

Bases: `Enum`

Zones to be used in combination with keyhole model and material properties.

`LIQUID = 2`

Liquid zone

`MUSHY = 1`

Mushy zone

`SOLID = 0`

Solid zone

`VAPOR = 3`

Vapor zone

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 System-Builder is that the operations are performed on all the previously selected databases. The system is then used to create calculations.

`create_and_select_species`(*stoichiometry: str*)

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. The created species will also be automatically selected.

Note: The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis *"()"* nor an underscore *"_"* is allowed in the chemical formula, while the special combination *"/-"* or *"/+"* can be used. Consult the Thermo-Calc database documentation for details about the syntax.

Parameters

`stoichiometry` – The stoichiometry of the species

Returns

This *`MultiDatabaseSystemBuilder`* object

`deselect_constituent_on_sublattice`(*phase_name: str*, *sublattice_no: int*, *constituent_name_to_deselect: str*)

Rejects a constituent on a sublattice in a phase in both the thermodynamic and the kinetic database.

Parameters

- **`phase_name`** – The name of the phase
- **`sublattice_no`** – The number of the sublattice (starting with 1)
- **`constituent_name_to_deselect`** – The name of the constituent to deselect

Returns

This *`MultiDatabaseSystemBuilder`* object

`deselect_phase`(*phase_name_to_deselect: str*)

Rejects a phase for both the thermodynamic and the kinetic database.

Parameters

`phase_name_to_deselect` – The phase name

Returns
This `MultiDatabaseSystemBuilder` object

`deselect_species`(*species_name: str*)

Removes the species from the system.

Parameters
`species_name` – The species

Returns
This `MultiDatabaseSystemBuilder` object

`get_system`() → *System*

Creates a new System object that is the basis for all calculation types. Several calculation types can be defined later from the object; these are independent.

Returns
A new `System` object

`select_constituent_on_sublattice`(*phase_name: str*, *sublattice_no: int*, *constituent_name_to_select: str*)

Selects a constituent on a sublattice in a phase in both the thermodynamic and the kinetic database.

Note: Previously the third parameter *constituent_name_to_select* had a wrong name, it has been corrected in version 2021b.

Parameters

- `phase_name` – The name of the phase
- `sublattice_no` – The number of the sublattice (starting with 1)
- `constituent_name_to_select` – The name of the constituent to select

Returns
This `MultiDatabaseSystemBuilder` object

`select_phase`(*phase_name_to_select: str*)

Selects a phase for both the thermodynamic and the kinetic database.

Parameters
`phase_name_to_select` – The phase name

Returns
This `MultiDatabaseSystemBuilder` object

`select_species`(*species_name: str*)

Adds the species to the system. Up to 1000 species can be defined in a single system.

Parameters
`species_name` – The species

Returns
This `MultiDatabaseSystemBuilder` object

`with_new_composition_set`(*composition_set:* CompositionSet)

Used to enter two or more composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.

The databases often create the typical composition sets for phases automatically when data are retrieved. The equilibrium calculations (using the default settings with global minimization) will usually add new composition sets if needed.

Note: Precipitation and diffusion calculations can require the user to define additional composition sets. E.g. in the case where the new composition set is needed in the configuration of the calculation.

Parameters
`composition_set` – the composition set

Returns
This *MultiDatabaseSystemBuilder* object

without_default_phases()

Rejects all the default phases from both the thermodynamic and the kinetic database, any phase now needs to be selected manually for the databases.

Returns
This *MultiDatabaseSystemBuilder* object

class tc_python.system.**System**(*system_instance*)

Bases: `object`

A system containing selections for databases, elements, phases etc.

Note: For the defined system, different calculations can be configured and run. **Instances of this class should always be created from a SystemBuilder**.

Note: The system object is **immutable**, i.e. it cannot be changed after 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:* ConversionUnit, *output_unit:* ConversionUnit, *dependent_component: str = ''*) → Dict[str, float]

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

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 (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*`)` → *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_phase_object(`*phase_name: str*`)` → *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_references()` → Dict[str, List[str]]

Provides a dictionary with database references per database in the selected system.

Returns
The database references

`get_species_in_system()` → List[str]

Returns the names of all species present in the selected system.

Note: The list does not contain any species 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
The list of species names

`get_species_object`(*species_name: str*) → *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

`get_system_data()` → *SystemData*

Returns the content of the database. This can be used to modify the parameters and functions and to change the current system by using `with_system_modifications()`.

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

Returns
The system data

`with_batch_equilibrium_calculation`(*default_conditions: bool = True*, *components: List[str] = []*) → *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()` → *PrecipitationCCTCalculation*

Creates a CCT diagram calculation.

Returns
A new `PrecipitationCCTCalculation` object

`with_isothermal_diffusion_calculation()` → *DiffusionIsoThermalCalculation*

Creates an isothermal diffusion calculation.

Returns
A new `DiffusionIsoThermalCalculation` object

`with_isothermal_precipitation_calculation()` → *PrecipitationIsoThermalCalculation*

Creates an isothermal precipitation calculation.

Returns
A new `PrecipitationIsoThermalCalculation` object

`with_material_to_material()` → *MaterialToMaterialCalculationContainer*

Provides access to all Material to Material calculations. The actual calculation needs to be chosen in the returned object.

Returns
A new `MaterialToMaterialCalculationContainer` object

`with_non_isothermal_diffusion_calculation()` → *DiffusionNonIsoThermalCalculation*

Creates a non-isothermal precipitation calculation.

Returns
A new `PrecipitationNonIsoThermalCalculation` object

`with_non_isothermal_precipitation_calculation()` → *PrecipitationNonIsoThermalCalculation*

Creates a non-isothermal precipitation calculation.

Returns
A new `PrecipitationNonIsoThermalCalculation` object

`with_phase_diagram_calculation`(*default_conditions: bool = True*, *components: List[str] = []*) → *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] = []*) → *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 = ''*, *debug_model: bool = False*) → *PropertyModelCalculation*

Creates a Property Model calculation.

The parameter *debug_model* is only used when debugging self-developed models.

Parameters

- **model** – The Property Model to be calculated.
- **path_to_models** – The path where the Property Models are installed. If no value is entered, the Property Models folder used by the normal Thermo-Calc application is used.
- **debug_model** – Used when debugging self-developed models.

Returns
A new `PropertyModelCalculation` object

with_scheil_calculation() → *ScheilCalculation*

Creates a Scheil solidification calculation.

Returns
A new `ScheilCalculation` object

with_single_equilibrium_calculation(*default_conditions: bool = True*, *components: List[str] = []*) → *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() → *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.

create_and_select_species(*stoichiometry: str*)

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. The created species will also be automatically selected.

Note: The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis *"()"* nor an underscore *"_"* is allowed in the chemical formula, while the special combination *"/-"* or *"/+"* can be used. Consult the Thermo-Calc database documentation for details about the syntax.

Parameters
`stoichiometry` – The stoichiometry of the species

Returns
This *SystemBuilder* object

`deselect_constituent_on_sublattice`(*phase_name: str*, *sublattice_no: int*, *constituent_name_to_deselect: str*)

Rejects a constituent on a sublattice in a phase in the last specified database only.

Parameters

- `phase_name` – The name of the phase
- `sublattice_no` – The number of the sublattice (starting with 1)
- `constituent_name_to_deselect` – The name of the constituent to deselect

Returns
This *SystemBuilder* object

`deselect_phase`(*phase_name_to_deselect: str*)

Rejects a phase in the last specified database only.

Parameters
`phase_name_to_deselect` – The name of the phase

Returns
This *SystemBuilder* object

`deselect_species`(*stoichiometry: str*)

Removes the species from the system.

Parameters
`stoichiometry` – The species

Returns
This *SystemBuilder* object

`get_system`() → *System*

Creates a new System object that is the basis for all calculation types. Several calculation types can be defined later from the object; these are independent.

Returns
A new *System* object

`select_constituent_on_sublattice`(*phase_name: str*, *sublattice_no: int*, *constituent_name_to_select: str*)

Selects a constituent on a sublattice in a phase in the last specified database only.

Note: Previously the third parameter *constituent_name_to_select* had a wrong name, it has been corrected in version 2021b.

Parameters

- **phase_name** – The name of the phase
- **sublattice_no** – The number of the sublattice (starting with 1)
- **constituent_name_to_select** – The name of the constituent to select

Returns
This `SystemBuilder` object

`select_database_and_elements`(*database_name: str*, *list_of_element_strings: List[str]*)

Selects a thermodynamic or kinetic database and its selected elements (that will be appended). After that, phases can be selected or unselected.

Parameters

- **database_name** – The database name, for example "FEDEMO"
- **list_of_element_strings** – A list of one or more elements as strings, for example ["Fe", "C"]

Returns
This `SystemBuilder` object

`select_phase`(*phase_name_to_select: str*)

Selects a phase in the last specified database only.

Parameters
phase_name_to_select – The name of the phase

Returns
This `SystemBuilder` object

`select_species`(*stoichiometry: str*)

Adds the species to the system. Up to 1000 species can be defined in a single system.

Parameters
stoichiometry – The species

Returns
This `SystemBuilder` object

`select_user_database_and_elements`(*path_to_user_database: str*, *list_of_element_strings: List[str]*)

Selects a thermodynamic database which is a user-defined database and select its elements (that will be appended).

Note: By using a r-literal, it is possible to use slashes on all platforms, also on Windows: *select_user_database_and_elements(r"my path/user_db.tdb", ["Fe", "Cr"]])*

Otherwise it is required to use **double** back-slashes on Windows as separator.

Note: On Linux and Mac the path is case-sensitive, also the file ending.

Parameters

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

- **`list_of_element_strings`** – A list of one or more elements as strings, for example [“Fe”, “C”]

Returns
This *`SystemBuilder`* object

`with_new_composition_set`(*composition_set:* CompositionSet)

Used to enter composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.

Parameters
`composition_set` – The composition set

Returns
This *`SystemBuilder`* object

`without_default_phases`()

Rejects all default phases in the last specified database only, any phase needs now to be selected manually for that database.

Returns
This *`SystemBuilder`* object

5.3 Module “entities”

class tc_python.entities.**CompositionSet**(*phase_name: str*)

Bases: `object`

Used by the method *`tc_python.system.SystemBuilder.with_new_composition_set()`* to enter two or more composition sets for a phase.

Parameters
`phase_name` – The name of the phase for which a new composition set is required

`set_major_constituents_for_sublattice`(*sublattice_index: int*, *major_constituents: List[str]*)

Specify the new major constituent(s) for the sublattice.

Default: If not specified, a default is automatically chosen based on the specified composition set.

Note: This is useful in order to make calculations converge faster and more easily (because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set). **The databases often set major constituents for several phases automatically when the data is retrieved.**

Parameters

- **`sublattice_index`** – Index of the sublattice to set the major constituents for (starting with *1*)
- **`major_constituents`** – Optional list of the major constituents, which must be selected from the phase constitution of the current system.

Returns
This *`CompositionSet`* object

class `tc_python.entities.`**`Element`**(*element*)

Bases: `object`

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

`get_enthalpy``()` → float

Returns the enthalpy of the element at 298 K, part of the stable element reference state (SER).

Returns
The enthalpy [J]

`get_entropy_diff_0_to_298k``()` → float

Returns the entropy difference 0 - 298 K of the element, part of the stable element reference state (SER).

Returns
The entropy difference 0 - 298 K [J/K]

`get_molar_mass``()` → float

Returns the molar mass of the element.

Returns
The molar mass [g/mol]

`get_name``()` → str

Returns the name of the element.

Returns
The element name

`get_stable_element_reference``()` → str

Returns the stable element reference (i.e. the stable phase at 298.15 K and 1 bar, reference for all element thermodynamic data).

Returns
The name of the stable element reference

`is_interstitial``()` → bool

Returns if the element is interstitial.

Note: In the diffusion simulations (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes.

Returns
If the element is interstitial

`is_special``()` → bool

Returns if the element is special (i.e. vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase)).

Returns
If the element is special

`is_valid``()` → bool

Returns if the element is valid. Non-valid elements are represented by an empty name.

Returns
If the element is valid

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[*Species*]

Returns the species of the phase.

Returns
A set containing the species

`get_species_for_composition_profile``()` → Set[*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[*Sublattice*]

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

Returns
A list containing the `Sublattice` objects

`get_type``()` → *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`(*value*)

Bases: `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 a species, making detailed information about the species accessible.

`get_all_elements()` → List[Tuple[*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()` → *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[*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.`**`AdditiveManufacturingCalculations`**(*additive_manufacturing_calculations*)

Bases: `object`

Provides access to the calculation objects for all Additive Manufacturing calculations.

`with_steady_state_calculation`(*moose_commands: Optional[Dict[str, str]] = None*) → *SteadyStateCalculation*

Creates a steady-state calculation for Additive Manufacturing.

Note: This computes the temperature distribution in a steady-state environment, either on a bare metal substrate or with a powder layer on the top, with the possibility to add fluid flow inside the melt pool.

Warning: It should not be necessary for most users to send commands directly to the FEM-solver, try to use the corresponding method implemented in the API instead.

Parameters
`moose_commands` – Additional commands (key-value pairs) directly sent to the FEM solver - this is a special option that is normally not needed

Returns
A new `SteadyStateCalculation` object

`with_transient_calculation`(*moose_commands: Optional[Dict[str, str]] = None*) → *TransientCalculation*

Creates a transient calculation for Additive Manufacturing.

Note: This computes the temperature distribution in a transient case with the given scanning strategy including multiple paths and layers and the possibility to add fluid flow inside the melt pool.

Warning: It should not be necessary for most users to send commands directly to the FEM-solver, try to use the corresponding method implemented in the API instead.

Parameters
`moose_commands` – Additional commands (key-value pairs) directly sent to the FEM solver - this is a special option that is normally not needed

Returns
A new `TransientCalculation` object

`with_transient_with_steady_state_calculation`(*moose_commands: Optional[Dict[str, str]] = None*) → *TransientWithSteadyStateCalculation*

Creates a transient calculation (with steady-state heat source) for Additive Manufacturing.

Note: This computes the temperature distribution in a transient case with the given scanning strategy including multiple paths and layers.

1. A steady-state simulation runs with the configured heat source and with the possibility to add fluid flow in the melt pool.
2. A volume heat source (based on the solution of steady-state calculation) is used in the transient simulation.

Tip: This type of calculation is significantly faster than fully transient calculations using `TransientCalculation`.

Warning: It should not be necessary for most users to send commands directly to the FEM-solver, try to use the corresponding method implemented in the API instead.

Parameters
`moose_commands` – Additional commands (key-value pairs) directly sent to the FEM solver - this is a special option that is normally not needed

Returns
A new `TransientWithSteadyStateCalculation` object

`class tc_python.server.`**`LoggingPolicy`**`(`*value*`)`

Bases: `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.`**`MetallurgyCalculations`**`(`*metallurgy_calculations*`)`

Bases: `object`

Provides access to the calculation objects for all Process Metallurgy calculations.

These are specialised calculations for working with metallurgical processes. Both equilibrium calculations and kinetic process simulations (Effective Equilibrium Reaction Zone model) are available.

`with_adiabatic_equilibrium_calculation``(`*database:* ProcessDatabase`)` → *AdiabaticEquilibriumCalculation*

Creates an adiabatic equilibrium calculation for Process Metallurgy.

Parameters
`database` – The thermodynamic database used in the calculation

Returns
A new `AdiabaticEquilibriumCalculation` object

`with_adiabatic_process_calculation``(`*database:* ProcessDatabase`)` → *ProcessSimulationCalculation*

Creates an adiabatic kinetic process simulation (EERZ, i.e. Effective Equilibrium Reaction Zone model).

Parameters
`database` – The thermodynamic database used in the calculation

Returns
A new `ProcessSimulationCalculation` object

`with_isothermal_equilibrium_calculation`(*database:* ProcessDatabase) → *IsoThermalEquilibriumCalculation*

Creates an isothermal equilibrium calculation for Process Metallurgy.

Parameters
`database` – The thermodynamic database used in the calculation

Returns
A new `IsoThermalEquilibriumCalculation` object

`class tc_python.server.ResultLoader`(*result_loader*)

Bases: `object`

Contains methods for loading results from previously done calculations.

`diffusion`(*path: str*) → *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*) → *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*) → *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*) → *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*) → *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*) → *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*) → *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*) → *SingleEquilibriumResult*

Loads a `SingleEquilibriumResult` from disc.

Parameters
path – path to the folder where result was previously saved.

Returns
A new `SingleEquilibriumResult` object which later can be used to get specific values from the calculated result

class tc_python.server.**SetUp**(*debug_logging=False*)

Bases: `object`

Starting point for all calculations.

Note: This class exposes methods that have no precondition, it is used for choosing databases and elements.

disable_caching()

A previously set cache folder is no longer used.

Note: Within the session, caching is activated and used through the default temporary directory.

Returns
This *SetUp* object

`get_database_info`(*database_short_name: str*) → 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 are 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`() → *ResultLoader*

Loads a previously calculated result from disk.

Note: This **only** works for results created by calling one of the `save_result()` methods on a *Result* class created from a calculation.

Returns
: A new `ResultLoader` object

`select_database_and_elements`(*database_name: str*, *list_of_elements: List[str]*) → *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]*) → *MultiDatabaseSystemBuilder*

Selects the thermodynamic and kinetic database at once, guarantees that the databases are added in the correct order. Further rejection or selection of phases applies to both databases.

Parameters

- **thermodynamic_db_name** – The thermodynamic database name, for example "FEDEMO"
- **kinetic_db_name** – The kinetic database name, for example "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]*) → *SystemBuilder*

Selects a user-defined database and selects the elements in it.

Note: By using a r-literal, it is possible to use slashes on all platforms, also on Windows: *select_user_database_and_elements(r"my path/user_db.tdb", ["Fe", "Cr"]])*

Otherwise it is required to use **double** back-slashes on Windows as separator.

Note: On Linux and Mac the path is case-sensitive, also the file ending.

Parameters

- **path_to_user_database** – The path to the database file ("database".TDB), defaults to the current working directory. Only filename is required if the database is located in the same folder as the script.
- **list_of_elements** – The list of the selected elements in that database, for example ["Fe", "C"]

Returns
A new `SystemBuilder` object

set_cache_folder(*path: str = ''*, *precision_for_floats: int = 12*)

Sets a folder where results from calculations and state of systems are saved. If at any time a calculation is run which has the exact same setting as a previous, the calculation is not re-run. The result is instead loaded from this folder.

Note: The same folder can be used in several scripts, and it can even be shared between different users. It can be a network folder.

Parameters

- **path** – path to the folder where results should be stored. It can be relative or absolute.
- **precision_for_floats** – The number of significant figures used when comparing if the calculation has the same setting as a previous.

Returns
This *SetUp* object

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

with_additive_manufacturing() → *AdditiveManufacturingCalculations*

Provides access to the calculation objects for all Additive Manufacturing calculations.

with_metallurgy() → *MetallurgyCalculations*

Provides access to the calculation objects for all Process Metallurgy calculations.

These are specialised calculations for working with metallurgical processes. Both equilibrium calculations and kinetic process simulations (Effective Equilibrium Reaction Zone model) are available.

class tc_python.server.**TCPython**(*logging_policy=LoggingPolicy.SCREEN*, *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:

```python
with TCPython() as session:
    session.select_database_and_elements(...)
```

Note: Each usage of *with TCPython()* causes significant overhead (starting a new process, stopping the old one, cleaning up the temporary disk space). Usually it is recommendable to call *with TCPython()* only once for each process, even if working in a loop. Instead you should pass the session or calculator object into the loop and use them there.

If necessary, beginning from version 2019a it is however possible to call *with TCPython* safely multiple times.

`tc_python.server.`**`start_api_server`**`(`*logging_policy=LoggingPolicy.SCREEN*, *log_file=None*, *debug_mode=False*, *is_unittest=False*, *do_throw_on_backend_hard_crash=True*, *port_number=0*`)`

Starts a process of the API server and sets up the socket communication with it.

Parameters

- **`logging_policy`** – Determines if the TC-Python log output is sent to the screen (*LoggingPolicy.SCREEN*), to file (*LoggingPolicy.FILE*) or nothing is logged at all (*LoggingPolicy.NONE*) **Default**: *LoggingPolicy.SCREEN*. Note that the log-handlers can also be adapted through the *tc_python.LOGGER* object at any time.
- **`log_file`** – The log-file relative to the current path or absolute, only relevant if *logging_policy=LoggingPolicy.FILE*. Log-output will be appended.
- **`debug_mode`** – If *True* it is tried to open a connection to an already running API-server. **This is only used for debugging the API itself**.
- **`is_unittest`** – Should be True if called by a unit test, **only to be used internally for development**.
- **`do_throw_on_backend_hard_crash`** – If *True* an *UnrecoverableCalculationException* will be thrown if the Java-backend crashes hard, if *False* the application will simply crash with a FORTRAN-stacktrace. *If `True` the exception can be caught outside of the `with`-clause and the application can continue, if `False` more information about the error is shown by the stacktrace..*
- **`port_number`** – The port number for the communication with the Java-backend server. **This is not required to be changed by normal users.**

Warning: Most users should use `TCPython` using a with-statement for automatic management of the resources (network sockets and temporary files). If you anyway need to use that method, make sure to call `stop_api_server()` **in any case using the try-finally-pattern**.

`tc_python.server.`**`start_matlab_server`**`(`*logging_policy=LoggingPolicy.SCREEN*, *log_file=None*, *debug_mode=False*, *is_unittest=False*, *do_throw_on_backend_hard_crash=True*, *port_number=0*`)`

`tc_python.server.`**`stop_api_server`**`(`*gateway_id: Optional[str] = None*`)`

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: `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*) → ActivityOfComponent

Creates a quantity representing the activity of a component.

Parameters

- **component** – The name of the component, use *ALL_COMPONENTS* to choose all components
- **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state is be used if this setting is set to *False*.

Returns

A new `ActivityOfComponent` object.

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

Creates a quantity representing the chemical diffusion coefficient of a phase [m^2/s].

Parameters

- **phase** – The name of the phase
- **diffusing_element** – The diffusing element
- **gradient_element** – The gradient element
- **reference_element** – The reference element (for example "Fe" in a steel)

Returns

A new `ChemicalDiffusionCoefficient` object.

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

Creates a quantity representing the chemical potential of a component [J].

Parameters

- **component** – The name of the component, use *ALL_COMPONENTS* to choose all components
- **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state is used if this setting is set to *False*.

Returns

A new `ChemicalPotentialOfComponent` object.

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

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*) → IntrinsicDiffusionCoefficient

Creates a quantity representing the intrinsic diffusion coefficient of a phase [m^2/s].

Parameters

- `phase` – The name of the phase
- `diffusing_element` – The diffusing element
- `gradient_element` – The gradient element
- `reference_element` – The reference element (for example "Fe" in a steel)

Returns
A new `IntrinsicDiffusionCoefficient` object.

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

Creates a quantity representing L" of a phase [m^2/s].

Parameters

- `phase` – The name of the phase
- `diffusing_element` – The diffusing element
- `gradient_element` – The gradient element
- `reference_element` – The reference element (for example "Fe" in a steel)

Returns
A new `Lbis` object.

`classmethod mass_fraction_of_a_component`(*component: str*) → MassFractionOfAComponent

Creates a quantity representing the mass fraction of a component.

Parameters
`component` – The name of the component or *ALL_COMPONENTS* to choose all components

Returns
A new `MassFractionOfAComponent` object.

`classmethod mass_fraction_of_a_phase`(*phase: str*) → MassFractionOfAPhase

Creates a quantity representing the mass fraction of a phase.

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

Returns
A new `MassFractionOfAPhase` object.

`classmethod mobility_of_component_in_phase`(*phase: str*, *component: str*) → MobilityOfComponentInPhase

Creates a quantity representing the mobility of a component in a phase [m^2/Js].

Parameters

- `phase` – The name of the phase
- `component` – The name of the component

Returns
A new `MobilityOfComponentInPhase` object.

classmethod mole_fraction_of_a_component(*component: str*) → MoleFractionOfAComponent

Creates a quantity representing the mole fraction of a component.

Parameters
component – The name of the component or *ALL_COMPONENTS* to choose all components

Returns
A new `MoleFractionOfAComponent` object.

classmethod mole_fraction_of_a_phase(*phase: str*) → MoleFractionOfAPhase

Creates a quantity representing the mole fraction of a phase.

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

Returns
A new `MoleFractionOfAPhase` object.

classmethod position_of_lower_boundary_of_region(*region: str*) → PositionOfLowerBoundaryOfRegion

Creates a quantity representing the position of lower boundary of a region [m].

Parameters
region – The name of the region

Returns
A new `PositionOfLowerBoundaryOfRegion` object.

classmethod position_of_upper_boundary_of_region(*region: str*) → PositionOfUpperBoundaryOfRegion

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() → 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*) → ThermoDynamicFactor

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() → Time

Creates a quantity representing the time [s].

classmethod total_mass_fraction_of_component(*component: str*) → TotalMassFractionOfComponent

Creates a quantity representing the total mass fraction of a component.

Parameters
`component` – The name of the component

Returns
A new `TotalMassFractionOfComponent` object.

classmethod total_mass_fraction_of_component_in_phase(*phase: str*, *component: str*) → TotalMassFractionOfComponentInPhase

Creates a quantity representing the total mass fraction of a component in a phase.

Parameters

- `phase` – The name of the phase
- `component` – The name of the component

Returns
A new `TotalMassFractionOfComponentInPhase` object.

classmethod total_mass_fraction_of_phase(*phase: str*) → TotalMassFractionOfPhase

Creates a quantity representing the total mass fraction of a phase.

Parameters
`phase` – The name of the phase.

Returns
A new `TotalMassFractionOfPhase` object.

classmethod total_mole_fraction_of_component(*component: str*) → TotalMoleFractionOfComponent

Creates a quantity representing the total mole fraction of a component.

Parameters
`component` – The name of the component

Returns
A new `TotalMoleFractionOfComponent` object.

classmethod total_mole_fraction_of_component_in_phase(*phase: str*, *component: str*) → TotalMoleFractionOfComponentInPhase

Creates a quantity representing the total mole fraction of a component in a phase.

Parameters

- `phase` – The name of the phase
- `component` – The name of the component

Returns
A new `TotalMoleFractionOfComponentInPhase` object.

classmethod total_volume_fraction_of_phase(*phase: str*) → TotalVolumeFractionOfPhase

Creates a quantity representing the total volume fraction of a phase.

Parameters
`phase` – The name of the phase.

Returns
A new `TotalVolumeFractionOfPhase` object.

classmethod tracer_diffusion_coefficient(*phase: str*, *diffusing_element: str*) → TracerDiffusionCoefficient

Creates a quantity representing tracer diffusion coefficient of a phase [m^2/s].

Parameters

- **phase** – The name of the phase
- **diffusing_element** – The diffusing element

Returns
A new `TracerDiffusionCoefficient` object.

classmethod u_fraction_of_a_component(*component: str*) → UFractionOfAComponent

Creates a quantity representing the u-fraction of a component.

Parameters
component – The name of the component

Returns
A new `UFractionOfAComponent` object.

classmethod user_defined_function(*expression: str*) → Function

Creates a quantity representing a user-defined function.

Parameters
expression – The function expression

Returns
A new `Function` object

classmethod velocity_of_lower_boundary_of_region(*region: str*) → VelocityOfLowerBoundaryOfRegion

Creates a quantity representing the velocity of lower boundary of a region [m/s].

Parameters
region – The name of the region

Returns
A new `VelocityOfLowerBoundaryOfRegion` object.

classmethod velocity_of_upper_boundary_of_region(*region: str*) → VelocityOfUpperBoundaryOfRegion

Creates a quantity representing the velocity of upper boundary of a region [m/s].

Parameters
region – The name of the region

Returns
A new `VelocityOfUpperBoundaryOfRegion` object.

classmethod width_of_region(*region: str*) → Function

Creates a quantity representing the width of a region [m].

Parameters
region – The name of the region

Returns
A new `WidthOfRegion` object.

`class tc_python.quantity_factory.`**`IndependentVariable`**

Bases: `AbstractQuantity`

Factory class providing quantities used for defining the independent variable in general diffusion result querying.

`classmethod` **`distance`**(*region: str = 'All'*) → Distance

Creates an independent variable representing the distance [m].

Returns
A new *Distance* object

`classmethod` **`time`**() → Time

Creates an independent variable representing the time [s].

Returns
A new *Time* object

`class tc_python.quantity_factory.`**`PlotCondition`**

Bases: `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'*) → DistanceCondition

Creates a plot condition representing the distance [m].

Change in version 2019b: Mandatory parameter *distancepoint* added

Parameters

- **`distancepoint`** – The distance from the lower interface of the region
- **`region`** – The name of the region or *All* to choose global.

Returns
A new *DistanceCondition* object

`classmethod` **`integral`**() → IntegralCondition

Creates an integral plot condition.

Returns
A new *IntegralCondition* object

`classmethod` **`interface`**(*region: str*, *interface_position:* InterfacePosition) → InterfaceCondition

Creates a plot condition representing an interface between two regions.

Parameters

- **`region`** – The name of the region used for defining the interface
- **`interface_position`** – The position of the interface relative to that region (lower or upper)

Returns
A new *InterfaceCondition* object

classmethod time(*timepoint: Union[float, str] = 'Last'*) → TimeCondition

Creates a plot condition representing the time [s].

Change in version 2019b: Lists of timepoints are no longer supported

Parameters
`timepoint` – The timepoint. Optionally “Last” can be used for the end of the simulation

Returns
A new *TimeCondition* object

class tc_python.quantity_factory.**ScheilQuantity**

Bases: `AbstractQuantity`

Factory class providing quantities used for defining a Scheil calculation result (*tc_python.scheil.ScheilCalculationResult*).

classmethod apparent_heat_capacity_per_gram() → ApparentHeatCapacityPerGram

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

Returns
A new `ApparentHeatCapacityPerGram` object.

classmethod apparent_heat_capacity_per_mole() → ApparentHeatCapacityPerMole

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

Returns
A new `ApparentHeatCapacityPerMole` object.

classmethod apparent_volumetric_thermal_expansion_coefficient() → ApparentVolumetricThermalExpansionCoeffici

Creates a quantity representing the apparent volumetric thermal expansion coefficient of the system [1/K].

Returns
A new `ApparentVolumetricThermalExpansionCoefficient` object.

classmethod average_composition_of_solid_phases_as_mass_fraction(*component: str*) → AverageCompositionOfSolidPhasesAsMass

Creates a quantity representing the average composition of solid phases [mass fraction] at the current Scheil step.

Parameters
`component` – The name of the component, use *ALL_COMPONENTS* to choose all components

Returns
A new `AverageCompositionOFSolidPhasesAsMassFraction` object.

classmethod average_composition_of_solid_phases_as_mole_fraction(*component: str*) → AverageCompositionOfSolidPhasesAsMole

Creates a quantity representing the average composition of solid phases [mole fraction] at the current Scheil step.

Parameters
`component` – The name of the component, use *ALL_COMPONENTS* to choose all components

Returns
A new `AverageCompositionOFSolidPhasesAsMoleFraction` object.

classmethod composition_of_phase_as_mole_fraction(*phase: str*, *component: str*) → CompositionOfPhaseAsMoleFraction

Creates a quantity representing the composition of a phase [mole-fraction].

Parameters

- **phase** – The name of the phase, use *ALL_PHASES* to choose all stable phases
- **component** – The name of the component, use *ALL_COMPONENTS* to choose all components

Returns
A new `CompositionOfPhaseAsMoleFraction` object.

classmethod composition_of_phase_as_weight_fraction(*phase: str*, *component: str*) → CompositionOfPhaseAsWeightFraction

Creates a quantity representing the composition of a phase [weight-fraction].

Parameters

- **phase** – The name of the phase, use *ALL_PHASES* to choose all stable phases
- **component** – The name of the component, use *ALL_COMPONENTS* to choose all components

Returns
A new `CompositionOfPhaseAsWeightFraction` object.

classmethod density_of_phase(*phase: str*) → DensityOfPhase

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

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

Returns
A new `DensityOfPhase` object.

classmethod density_of_system() → DensityOfSystem

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

Returns
A new `DensityOfSystem` object.

classmethod distribution_of_component_of_phase(*phase: str*, *component: str*) → DistributionOfComponentOfPhase

Creates a quantity representing the (molar) fraction of the specified component being present in the specified phase compared to the overall system [-]. This corresponds to the degree of segregation to that phase.

Parameters

- **phase** – The name of the phase
- **component** – The name of the component

Returns
A new `DistributionOfComponentOfPhase` object.

classmethod heat_per_gram() → HeatPerGram

Creates a quantity representing the total heat release from the liquidus temperature down to the current temperature [J/g].

Note: The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*`latent_heat_per_mole()`* and *`latent_heat_per_gram()`*), and the other is the heat related to the specific heat of liquid and solid phases (*`heat_per_mole()`* and *`heat_per_gram()`*).

Returns
A new `HeatPerGram` object.

classmethod heat_per_mole() → HeatPerMole

Creates a quantity representing the total heat release from the liquidus temperature down to the current temperature [J/mol].

Note: The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*`latent_heat_per_mole()`* and *`latent_heat_per_gram()`*), and the other is the heat related to the specific heat of liquid and solid phases (*`heat_per_mole()`* and *`heat_per_gram()`*).

Returns
A new `HeatPerMole` object.

classmethod latent_heat_per_gram() → LatentHeatPerGram

Creates a quantity representing the cumulated latent heat release from the liquidus temperature down to the current temperature [J/g].

Note: The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*`latent_heat_per_mole()`* and *`latent_heat_per_gram()`*), and the other is the heat related to the specific heat of liquid and solid phases (*`heat_per_mole()`* and *`heat_per_gram()`*).

Returns
A new `LatentHeatPerGram` object.

classmethod latent_heat_per_mole() → LatentHeatPerMole

Creates a quantity representing the cumulated latent heat release from the liquidus temperature down to the current temperature [J/mol].

Note: The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*`latent_heat_per_mole()`* and *`latent_heat_per_gram()`*), and the other is the heat related to the specific heat of liquid and solid phases (*`heat_per_mole()`* and *`heat_per_gram()`*).

Returns
A new `LatentHeatPerMole` object.

classmethod mass_fraction_of_a_solid_phase(*phase: str*) → MassFractionOfASolidPhase

Creates a quantity representing the mass fraction of a solid phase.

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

Returns
A new `MassFractionOfASolidPhase` object.

classmethod mass_fraction_of_all_liquid() → MassFractionOfAllLiquid

Creates a quantity representing the total mass fraction of all the liquid phase.

Returns
A new `MassFractionOfAllLiquid` object.

classmethod mass_fraction_of_all_solid_phases() → MassFractionOfAllSolidPhase

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

Returns
A new `MassFractionOfAllSolidPhase` object.

classmethod molar_volume_of_phase(*phase: str*) → MolarVolumeOfPhase

Creates a quantity representing the molar volume of a phase [m^3/mol].

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

Returns
A new `MolarVolumeOfPhase` object.

classmethod molar_volume_of_system() → MolarVolumeOfSystem

Creates a quantity representing the molar volume of the system [m^3/mol].

Returns
A new `MolarVolumeOfSystem` object.

classmethod mole_fraction_of_a_solid_phase(*phase: str*) → MoleFractionOfASolidPhase

Creates a quantity representing the molar fraction of a solid phase.

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

Returns
A new `MoleFractionOfASolidPhase` object.

classmethod mole_fraction_of_all_liquid() → MoleFractionOfAllLiquid

Creates a quantity representing the total molar fraction of all the liquid phase.

Returns
A new `MoleFractionOfAllLiquid` object.

classmethod mole_fraction_of_all_solid_phases() → MoleFractionOfAllSolidPhases

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

Returns
A new `MoleFractionOfAllSolidPhases` object.

classmethod site_fraction_of_component_in_phase(*phase: str*, *component: str*, *sub_lattice_ordinal_no: int = 0*) → SiteFractionOfComponentInPhase

Creates a quantity representing the site fractions [-].

Parameters

- `phase` – The name of the phase, use *ALL_PHASES* to choose all stable phases

- **component** – The name of the component, use *ALL_COMPONENTS* to choose all components
- **sub_lattice_ordinal_no** – The ordinal number (i.e. 1, 2, . . .) of the sublattice of interest, use None to choose all sublattices

Note: Detailed information about the sublattices can be obtained by getting the *Phase* object of a phase from the *System* object using `tc_python.system.System.get_phase_in_system`. For each phase the sublattices are obtained by using `tc_python.system.Phase.get_sublattices`. The order in the returned list is equivalent to the sublattice ordinal number expected, **but note that the ordinal numbers start with 1**.

Returns
A new `SiteFractionOfComponentInPhase` object.

`classmethod` **`temperature()`** → Temperature

Creates a quantity representing the temperature [K].

Returns
A new `Temperature` object.

`classmethod` **`volume_fraction_of_a_solid_phase`**(*phase: str*) → VolumeFractionOfASolidPhase

Creates a quantity representing the volume fraction of a solid phase.

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

Returns
A new `VolumeFractionOfASolidPhase` object.

`classmethod` **`volume_fraction_of_all_liquid()`** → VolumeFractionOfAllLiquid

Creates a quantity representing the total volume fraction of all the liquid phase.

Returns
A new `VolumeFractionOfAllLiquid` object.

`classmethod` **`volume_fraction_of_all_solid_phases()`** → VolumeFractionOfAllSolidPhases

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

Returns
A new `VolumeFractionOfAllSolidPhases` object.

`class tc_python.quantity_factory.`**`ThermodynamicQuantity`**

Bases: `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*) → ActivityOfComponent

Creates a quantity representing the activity of a component [-].

Parameters

- `component` – The name of the component, use *ALL_COMPONENTS* to choose all components
- `use_ser` – Use Stable-Element-Reference(SER). The user-defined reference state is used if this setting is set to *False*.

Returns
A new `ActivityOfComponent` object.

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

Creates a quantity representing the chemical diffusion coefficient of a phase [m^2/s].

Parameters

- `phase` – The name of the phase
- `diffusing_element` – The diffusing element
- `gradient_element` – The gradient element
- `reference_element` – The reference element (for example "Fe" in a steel)

Returns
A new `ChemicalDiffusionCoefficient` object.

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

Creates a quantity representing the chemical potential of a component [J].

Parameters

- `component` – The name of the component, use *ALL_COMPONENTS* to choose all components
- `use_ser` – Use Stable-Element-Reference(SER). The user-defined reference state is used if this setting is set to *False*.

Returns
A new `ChemicalPotentialOfComponent` object.

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

Creates a quantity representing the composition of a phase [mole-fraction].

Parameters

- `phase` – The name of the phase, use *ALL_PHASES* to choose all stable phases
- `component` – The name of the component, use *ALL_COMPONENTS* to choose all components

Returns
A new `CompositionOfPhaseAsMoleFraction` object.

`classmethod composition_of_phase_as_weight_fraction`(*phase: str*, *component: str*) → CompositionOfPhaseAsWeightFraction

Creates a quantity representing the composition of a phase [weight-fraction].

Parameters

- `phase` – The name of the phase, use *ALL_PHASES* to choose all stable phases

- **component** – The name of the component, use *ALL_COMPONENTS* to choose all components

Returns
A new `CompositionOfPhaseAsWeightFraction` object.

classmethod gibbs_energy_of_a_phase(*phase: str*, *use_ser: bool = False*) → GibbsEnergyOfAPhase

Creates a quantity representing the Gibbs energy of a phase [J].

Parameters

- **phase** – The name of the phase or *ALL_PHASES* to choose all phases
- **use_ser** – Use Stable-Element-Reference(SER). The user-defined reference state will be used when this setting is set to False.

Returns
A new `GibbsEnergyOfAPhase` object.

classmethod mass_fraction_of_a_component(*component: str*) → MassFractionOfAComponent

Creates a quantity representing the mass fraction of a component.

Parameters
component – The name of the component or *ALL_COMPONENTS* to choose all components

Returns
A new `MassFractionOfAComponent` object.

classmethod mass_fraction_of_a_phase(*phase: str*) → MassFractionOfAPhase

Creates a quantity representing the mass fraction of a phase.

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

Returns
A new `MassFractionOfAPhase` object.

classmethod mole_fraction_of_a_component(*component: str*) → MoleFractionOfAComponent

Creates a quantity representing the mole fraction of a component.

Parameters
component – The name of the component or *ALL_COMPONENTS* to choose all components

Returns
A new `MoleFractionOfAComponent` object.

classmethod mole_fraction_of_a_phase(*phase: str*) → MoleFractionOfAPhase

Creates a quantity representing the mole fraction of a phase.

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

Returns
A new `MoleFractionOfAPhase` object.

classmethod normalized_driving_force_of_a_phase(*phase: str*) → NormalizedDrivingForceOfAPhase

Creates a quantity representing normalized driving force of a phase [-].

Warning: A driving force calculation requires that the respective phase has been set to the state *DORMANT*. The parameter *All* is only reasonable if all phases have been set to that state.

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

Returns
A new `DrivingForceOfAPhase` object.

`classmethod pressure()` → Pressure

Creates a quantity representing the pressure [Pa].

Returns
A new `Pressure` object.

`classmethod system_size()` → SystemSize

Creates a quantity representing the system size [mol].

Returns
A new `SystemSize` object.

`classmethod temperature()` → Temperature

Creates a quantity representing the temperature [K].

Returns
A new `Temperature` object.

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

Creates a quantity representing tracer diffusion coefficient of a phase [m^2/s].

Parameters

- `phase` – The name of the phase
- `diffusing_element` – The diffusing element

Returns
A new `TracerDiffusionCoefficient` object.

`classmethod u_fraction_of_a_component(`*component: str*`)` → UFractionOfAComponent

Creates a quantity representing the u-fraction of a component.

Parameters
`component` – The name of the component

Returns
A new `UFractionOfAComponent` object.

`classmethod user_defined_function(`*expression: str*`)` → Function

Creates a quantity representing a user-defined function.

Parameters
`expression` – The function expression

Returns
A new `Function` object

`classmethod volume_fraction_of_a_phase(`*phase: str*`)` → VolumeFractionOfAPhase

Creates a quantity representing the volume fraction of a phase.

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

Returns
A new `VolumeFractionOfAPhase` object.

5.6 Module “utils”

class `tc_python.utils.`**`CompositionType`**(*value*)

Bases: `Enum`

The type of composition.

`COMPONENT = 1`

Composition given per component, this will be identical to *ELEMENT* in case of metals.

`ELEMENT = 0`

Composition given per element.

class `tc_python.utils.`**`CompositionUnit`**(*value*)

Bases: `Enum`

The composition unit.

`MASS_FRACTION = 1`

Mass fraction.

`MASS_PERCENT = 0`

Mass percent.

`MOLE_FRACTION = 3`

Mole fraction.

`MOLE_PERCENT = 2`

Mole percent.

class `tc_python.utils.`**`ConversionUnit`**(*value*)

Bases: `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.`**`GasAmountUnit`**(*value*)

Bases: `Enum`

The amount of a gas.

`KILOGRAM = 1`

Kilogram.

NORM_CUBIC_METER = 0

Norm cubic meter (according to ISO 2533, p=101325 Pa, T=288.15 K, typically used for trading of gas bottles). Other definitions vary only slightly.

class tc_python.utils.**GasCompositionUnit**(*value*)

Bases: `Enum`

The composition unit for a gas.

MASS_FRACTION = 1

Mass fraction.

MASS_PERCENT = 0

Mass percent.

MOLE_FRACTION = 3

Mole fraction.

MOLE_PERCENT = 2

Mole percent.

VOLUME_FRACTION = 5

Volume fraction.

VOLUME_PERCENT = 4

Volume percent.

class tc_python.utils.**GasRateUnit**(*value*)

Bases: `Enum`

The rate of a gas flow.

KILOGRAM_PER_SEC = 1

Kilogram per second.

NORM_CUBIC_METER_PER_SEC = 0

Norm cubic meter per second (according to ISO 2533, p=101325 Pa, T=288.15 K, typically used for trading of gas bottles). Other definitions vary only slightly.

class tc_python.utils.**InterfacePosition**(*value*)

Bases: `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.**PhaseUnit**(*value*)

Bases: `Enum`

The units available for a phase fraction.

MASS_FRACTION = 1

Mass fraction.

MOLE_FRACTION = 0

Mole fraction.

VOLUME_FRACTION = 2

Volume fraction.

class tc_python.utils.**ResultValueGroup**(*result_line_group_java*)

Bases: `object`

A x-y-dataset representing a line data calculation result (i.e. a Thermo-Calc *quantity 1* vs. *quantity 2*).

Warning: Depending on the calculator, the dataset might contain *NaN*-values to separate the data between different subsets.

Variables

- **label** – a str describing what the data corresponds to
- **x** – list of floats representing the first quantity ("x-axis")
- **y** – list of floats representing the second quantity ("y-axis")

get_label() → str

Accessor for the line label :return the line label

get_x() → List[float]

Accessor for the x-values :return the x values

get_y() → List[float]

Accessor for the y-values :return the y values

class tc_python.utils.**TemperatureProfile**

Bases: `object`

Represents a time-temperature profile used by non-isothermal calculations.

Note: The total simulation time can differ from the defined temperature profile. Constant temperature is assumed for any timepoint after the end of the defined profile.

add_time_temperature(*time: float*, *temperature: float*)

Adds a time-temperature point to the non-isothermal temperature profile.

Parameters

- **time** – The time [s]
- **temperature** – The temperature [K]

Returns

This *TemperatureProfile* object

5.7 Module "propertymodel_sdk"

class `tc_python.propertymodel_sdk.`**`CCTResult`**(*quantity_id: str*, *description: str*)

Bases: `ResultQuantity`

Represents a Continuous Cooling (CCT) result.

Parameters

- **`quantity_id`** – The id of this result
- **`description`** – The description of this result

`add_time_temperature`(*time_temperature_id: str*, *description: str*)

Adds a time-temperature pair to the result.

Parameters

- **`time_temperature_id`** – The id of the time-temperature pair
- **`description`** – The description of the time-temperature pair

`temperature_suffix = ' (T)'`

The temperature suffix of a `CCTResult`

`time_suffix = ' (t)'`

The time suffix of a `CCTResult`

class `tc_python.propertymodel_sdk.`**`CCTResultValues`**(*cooling_rate: float = -1.0*, *cooling_rate_start_temperature: float = -1.0*, *cooling_rate_end_temperature: float = -1.0*)

Bases: `object`

Represents Continuous Cooling (CCT) result values.

Parameters

- **`cooling_rate`** – The cooling rate [K/s]
- **`cooling_rate_start_temperature`** – The start temperature of cooling [K]
- **`cooling_rate_end_temperature`** – The end temperature of cooling [K]

`set_result_time_temperature`(*time_temperature_id: str*, *time: float*, *temperature: float*)

Sets a time-temperature pair of the result.

Parameters

- **`time_temperature_id`** – The id of the time-temperature pair
- **`time`** – The time [s]
- **`temperature`** – The temperature [K]

class `tc_python.propertymodel_sdk.`**`CalculationContext`**(*system: System*, *model_utils=None*)

Bases: `object`

Represents the interface of the Property Model with the Thermo-Calc application and the rest of the TC-Python functionality.

Parameters

- **`system`** – The system object of this calculation

- `model_utils` – The model utils object

`get_argument_ids()` → Set[str]

Returns a list with the arguments of the models. Including arguments created from dynamic parameters.

`get_dependent_component()` → str

Obtains the dependent component from the UI

Note: The dependent component is that which has no composition specified explicitly, typically this is the major element of the material (such as Fe, Al, Ni, . . .)

Returns
The dependent component

`get_element_names_in_camel_case()`

Obtains the elements in the system. The dependent component is not included.

Returns
A list of the elements in the system, each written in camel case.

`get_mass_fractions()` → Dict[str, float]

Obtains the current composition from the UI as mass-fraction.

Note: In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

Returns
The composition (key: component, value: content) [mass-fraction]

`get_mass_percents()` → Dict[str, float]

Obtains the current composition from the UI in mass-percent.

Note: In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

Returns
The composition (key: component, value: content) [mass-percent]

`get_mole_fractions()` → Dict[str, float]

Obtains the current composition from the UI as mole-fraction.

Note: In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

Returns
The composition (key: component, value: content) [mole-fraction]

get_mole_percents() → Dict[str, float]

Obtains the current composition from the UI in mole-percent.

Note: In case of stepping over one or multiple axis, the returned data will represent the composition at the current step.

Returns
The composition (key: component, value: content) [mole-percent]

get_temperature() → float

Obtains the current temperature from the UI.

Returns
The temperature [K]

get_ui_boolean_value(*component_id: str*) → bool

Obtains the value from the specified checkbox UI component.

Parameters
component_id – Id of the checkbox

Returns
The setting of the checkbox

get_ui_condition_list(*component_id: str*) → *ConditionListEntry*

Used to get the selected condition from components of type UIConditionListComponent :param component_id: Id of the list UI component :return: The selected condition

get_ui_float_value(*component_id: str*) → float

Obtains the value from the specified UI component.

Parameters
component_id – Id of the UI component

Returns
The value

get_ui_list_value(*component_id: str*) → str

Obtains the selected entry from a UI component list. If a special element (such as *ANY*, *NONE*, ...) is selected, the corresponding locale-independent placeholder is provided.

Parameters
component_id – Id of the list UI component

Returns
The selected entry

get_ui_string_value(*component_id: str*) → str

Obtains the selected entry from a UI component text field.

Parameters
component_id – Id of the string UI component

Returns
The selected entry

get_ui_temperature_value(*component_id: str*) → float

Obtains the temperature from the specified temperature UI component.

Parameters

component_id – Id of the temperature UI component

Returns

The temperature [K], note that input unit of the UI is specified in the model panel. If required, the temperature is automatically converted to K.

set_result_cct_values(*quantity_id: str*, *r:* CCTResultValues)

Sets the value of a previously defined result quantity (of type *CCTResultValues*) for further usage in the Thermo-Calc application for plotting, etc.

Parameters

- **quantity_id** – unique id of the result quantity
- **r** – the *CCTResultValues* to be set

set_result_quantity_value(*quantity_id: str*, *value: float*, *parameter: str = ''*)

Sets the value of a previously defined result quantity for further usage in the Thermo-Calc application for plotting, etc.

Note: Any result quantity that remains unset is automatically set to *NaN*.

Parameters

- **quantity_id** – Unique id of the result quantity
- **parameter** – Use if result is parameterized. f.i. "per phase"
- **value** – The value to be set

set_single_equilibrium_result(*quantity_id: str*, *r:* SingleEquilibriumResult)

class tc_python.propertymodel_sdk.**ConditionListEntry**

Bases: `object`

Used in combination with components of type UIConditionListComponent.

Contains the element, if the selected condition is a composition Contains the Console Mode syntax of the selected condition. Contains the unit of the selected condition

class tc_python.propertymodel_sdk.**PropertyModel**(*_locale: str = 'en-US'*)

Bases: `object`

The abstract base class for all property models.

Note: Every Property Model needs to implement most of the abstract methods of this class. However, some abstract methods are optional and should only be implemented if required.

Note: If overwriting the constructor in a Property Model, the constructor of the implemented class must have the identical signature and should pass the parameters to this base class constructor.

Tip: It is possible to switch off **internal INFO-log messages coming from the calculation engine** by changing the log-level on the TC-Python log object like this: *logging.getLogger("tc_python").setLevel(logging.ERROR)*.

Parameters
`_locale` – The locale to be used, **this is an internal parameter and is of no meaning to the end-user**

Variables
`logger` – logger object that is connected to the Thermo-Calc UI (*INFO*- and *WARNING*-level will be printed as *INFO*, *ERROR*-level as *ERROR*), it can be accessed like this: *self.logger.info("Some message")*

abstract add_button_callback(*component_id: str*, *ui_components: Dict[*UIComponent*, int]*) → List[*UIComponent*]

Implement this method if you have one or more UI components on which you called `UIComponent.enable_add_button()`, which adds a + button next to the component.

This method will be executed when you press any such + button.

This method is typically used to add more UI components dynamically and the method must return a list of the UI components to be added.

This method can optionally be implemented by a Property Model.

Parameters

- `component_id` – The id of the UI component next to the pressed + button
- `ui_components` – dict with the components and the index of the current ui components of the model. Including arguments created in previous calls to add_button_callback.

Returns
A list of *UIComponent* objects to be added

abstract add_callback(*component_id: str*, *ui_components: Dict[*UIComponent*, int]*, *old_value*, *new_value*)

TODO: docstring

abstract after_evaluations()

Called by the Thermo-Calc application immediately after the last model evaluation (using the method `PropertyModel.evaluate_model()`). Use this method for any required cleanup.

This method can optionally be implemented by a Property Model.

abstract before_evaluations(*context:* CalculationContext)

Called by the Thermo-Calc application immediately before the first model evaluation (using the method `PropertyModel.evaluate_model()`). Use this method for any required preparations.

This method can optionally be implemented by a Property Model.

Parameters
`context` – The calculation context

abstract evaluate_model(*context:* CalculationContext)

Called by the Thermo-Calc application when the model should be actually calculated. **This is the main-method of the Property Model that contains the actual calculation code.**

This method needs to be implemented by all property models.

Parameters

`context` – The calculation context, this provides access to the Thermo-Calc application and all other TC-Python modules

`abstract get_license_key()` → str

Provides the license key of the model.

This method can optionally be implemented by a Property Model.

`abstract provide_calculation_result_quantities()` → List[*ResultQuantity*]

Called by the Thermo-Calc application when the model should provide its result quantity objects.

This method needs to be implemented by all property models.

Returns

Result quantity objects of the model (to be filled later with results in the method *`PropertyModel.evaluate_model()`*)

`abstract provide_model_category()` → List[str]

Called by the Thermo-Calc application when the model should provide its category (shown in the Thermo-Calc model tree).

This method needs to be implemented by all property models.

Returns

Category of the model, it may be present in several categories

`abstract provide_model_description()` → str

Called by the Thermo-Calc application when the model should provide its detailed description.

This method needs to be implemented by all property models.

Returns

Description text for the model

`abstract provide_model_name()` → str

Called by the Thermo-Calc application when the model should provide its name (shown in the Thermo-Calc model tree).

This method needs to be implemented by all property models.

Returns

Name of the model

`abstract provide_model_parameters()` → Dict[str, float]

Called by the Thermo-Calc application when the model should provide all model parameters and their current values.

This method can optionally be implemented by a Property Model.

Note: These are internal variables of the Property Model that are intended to be modified from the outside. Typically this is used to adjust their values in a optimizer during the development of the model.

Returns

The model parameter ids and their current values [unit according to the parameter meaning]

abstract provide_ui_panel_components`()` → List[*UIComponent*]

Called by the Thermo-Calc application when the model should provide its UI components for the model panel to be plotted. This happens also whenever a model gets checked in the model tree.

This method needs to be implemented by all property models.

Returns
Model UI panel components in the order to be presented in the model panel

abstract remove_button_callback(*component_id: str*, *ui_components: Dict[*UIComponent*, int]*) → List[str]

Implement this method if you have one or more UI components on which you called `UIComponent.enable_remove_button()`, which adds a - button next to the component.

This method will be executed when you press any such - button.

This method is typically used to remove UI components dynamically and the method must return a list of the ids of the components that are going to be removed.

This method can optionally be implemented by a Property Model.

Parameters

- **component_id** – the id of the UI component next to the pressed - button
- **ui_components** – list with the components and the index of the current ui components of the model. Including arguments created in previous calls to add_button_callback.

Returns
a list of UI component ids that are required to be removed

abstract set_model_parameter(*model_parameter_id: str*, *value: float*)

Called by the Thermo-Calc application when a model parameter should be reset.

This method can optionally be implemented by a Property Model.

Note: These are internal variables of the Property Model that are intended to be modified from the outside. Typically this is used to adjust their values in a optimizer during the development of the model.

Parameters

- **model_parameter_id** – The parameter id
- **value** – The value [unit according to the parameter meaning]

class tc_python.propertymodel_sdk.ResultQuantity(*quantity_id: str*, *description: str*, *quantity_type: ResultQuantityType*)

Bases: `object`

Defines a calculation result quantity of a Property Model that is identified by a unique id.

Parameters

- **quantity_id** – Unique id of the quantity
- **description** – Description of the quantity (shown in the Thermo-Calc UI)
- **quantity_type** – Type of the quantity (defines the unit)

`get_description()` → str

Obtains the description of the quantity.

Returns
Description of the quantity

`get_id()` → str

Obtains the id of the quantity.

Returns
Unique id of the quantity

`get_type()` → *ResultQuantityType*

Obtains the type of quantity.

Returns
Type of the quantity

`class tc_python.propertymodel_sdk.ResultQuantityType(value)`

Bases: `Enum`

Defining the type of a result quantity.

`CCT_QUANTITY = 5`

A cct quantity

`ENERGY_QUANTITY = 2`

An energy quantity

`GENERAL_QUANTITY = 0`

A general quantity

`LENGTH_QUANTITY = 7`

A length in quantity

`SINGLE_EQUILIBRIUM_QUANTITY = 6`

A cct quantity

`STRENGTH_QUANTITY = 8`

A strength quantity

`SURFACE_ENERGY_QUANTITY = 3`

A surface energy quantity

`TEMPERATURE_QUANTITY = 1`

A temperature quantity

`TIME_QUANTITY = 4`

A time quantity

`class tc_python.propertymodel_sdk.SpecialListMarkers`

Bases: `object`

Placeholders for special list elements that are locale-dependent. They will be provided by UI list components if a special marker has been selected.

`ANY_LIST_MARKER = 'ANY'`

Marker that represents "Any"

NONE_LIST_MARKER = 'NONE'

Marker that represents "None"

class tc_python.propertymodel_sdk.**UIBooleanComponent**(*component_id: str*, *name: str*, *description: str*, *setting: bool*)

Bases: *UIComponent*

Checkbox UI component of the model panel.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **setting** – Initial setting of the checkbox

connect_component_enableability(*dependent_component_id: str*)

Connects the state enabled of any other UI component of the model panel to the value of this boolean component.

Parameters

dependent_component_id – Id of the UI element to be dependent on this boolean component

connect_component_visibility(*dependent_component_id: str*)

Connects the visibility of any other UI component of the model panel to the value of this boolean component.

Parameters

dependent_component_id – Id of the UI element to be dependent on this boolean component

enable_add_button()

Adds a + button to the right of the UI component.

Returns

This UI component

enable_remove_button()

Adds a - button to the right of the UI component.

Returns

This UI component

get_dependent_components() → List[str]

Obtains a list containing all UI elements currently connected regarding their visibility.

Returns

A list with the component id of all UI elements currently connected

get_setting() → bool

Obtains the setting of the checkbox.

Returns

The setting of the checkbox

`remove_component_visibility`(*dependent_component_id: str*)

Removes the visibility connection to a UI component that has been previously connected.

Parameters
`dependent_component_id` – Id of the previously connection UI element

`set_index`(*index: int = -1*)

Sets the position in the graphical user interface.

Parameters
`index` – The position

Returns
This UI component

class `tc_python.propertymodel_sdk.UIComponent`(*component_id: str*, *name: str*, *description: str*)

Bases: `object`

Abstract Base class for all UI components of the model panel.

Never make an instance of UIComponent, always use the sub-classes. For instance UIStringComponent.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component

`get_description`() → str

Obtains the additional description of the component.

Returns
Additional description of the component

`get_id`() → str

Obtains the unique id of the component.

Returns
Unique id of the component

`get_name`() → str

Obtains the name of the component.

Returns
Name of the component, will be presented in the model panel

`set_enabled`(*enabled*)

Sets whether the component should be enabled or not

Parameters
`enabled` –

Returns
This UI component

`set_has_callback`(*has_callback*)

`set_visible`(*visible*)

Sets the visibility of the component

Parameters
`visible` –

Returns
This UI component

class `tc_python.propertymodel_sdk.`**`UIConditionListComponent`**(*component_id: str*, *name: str*, *description: str*)

Bases: *UIComponent*

System condition list UI component of the model panel.

Parameters

- **`component_id`** – Unique id of the component
- **`name`** – Name of the component, will be presented in the model panel
- **`description`** – Additional description of the component

class `tc_python.propertymodel_sdk.`**`UIFloatComponent`**(*component_id: str*, *name: str*, *description: str*, *value: float*)

Bases: *UIComponent*

General real value text field UI component of the model panel.

Parameters

- **`component_id`** – Unique id of the component
- **`name`** – Name of the component, will be presented in the model panel
- **`description`** – Additional description of the component
- **`value`** – Initial setting of the text field

`enable_add_button`()

Adds a + button to the right of the UI component.

Returns
This UI component

`enable_remove_button`()

Adds a - button to the right of the UI component.

Returns
this UI component

`get_value`() → float

Obtains the setting of the text field.

Returns
The setting of the text field

`set_index`(*index: int = -1*)

Sets the position in the graphical user interface.

Parameters
`index` – The position

Returns
This UI component

class `tc_python.propertymodel_sdk.`**`UIGeneralListComponent`**(*component_id: str*, *name: str*, *description: str*, *content: List[Tuple[str, str]]*, *selected_entry: str = ''*)

Bases: *UIComponent*

General list UI component of the model panel that can contain any strings.

Parameters

- **`component_id`** – Unique id of the component
- **`name`** – Name of the component, will be presented in the model panel
- **`description`** – Additional description of the component
- **`content`** – Entries of the list, they need to contain a locale-independent id and a localized content string, for example: *[("ENTRY_1_ID", "entry 1"), (ENTRY_2_ID", "entry 2")]*
- **`selected_entry`** – Entry to be initially selected. If omitted, by default the first element is selected.

`connect_component_visibility`(*dependent_component_id: str*, *selected_item_to_set_visible: str*)

Connects the visibility of any other UI component of the model panel to the selection of a certain entry of the list.

Parameters

- **`dependent_component_id`** – Id of the UI element to be dependent on the chosen element
- **`selected_item_to_set_visible`** – Entry (locale independent id) of the list to be chosen to set the dependent component visible

`enable_add_button`()

Adds a + button to the right of the UI component.

Returns

This UI component

`enable_remove_button`()

Adds a - button to the right of the UI component.

Returns

This UI component

`get_content`() → List[Tuple[str, str]]

Obtains the entries of the list.

Returns

Entries of the list, they need to contain a locale-independent id and a localized content string, for example: *[("ENTRY_1_ID", "entry 1"), (ENTRY_2_ID", "entry 2")]*

`get_dependent_components`() → Dict[str, List[str]]

Obtains a dictionary containing all UI elements currently connected regarding their visibility.

Returns

All UI elements currently connected (key: dependent component id, value: required list entries to set it visible)

`get_selected_entry`() → str

Obtains the initially selected entry.

Returns

Initially selected entry. If empty, the first element is selected.

remove_component_visibility(*dependent_component_id: str*)

Removes the visibility connection to a UI component that has been previously connected.

Parameters
dependent_component_id – Id of the previously connection UI element

set_index(*index: int = -1*)

Sets the position in the graphical user interface.

Parameters
index – The position

Returns
This UI component

class tc_python.propertymodel_sdk.**UIPhaseListComponent**(*component_id: str*, *name: str*, *description: str*, *default_phase: str = ''*, *any_marker_setting: bool = False*)

Bases: *UIComponent*

Phase list UI component of the model panel.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **default_phase** – Default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. If an ANY-marker is added, this is chosen as the default element.
- **any_marker_setting** – Defines if an entry "ANY PHASE" should be added to the phase list, if set to true this overrides any default phase setting

enable_add_button()

Adds a + button to the right of the UI component.

Returns
This UI component

enable_remove_button()

Adds a - button to the right of the UI component.

Returns
This UI component

get_any_marker_setting() → bool

Obtains the setting if any entry "ANY PHASE" is added to the phase list.

Returns
If an entry "ANY PHASE" is added to the phase list, if set to true this overrides any default phase setting

get_default_phase() → str

Obtains the default phase.

Returns
Default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. If an ANY-marker is added, this is chosen as the default element.

`set_index`(*index: int = -1*)

Sets the position in the graphical user interface.

Parameters
`index` – The position

Returns
This UI component

`class tc_python.propertymodel_sdk.UISectionDividerComponent`(*component_id: str*, *name: str*, *description: str*)

Bases: *UIComponent*

General text field UI component of the model panel.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `string` – Initial setting of the text field

`get_value`() → str

Obtains the setting of the text field.

Returns
The setting of the text field

`set_index`(*index: int = -1*)

Sets the position in the graphical user interface.

Parameters
`index` – The position

Returns
This UI component

`class tc_python.propertymodel_sdk.UIStringComponent`(*component_id: str*, *name: str*, *description: str*, *string: str*)

Bases: *UIComponent*

General text field UI component of the model panel.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `string` – Initial setting of the text field

`enable_add_button`()

Adds a + button to the right of the UI component.

Returns
This UI component

`enable_remove_button()`

Adds a - button to the right of the UI component.

Returns
This UI component

`get_value()` → str

Obtains the setting of the text field.

Returns
The setting of the text field

`set_index`(*index: int* = *-1*)

Sets the position in the graphical user interface.

Parameters
`index` – The position

Returns
This UI component

class `tc_python.propertymodel_sdk.UITemperatureComponent`(*component_id: str*, *name: str*, *description: str*, *temp: float*)

Bases: *UIComponent*

Temperature value text field UI component of the model panel.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `temp` – Initial temperature to be set in the text field (unit defined by the user in the Thermo-Calc system)

`enable_add_button()`

Adds a + button to the right of the UI component.

Returns
This UI component

`enable_remove_button()`

Adds a - button to the right of the UI component.

Returns
This UI component

`get_temp()` → float

Obtains the temperature set in the text field.

Returns
The temperature to be set in the text field (unit defined by the user in the Thermo-Calc system)

`set_index`(*index: int* = *-1*)

Sets the position in the graphical user interface.

Parameters
`index` – The position

Returns
This UI component

`tc_python.propertymodel_sdk.create_boolean_ui_component`(*component_id: str*, *name: str*, *description: str*, *initial_setting: bool*) → *UIBooleanComponent*

Creates a UI checkbox component for a boolean value. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **initial_setting** – Initial setting of the checkbox

Returns
The created component

`tc_python.propertymodel_sdk.create_condition_list_ui_component`(*component_id: str*, *name: str*, *description: str*) → *UIConditionListComponent*

Creates a UI list component for all conditions defined in the system. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component

Returns
The created component

`tc_python.propertymodel_sdk.create_energy_quantity`(*quantity_id: str*, *description: str*) → *ResultQuantity*

Creates a UI energy result quantity (in J). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** – Unique id of the result quantity
- **description** – Additional description of the result quantity

Returns
The created result quantity

`tc_python.propertymodel_sdk.create_float_ui_component`(*component_id: str*, *name: str*, *description: str*, *value: float*) → *UIFloatComponent*

Creates a UI text field component for a real number. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel

- **description** – Additional description of the component
- **value** – Initial setting of the text field

Returns
The created component

`tc_python.propertymodel_sdk.`**`create_general_quantity`**(*quantity_id: str*, *description: str*) → *ResultQuantity*

Creates a general result quantity that can contain any type of result (without a unit). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** – Unique id of the result quantity
- **description** – Additional description of the result quantity

Returns
The created result quantity

`tc_python.propertymodel_sdk.`**`create_length_quantity`**(*quantity_id: str*, *description: str*) → *ResultQuantity*

Creates a length result quantity. When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** – Unique id of the result quantity
- **description** – Additional description of the result quantity

Returns
The created result quantity

`tc_python.propertymodel_sdk.`**`create_list_ui_component`**(*component_id: str*, *name: str*, *description: str*, *entry_list: List[Tuple[str, str]]*, *selected_entry: str = ''*) → *UIGeneralListComponent*

Creates a UI list component for string entries. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** – Unique id of the component
- **name** – Name of the component, will be presented in the model panel
- **description** – Additional description of the component
- **entry_list** – Entries of the list, they need to contain a locale-independent id and a localized content string, for example: *[("ENTRY_1_ID", "entry 1"), (ENTRY_2_ID", "entry 2")]*
- **selected_entry** – Entry to be initially selected. If omitted, by default the first element is selected.

Returns
The created component

`tc_python.propertymodel_sdk.`**`create_phase_list_ui_component`**(*component_id: str*, *name: str*, *description: str*, *default_phase: str = ''*, *any_marker: bool = False*) → *UIPhaseListComponent*

Creates a UI list component for all phases defined in the system. It is possible to select a default phase that is supposed to be the **expected phase selection** for that list. The value of that component can later be accessed during the model evaluation.

A **default** phase is the phase that is initially selected and re-selected as soon as a currently selected phase is removed. If the default phase is not available, a "NONE"-marker will be created and used instead of the default phase. A typical use case for the default phase setting is a phase list that expects to contain the LIQUID-phase of a system.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `default_phase` – Default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. **If an ANY-marker is added, this is chosen as the default element.**
- `any_marker` – Defines if an entry "ANY PHASE" should be added to the phase list, if set to true this overrides any default phase setting

Returns
The created component

`tc_python.propertymodel_sdk.`**`create_section_divider_ui_component`**(*component_id: str*, *name: str*, *description: str*) → *UISectionDividerComponent*

Creates an empty UI component acting as a spacer. :param component_id: Unique id of the component :return: The created component

`tc_python.propertymodel_sdk.`**`create_strength_quantity`**(*quantity_id: str*, *description: str*) → *ResultQuantity*

Creates a strength result quantity. When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- `quantity_id` – Unique id of the result quantity
- `description` – Additional description of the result quantity

Returns
The created result quantity

`tc_python.propertymodel_sdk.`**`create_string_ui_component`**(*component_id: str*, *name: str*, *description: str*, *string: str*) → *UIStringComponent*

Creates a UI text field component. The value of that component can later be accessed during the model evaluation.

Parameters

- `component_id` – Unique id of the component
- `name` – Name of the component, will be presented in the model panel
- `description` – Additional description of the component
- `string` – Initial setting of the text field

Returns
The created component

`tc_python.propertymodel_sdk.`**`create_surface_energy_quantity`**(*quantity_id: str*, *description: str*) → *ResultQuantity*

Creates an energy result quantity (in J). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **`quantity_id`** – Unique id of the result quantity
- **`description`** – Additional description of the result quantity

Returns
The created result quantity

`tc_python.propertymodel_sdk.`**`create_temperature_quantity`**(*quantity_id: str*, *description: str*) → *ResultQuantity*

Creates a temperature result quantity (in K). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **`quantity_id`** – Unique id of the result quantity
- **`description`** – Additional description of the result quantity

Returns
The created result quantity

`tc_python.propertymodel_sdk.`**`create_temperature_ui_component`**(*component_id: str*, *name: str*, *description: str*, *initial_temp: float*) → *UITemperatureComponent*

Creates a UI text field component for a temperature value. The value of that component can later be accessed during the model evaluation.

Parameters

- **`component_id`** – Unique id of the component
- **`name`** – Name of the component, will be presented in the model panel
- **`description`** – Additional description of the component
- **`initial_temp`** – Initial temperature to be set in the text field. (The unit of initial_temp is Kelvin. The value in the text field will be automatically converted using the unit chosen by the user.)

Returns
The created component

`tc_python.propertymodel_sdk.`**`create_time_quantity`**(*quantity_id: str*, *description: str*) → *ResultQuantity*

Creates a time result quantity (in s). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **`quantity_id`** – Unique id of the result quantity
- **`description`** – Additional description of the result quantity

Returns
The created result quantity

5.8 Module "exceptions"

exception `tc_python.exceptions.`**`APIServerException`**

Bases: *`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: *`TCException`*

An exception that occurred during a calculation.

exception `tc_python.exceptions.`**`ComponentNotExistingException`**

Bases: *`GeneralException`*

The selected component is not existing.

exception `tc_python.exceptions.`**`DatabaseException`**

Bases: *`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: *`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: *`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: *`CalculationException`*

General error occurring while a calculation is performed.

exception `tc_python.exceptions.`**`GeneralException`**

Bases: *`TCException`*

A general exception that might occur in different situations.

exception `tc_python.exceptions.`**`InvalidCalculationConfigurationException`**

Bases: *`CalculationException`*

Thrown when errors are detected in the configuration of the calculation.

exception `tc_python.exceptions.`**`InvalidCalculationStateException`**

Bases: *`CalculationException`*

Trying to access an invalid calculation object that was invalidated by calling *invalidate* on it.

exception `tc_python.exceptions.`**`InvalidNumberOfResultGroupsException`**

Bases: *`ResultException`*

A calculation result contains several result groups, which is not supported for the used method.

exception `tc_python.exceptions.`**`InvalidResultConfigurationException`**

Bases: *`ResultException`*

A calculation result configuration is invalid.

exception `tc_python.exceptions.`**`InvalidResultStateException`**

Bases: *`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: *`GeneralException`*

No valid license for the API or any Thermo-Calc product used by it found.

exception `tc_python.exceptions.`**`NoDataForPhaseException`**

Bases: *`ResultException`*

There is no result data available for a selected phase.

exception `tc_python.exceptions.`**`NotAllowedOperationException`**

Bases: *`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: *`GeneralException`*

The selected phase is not existing, so no data can be provided for it.

exception `tc_python.exceptions.`**`ResultException`**

Bases: *`TCException`*

An exception that occurred during the configuration of a calculation result.

exception `tc_python.exceptions.`**`SyntaxException`**

Bases: *`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: *`CalculationException`*

The calculation reached a state where no further actions are possible, this happens most often due to a FORTRAN-hard crash in the API server backend.

Note: It is possible to catch that exception outside of the *with*-clause context and to continue by setting up a new context (i.e. by a new *with TCPython() as session*).

`tc_python.exceptions.`**`handle_exception`**`(`*e*`)`

5.9 Module "abstract_base"

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**.

`get_system_data``()` → *SystemData*

Returns the content of the database for the currently loaded system. This can be used to modify the parameters and functions and to change the current system by using *`with_system_modifications()`*.

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

Returns

The system data

`invalidate``()`

Invalidates the object and frees the disk space used by it. *This is only required if the disk space occupied by the object needs to be released during the calculation.* No data can be retrieved from the object afterwards.

`with_system_modifications`(*system_modifications:* SystemModifications)

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

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

Parameters

`system_modifications` – The system modification to be performed

Returns

class `tc_python.abstract_base.`**`AbstractResult`**(*result*)

Bases: `object`

Abstract base class for results. This can be used to query for specific values .

`invalidate``()`

Invalidates the object and frees the disk space used by it. *This is only required if the disk space occupied by the object needs to be released during the calculation.* No data can be retrieved from the object afterwards.

class `tc_python.abstract_base.`**`PhaseParameter`**(*parameter_name: Union[str, object]*)

Bases: `object`

Database phase parameter expression used by *`SystemModifications.set()`*.

Parameters
: `parameter_name` – The phase parameter name

`get_intervals()` → List[*TemperatureInterval*]

Returns the list of all defined intervals.

Returns
: The defined temperature intervals

`get_lower_temperature_limit()` → float

Returns the lower temperature limit.

Returns
: The lower temperature limit in K

`get_name()` → str

Returns the name of the phase parameter.

Returns
: The name of the phase parameter.

`remove_all_intervals()`

Removes all previously defined temperature intervals.

Returns
: This `PhaseParameter` object

`remove_interval_with_upper_limit`(*upper_temperature_limit: float*)

Removes a previously defined temperature interval with matching upper temperature limit.

If no such interval exists, an exception is thrown.

Returns
: This `PhaseParameter` object

`set_expression_with_upper_limit`(*parameter_expression: str*, *upper_temperature_limit: float = 6000.0*)

Adds/overwrites a parameter expression for a temperature interval.

Default value of the upper limit of the interval: 6000 K

Note: The lower temperature limit is either defined by the lower temperature limit given with `PhaseParameter.set_lower_temperature_limit()` or by the upper temperature limit of the adjacent interval.

Note: If there is an existing interval with exactly the same *upper_temperature_limit*, that interval is overwritten, otherwise the interval is added.

Parameters

- `parameter_expression` – The parameter expression, example: *+V34*T*LN(T)+V35*T**2+V36*T**(-1)+V37*T**3")*
- `upper_temperature_limit` – The upper temperature limit for which the expression should be used

Returns
: This `PhaseParameter` object

set_interval(*interval: TemperatureInterval*)

Adds/overwrites a temperature interval.

Note: The lower temperature limit is either defined by the lower temperature limit given with *PhaseParameter.set_lower_temperature_limit()* or by the upper temperature limit of the adjacent interval.

Note: If there is an existing interval with exactly the same *upper_temperature_limit*, that interval is overwritten, otherwise the interval is added.

Returns
This *PhaseParameter* object

set_lower_temperature_limit(*lower_temperature_limit: float = 298.15*)

Sets the lower temperature limit of the phase parameter.

Default: 298.15 K

Parameters
lower_temperature_limit – The lower temperature limit in K

Returns
This *PhaseParameter* object

class tc_python.abstract_base.**SystemData**(*system_data*)

Bases: `object`

Provides information about the parameters and functions of a user database. The obtained objects can be used to modify the database using `with_system_modifications()` of all calculators.

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

---

get_phase_parameter(*parameter: str*) → *PhaseParameter*

Returns a phase parameter.

Example:

system_data.get_phase_parameter('G(HCP_A3,FE:VA;0)')

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

Note: For details about the syntax search the Thermo-Calc help for *GES* (the name for the Gibbs Energy System module in Console Mode).

Parameters
parameter – The name of the phase parameter (for example: *"G(LIQUID,FE;0)"*)

Returns
The phase parameter

get_phase_parameter_names() → List[str]

Returns all phase parameters present in the current system.

Returns
The list of phase parameters

get_system_function(*f: str*) → *SystemFunction*

Returns a system function.

Note: The parameter 'f' was previously called 'function' but was renamed.

Example:

system_data.get_system_function('GHSERCR')

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

Note: For details about the syntax search the Thermo-Calc help for *GES* (the name for the Gibbs Energy System module in Console Mode).

Parameters
f – The name of the system function (for example: *"GHSERCR"*)

Returns
The system function

get_system_function_names() → List[str]

Returns all system functions present in the current system.

Returns
The list of system functions

class tc_python.abstract_base.**SystemFunction**(*function_name: Union[str, object]*)

Bases: `object`

Database function expression used by `SystemModifications.set()`.

Parameters
function_name – The function name

get_intervals() → List[*TemperatureInterval*]

Returns the list of all defined intervals.

Returns
The defined temperature intervals

get_lower_temperature_limit() → float

Returns the lower temperature limit.

Returns
The lower temperature limit in K

`get_name()` → str

Returns the name of the system function.

Returns
The name of the system function

`remove_all_intervals()`

Removes all previously defined temperature intervals.

Returns
This `SystemFunction` object

`remove_interval_with_upper_limit`(*upper_temperature_limit: float*)

Removes a previously defined temperature interval with matching upper temperature limit.

If no such interval exists, an exception is thrown.

Returns
This `SystemFunction` object

`set_expression_with_upper_limit`(*function_expression: str*, *upper_temperature_limit: float = 6000.0*)

Adds/overwrites a function expression for a temperature interval.

Default value of the upper limit of the interval: 6000 K

Note: The lower temperature limit is either defined by the lower temperature limit given with `SystemFunction.set_lower_temperature_limit()` or by the upper temperature limit of the adjacent interval.

Note: If there is an existing interval with exactly the same *upper_temperature_limit*, that interval is overwritten, otherwise the interval is added.

Parameters

- **function_expression** – The function expression, example: *+V34*T*LN(T)+V35*T**2+V36*T**(-1)+V37*T**3")*
- **upper_temperature_limit** – The upper temperature limit for which the expression should be used

Returns
This `SystemFunction` object

`set_interval`(*interval:* TemperatureInterval)

Adds/overwrites a temperature interval.

Note: The lower temperature limit is either defined by the lower temperature limit given with `SystemFunction.set_lower_temperature_limit()` or by the upper temperature limit of the adjacent interval.

Note: If there is an existing interval with exactly the same *upper_temperature_limit*, that interval is overwritten, otherwise the interval is added.

Returns
This *SystemFunction* object

set_lower_temperature_limit(*lower_temperature_limit: float = 298.15*)

Sets the lower temperature limit of the system function.

Default: 298.15 K

Parameters
lower_temperature_limit – The lower limit in K

Returns
This *SystemFunction* object

class tc_python.abstract_base.**SystemModifications**

Bases: `object`

Functionality to modify a user database during a calculation by changing phase parameters and system functions.

The actual changes are **only applied** by using *tc_python.abstract_base.AbstractCalculation.with_system_modifications()* on a calculator object.

run_ges_command(*ges_command: str*)

Sends a GES-command. **This is actually applied when running `with_system_modifications` on a calculator object.**

Example: *run_ges_command("AM-PH-DE FCC_A1 C_S 2 Fe:C")* for adding a second composition set to the FCC_A1 phase with *Fe* as major constituent on first sublattice and *C* as major constituent on second sublattice.

Note: For details about the syntax search the Thermo-Calc help for *GES* (the name for the Gibbs Energy System module in Console Mode).

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

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

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

Returns
This *SystemModifications* object

set(*parameter_or_function: Union[PhaseParameter, SystemFunction]*)

Overwrites or creates a phase parameter or system function.

Example: *system_modifications.set(PhaseParameter('G(LIQUID,FE;0)').set_expression_with_upper_limit('+1.2*GFELIQ*

Example: *system_modifications.set(SystemFunction("DGDEF").set_expression_with_upper_limit('+10.0-R*T', 1000).set_expression_with_upper_limit('+20.0-R*T', 3000))*

Note: The old parameter/function is **overwritten** and any temperature intervals not defined are lost.

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

Returns
This `SystemModifications` object

`class tc_python.abstract_base.TemperatureInterval`(*expression: Union[str, object]*, *upper_temperature_limit: float*)

Bases: `object`

Temperature interval expression used by the classes `SystemFunction` and `PhaseParameter`.

Parameters

- **`expression`** – The temperature function expressed in Thermo-Calc database syntax.
- **`upper_temperature_limit`** – The upper temperature limit in K

`get_expression()` → str

Returns the function expression of this temperature interval.

Returns
The temperature function expression

`get_upper_temperature_limit()` → float

Returns the upper limit of this temperature interval.

Returns
The upper temperature limit in K

`set_expression`(*expression: str*)

Sets the function expression of this temperature interval.

Parameters
`expression` – The temperature function expression

`set_upper_temperature_limit`(*upper_temperature_limit: float*)

Sets the upper limit of this temperature interval.

Parameters
`upper_temperature_limit` – The upper temperature limit in K

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://download.thermocalc.com/downloads/support/diagnostics-py/2024a/tc-python-
↪diagnostic-script-2024a.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 = '2024a'

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 (needs to be at least Python 3.8, Python 2.x is not supported):')
print(sys.version)
if sys.version_info[0] < 3 or sys.version_info[1] < 8:
    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, '
```

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```
      'TC-Python must be installed into \nEACH separate environment used!)')
print(sys.executable)

import os
print('')
print('Thermo-Calc ' + version + ' installation directory: (must be a valid path to a␣
↪complete installation of ' + version + ')')
tc_env_variable = 'TC' + version[2:].upper() + '_HOME'
try:
    print(os.environ[tc_env_variable])
except:
    print('No Thermo-calc environment variable for ' + version + ' was found. (' + tc_
↪env_variable + ')')

print('')
print('Url of license server: (if license server is NO-NET, you need a local license␣
↪file)')
try:
    print(os.environ['LSHOST'])
except:
    print('No Thermo-calc license server url was found. (LSHOST)')


print('')
print('Path to local license file: (only necessary if not using license server)')
try:
    print(os.environ['LSERVRC'])
except:
    print('No path to local license file was found. (LSERVRC)')


import tc_python
numerical_version = version[:-1]
if version[-1] == 'a':
    numerical_version += '.1.*'
elif version[-1] == 'b':
    numerical_version += '.2.*'
print('')
print('TC-Python version: (needs to be ' + numerical_version + ')')
print(tc_python.__version__)


with tc_python.TCPython() as session:
    print('')
    print('Lists the databases: (should be a complete list of the installed databases␣
↪that you have license for or do not require license)')
    print(session.get_databases())
```

6.2 "No module named tc_python" error on first usage

This problem occurs because your used Python interpreter cannot find the TC-Python package. We expect that you have installed the TC-Python package in your **Python system interpreter** following the instructions in the *Installation Guide*.

Normally the error message "*No module named tc_python*" is caused by unintentionally configuring a PyCharm project to use a so-called **Virtual Environment**. This happens unfortunately by default when creating a new PyCharm project with not changing the default settings.

Note: A Virtual Environment is basically a separate and completely independent copy of the system-wide Python interpreter. It does not contain any packages.

On Windows systems we recommend to use the Anaconda Python Distribution as Python interpreter. However, the instructions given here are valid for any operating system and distribution.

Since TC-Python 2018b we do recommend to **not use Virtual Environments** unless there is a reasonable use case for that.

There are two possible solutions to fix the problem:

1. The quick fix for your problem is to run

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

   within the *Terminal window* of the opened PyCharm project. This *Terminal window* automatically runs within the *Virtual Environment* configured for the project (if any). You can see the name of the *Virtual Environment* at the beginning of each command prompt line (here it is called *venv*):

   ```
   Microsoft Windows [Version 10.0.16299.431]
   (c) 2017 Microsoft Corporation. All rights reserved.

   (venv) C:\Users\User\Documents\>
   ```

   The command will consequently **install TC-Python also within that Virtual Environment automatically**. The Terminal window can be found at the bottom of the IDE. Note that it might be necessary to enable these buttons first by selecting the menu entry **View→Tool Buttons**.

2. The better fix is to change your project **to use the system interpreter**. This is described in detail in the section *Fixing potential issues with the environment* in Step 5 of the *Installation Guide*.

   It is recommendable to use that approach also for all your future projects.

Both fixes will only change the configuration of the opened project. Further useful information can be found in the section *Python Virtual Environments*.

6.3 "pip install" fails with "Failed to establish a new network connection" or similar

If *pip install* fails with a network related error (might also be "*socket not available*", "*retrying after connection broken*", . . .) it is often due to the computer being behind a proxy-server, this is common in large organizations. Of course also the network connection might be broken.

TC-Python has dependencies to a few other packages:

- *py4j*
- *jproperties* (has transient dependency *six*)
- *pyvista* (*optional, only for Additive Manufacturing result plotting and data extraction*, it has a number of transient dependencies)

1. The recommended approach is to simply use *pip*. It will resolve the dependencies automatically by downloading them from the *PyPI*-repository server (https://pypi.org). If your computer is located behind a proxy-server, the connection to the repository will fail. In that case it is necessary to configure *pip* with the detailed configuration of the proxy server:

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

2. Another alternative is to manually download the latest `*.whl`-file of each dependency from the repository server (https://pypi.org -> *Search projects*) and to install it manually using:

```
pip install py4j-#.#.#-py2.py3-none-any.whl
...
```

The actual actual version number needs to be inserted into the file name. The downside of this approach is that updates to that package have to be fully manual also in the future. Additionally it is also necessary to install all transient dependencies in that way.

PYTHON MODULE INDEX