# TC-Toolbox for MATLAB® Documentation

***Release 2022b***

**Thermo-Calc Software AB**

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# CONTENTS

CHAPTER

ONE

# QUICK INSTALLATION GUIDE

This guide helps you to get a working TC-Toolbox for MATLAB® installation. It is only a short guideline, please refer to the **Thermo-Calc Installation Guides** for more details if required.

The present documentation is also included in your installation as a PDF-file. 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-Toolbox for MATLAB®.

**Note:** TC-Toolbox for MATLAB® is available for Windows.

## 1.1 Installing TC-Toolbox for MATLAB®

### 1.1.1 Automatic Installation of TC-Toolbox

When the following conditions are met, Thermo-Calc automatically installs the TC-Toolbox for MATLAB® component on your computer.

1. MATLAB® is already installed.
2. There is only one Windows user on the computer where TC-Toolbox is being installed.

**Note:** Administrator privileges are needed when you start the Thermo-Calc installer.

Then follow the regular installation instructions for Thermo-Calc, choosing whether you use a Standalone or Network installation.

### 1.1.2 Manual Installation of TC-Toolbox

The installation is not automatic if:

- There are multiple Windows users on the same machine, or
- The installer cannot find the directory path to the MATLAB® installation.

#### 1.1.2.1 Multiple Windows Users on Same Machine

If there are multiple Windows users on the same machine, then the following manual steps are done at the end of the automatic installation.

1. A message at the end of the Thermo-Calc installation process displays with instructions.
2. An Explorer window automatically opens to this folder `C:\Users\<user>\Documents\Thermo-Calc\2022b\SDK\TC-Toolbox-MATLAB`.
3. Double-click the `InstallTCToolboxMATLAB.cmd` file to finalize the process. This briefly launches MATLAB® and installs TC-Toolbox.

#### 1.1.2.2 Installer Cannot Find the MATLAB® Installation Directory

1. Start the version of MATLAB® that you want to install TC-Toolbox in.
2. Open and run the script `C:\Users\<user>\Documents\Thermo-Calc\2022b\SDK\TC-Toolbox-MATLAB\setupTCToolbox.m`.

For more information, se the more detailed instructions given in the **Thermo-Calc Installation Guides**.

### 1.1.3 Check the Installation

To check if the installation was successful start MATLAB® and run, for example, the diagnostics script, which is located in the folder `C:\Users\<user>\Documents\Thermo-Calc\2022b\SDK\TC-Toolbox-MATLAB\Examples\Miscellaneous`.

Alternatively open the **Add-Ons** menu (in the **HOME** tab) in MATLAB® and choose **Manage Add-Ons**. If the toolbox is installed it will be included in this list.

## 1.2 Uninstalling TC-Toolbox for MATLAB®

If you are logged in as a **user with administrator rights, and have Thermo-Calc installed for this user**, then the uninstallation is automatically done at the same time as a full Thermo-Calc uninstallation. Otherwise a manual step is required:

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**Note:** To uninstall the TC-Toolbox for MATLAB® if it is not uninstalled by the Thermo-Calc uninstaller, start MATLAB® and select (in the **HOME** tab) **Manage Add-Ons** from the **Add-Ons** menu. Right-click TC-Toolbox and choose **Uninstall**.

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CHAPTER

TWO

# ARCHITECTURE OVERVIEW

TC-Toolbox contains classes of these types:

- `TCToolbox` – 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.

## 2.1 TCToolbox

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

You can think of this as the start of a "wizard".

You use it to select databases and elements and then in the next step, configure the system.

**Example:**

```
import tc_toolbox.*

session = TCToolbox();
session.select_database_and_elements(...
% e.t.c.
% ...
```

**Note:** When your MATLAB® script runs a row like this:

```
session = TCToolbox();
```

a process running a calculation server starts. Your code, via TC-Toolbox, uses socket communication to send and receive messages to and from that server.

When you remove the variable *session* from the MATLAB® workspace, the calculation server automatically shuts down, and all temporary files are deleted.

**Note:** You can set up a folder location to re-use results from saved calculations. This folder can be a network folder and shared by many users. This is done using the method `set_cache_folder()`.

```
import tc_toolbox.*

session = TCToolbox();
session.set_cache_folder("cache")
```

Once the cache folder is created, if a previous TC-Toolbox 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.

**Example:**

```
import tc_toolbox.*

session = TCToolbox();
%... 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')
```

## 2.2 SystemBuilder and System

A `SystemBuilder` is returned when you have selected your database and elements in `TCToolbox`.

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

**Example:**

```
import tc_toolbox.*

session = TCToolbox();
start.select_database_and_elements("ALDEMO", ["Al", "Sc"]).select_phase("FCC_A1")
% e.t.c
```

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

- 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.

## 2.3 Calculation

All available calculation types are set up in a similar way, some calculations have many settings. But default values are used where it is applicable, and are overridden if you specify something different.

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**Tip:** Review the TC-Toolbox examples included with the Thermo-Calc installation to see how calculations are used for various solutions.

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

### 2.3.1 Single Equilibrium Calculations

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

This is done 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`.

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

---

**Example:**

```
import tc_toolbox.*

session = TCToolbox();

sys = session.select_database_and_elements("FEDEMO", ["Fe", "Cr", "C"]).get_system();
calculation = sys.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();

gibbs_energy = calculation.get_value_of("G")
```

### 2.3.2 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 MATLAB® and TC-Toolbox.

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**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).

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**Example:**

```
import tc_toolbox.*

session = TCToolbox();
session.set_cache_folder("_cache");

system_builder = session.select_database_and_elements("NIDEMO", ["Ni", "Al", "Cr"]);
system_builder.without_default_phases();
system_builder.select_phase('BCC_A2');
sys = system_builder.get_system();
batch_calculation = sys.with_batch_equilibrium_calculation();

batch_calculation.set_condition("T", 800);
batch_calculation.set_condition("X(Al)", 1E-2);
batch_calculation.set_condition("X(Cr)", 1E-2);
batch_calculation.disable_global_minimization();

list_of_x_Al = linspace(1e-4, 10e-2, 10);
list_of_x_Cr = linspace(1e-4, 15e-2, 10);
list_of_density = [];
equilibria = {};

i = 1;
for x_Al = list_of_x_Al
    for x_Cr = list_of_x_Cr
        equilibria{i} = {{"X(Al)", x_Al} {"X(Cr)", x_Cr}};
        i = i+1;
    end
end

batch_calculation.set_conditions_for_equilibria(equilibria);

results = batch_calculation.calculate(["BM", "VM"], 100);

masses = results.get_values_of("BM");
volumes = results.get_values_of('VM');
density = 1e-3 * masses ./ volumes
```

### 2.3.3 Precipitation Calculations

All the configuration settings for the *Precipitation Calculator* in Graphical Mode are available for this calculation. However, you must at least enter a matrix phase, a precipitate phase, temperature, simulation time, and compositions.

**Example:**

```
import tc_toolbox.precipitation.*
import tc_toolbox.*

session = TCToolbox();
session.set_cache_folder("_cache");

system_builder = session.select_thermodynamic_and_kinetic_databases_with_elements(
↪"ALDEMO", "MALDEMO", ["Al","Sc"]);
sys = system_builder.get_system();

precipitationCalculation = sys.with_isothermal_precipitation_calculation();
precipitationCalculation.set_composition("Sc", 0.18);
precipitationCalculation.set_temperature(623.15);
precipitationCalculation.set_simulation_time(1e5);
precipitationCalculation.with_matrix_phase(MatrixPhase("FCC_A1")...
                                           .add_precipitate_phase(PrecipitatePhase(
↪"AL3SC")));

result = precipitationCalculation.calculate();
[time, meanRadius] = result.get_mean_radius_of("AL3SC");
```

### 2.3.4 Scheil Calculations

All Scheil calculation settings available in Graphical Mode (using the *Scheil Calculator*) or Console Mode (using the Scheil module) are available for this calculation. The minimum you need to specify are the elements and compositions. Everything else is set to a default value.

**Example:**

```
import tc_toolbox.*

session = TCToolbox();
sys = session.select_database_and_elements("FEDEMO", ["Fe", "C"]).get_system();
temperature_vs_mole_fraction_of_solid = sys.with_scheil_calculation()...
                                           .set_composition("C", 0.3)...
                                           .calculate()...
                                           .get_values_of(ScheilQuantity.
↪temperature(),...
                                                          ScheilQuantity.mole_
↪fraction_of_all_solid_phases());
```

### 2.3.5 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. All other settings use the default values unless specified otherwise.

**Example:**

```
import tc_toolbox.*
import tc_toolbox.step_or_map_diagrams.*

session = TCToolbox();
    property_diagram = session...
             .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"));
```

### 2.3.6 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. All other settings use the default values unless specified otherwise.

**Example:**

```
import tc_toolbox.*
import tc_toolbox.step_or_map_diagrams.*

session = TCToolbox();
    property_diagram = session...
             .select_database_and_elements("FEDEMO", ["Fe", "C"])...
             .get_system()...
             .with_phase_diagram_calculation()...
                 .with_first_axis(CalculationAxis(ThermodynamicQuantity.temperature()).
↪..
                                  .set_min(500)...
                                  .set_max(3000))...
                 .with_second_axis(CalculationAxis(ThermodynamicQuantity.mole_fraction_
↪of_a_component("C"))...
                                   .set_min(0)...
                                   .set_max(1))...
                 .set_condition(ThermodynamicQuantity.mole_fraction_of_a_component("C
↪"), 0.01)...
                 .calculate()...
```

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```
                .get_values_grouped_by_stable_phases_of(ThermodynamicQuantity.mass_
↪fraction_of_a_component("C"),...
                                                        ThermodynamicQuantity.
↪temperature());
```

### 2.3.7 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:**

```
import tc_toolbox.diffusion.*
import tc_toolbox.*

session = TCToolbox();

tc_system = session...
    .select_thermodynamic_and_kinetic_databases_with_elements("FEDEMO", "MFEDEMO", [
↪"Fe", "Ni"])...
    .get_system();

calculator = tc_system...
                .with_isothermal_diffusion_calculation()...
                .set_temperature(1400.0)...
                .set_simulation_time(108000.0)...
                .add_region(Region("Austenite")...
                            .set_width(100E-6)...
                            .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"));

results = calculator.calculate();

[distance, mass_frac_ni] = results.get_mass_fraction_of_component_at_time("Ni",␣
↪SimulationTime.LAST);
```

### 2.3.8 Property Model Calculations

For Property Model calculations, all the configuration settings for the *Property Model Calculator* in Graphical Mode are available for this calculation. The minimum you need to specify are elements, composition, and which Property Model you want to use.

**Example:**

```
import tc_toolbox.*

session = TCToolbox();
"Available property models: " + session.get_property_models()
```

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```
property_model = session...
                    .select_database_and_elements("FEDEMO", ["Fe", "C"])...
                    .get_system()...
                    .with_property_model_calculation("Driving Force")...
                    .set_composition("C", 1.0)...
                    .set_argument("matrix", "LIQUID")...
                    .set_argument("precipitate", "GRAPHITE");

"Available arguments: " + property_model.get_arguments()
result = property_model.calculate();

"Available result quantities: " + result.get_result_quantities()
driving_force = result.get_value_of("normalizedDrivingForce")
```

### 2.3.9 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:**

```
import tc_toolbox.*
import tc_toolbox.material_to_material.*;

independent_elements = ["Cr", "Ni"];
a_comp = [10.0, 15.0];
b_comp = [15.0, 10.0];

activity_elements = ["C"];
activities = [0.1];

session = TCToolbox();

material_to_material_property_diagram = session...
    .select_database_and_elements("FEDEMO", ["Fe", "Cr", "Ni", "C"])...
    .get_system()...
    .with_material_to_material()...
        .with_property_diagram_calculation()...
        .set_material_a(containers.Map(independent_elements, a_comp), "Fe")...
        .set_material_b(containers.Map(independent_elements, b_comp), "Fe")...
        .set_activities(containers.Map(activity_elements, activities))...
        .with_constant_condition(ConstantCondition.temperature(800 + 273.15))...
        .with_axis(MaterialToMaterialCalculationAxis.fraction_of_material_b());

result = material_to_material_property_diagram.calculate();
data = result.get_values_grouped_by_quantity_of(...
    Constants.MATERIAL_B_FRACTION,...
    ThermodynamicQuantity.volume_fraction_of_a_phase(Constants.ALL_PHASES));

for k = data.keys()
    group = data(k{1});
```

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```
    fractions_of_b = group.get_x();
    volume_fraction_of_phase = group.get_y();
    phase_name = group.get_label();
end
```

### 2.3.10 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 type of calculations:

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

**Equilibrium calculation example:**

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

```
import tc_toolbox.process_metallurgy.base.*;
import tc_toolbox.process_metallurgy.equilibrium.*;
import tc_toolbox.*

session = tc_toolbox.TCToolbox();

metal = EquilibriumAddition(containers.Map(["Fe", "C", "Si"], {NaN, 4.5, 1.0}), 100e3,
↪ 1650 + 273.15);
slag = EquilibriumAddition(containers.Map(["CaO", "Al2O3"], {75, 25}), 3e3, 1600 +␣
↪273.15);
gas = EquilibriumGasAddition(containers.Map({'O2'}, {100}), 1000, 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();

disp("Stable phases:")
disp(result.get_stable_phases())
disp("Temperature: " + result.get_temperature() + " K");
```

**Process simulation example:**

TC-Toolbox 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:

```
import tc_toolbox.process_metallurgy.base.*;
import tc_toolbox.process_metallurgy.process.*;
import tc_toolbox.*

session = tc_toolbox.TCToolbox();


calc = (session.with_metallurgy()...
        .with_adiabatic_process_calculation(ProcessDatabase.OXDEMO)...
        .set_end_time(15 * 60));

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

steel_zone.add_addition(SingleTimeAddition(containers.Map(["Fe", "C", "Si"], {NaN, 4.
↪5, 1.0}), 120e3,...
                                           1600 + 273.15), 0);
slag_zone.add_addition(SingleTimeAddition(containers.Map(["CaO", "SiO2"], {75, 25}),␣
↪1.2e3,...
                                          1500 + 273.15,...
                                          CompositionUnit.MOLE_PERCENT), 0);

steel_zone.add_continuous_addition(ContinuousGasAddition(containers.Map({'O2'}, {100}
↪), 1,...
                                                         GasRateUnit.NORM_CUBIC_METER_
↪PER_SEC));

calc.with_reaction_zone(ReactionZone(10.0,...
                                     steel_zone, 1.0e-5,...
                                     slag_zone, 1.0e-6));

result = calc.calculate();

disp("Stable phases in the steel melt:")
disp(result.get_stable_phases('metal'))
disp("C-content in steel vs. time:")
compositions = result.get_composition_of_phase_group('metal', PhaseGroup.ALL_METAL);
disp(compositions('C'))
```

## 2.4 Result

All calculations have a method called `calculate()` that starts the calculations and when finished, returns a `Result`.

The `Result` classes have very different methods, depending on the type of calculation.

The `Result` is used to get numerical values from a calculation that has run.

The `Result` can be saved to disk by the method `save_to_disk()`.

Previously saved results can be loaded by the method `load_result_from_disk()` on the `SetUp` class.

**Example:**

```
% code above sets up the calculation
r = calculation.calculate()
time, meanRadius = r.get_mean_radius_of("AL3SC")
```

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

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

**Example:**

```
% ...
% some code to set up a single equilibrium calculation
% ...

single_eq_result = single_eq_calculation.calculate_with_state()

% ...
% some code to set up a precipitation calculation
% ...

prec_result = precipitation_calculation.calculate()

% ...
% some code to set up a Scheil calculation
% ...

scheil_result = scheil_calculations.calculate()

% now it is possible to get results from the single equilibrium calculation,
% without having to re-run it (because it has been calculated with saving of the␣
↪state)

gibbs = single_eq_result.get_value_of("G")
```

CHAPTER

THREE

# BEST PRACTICES

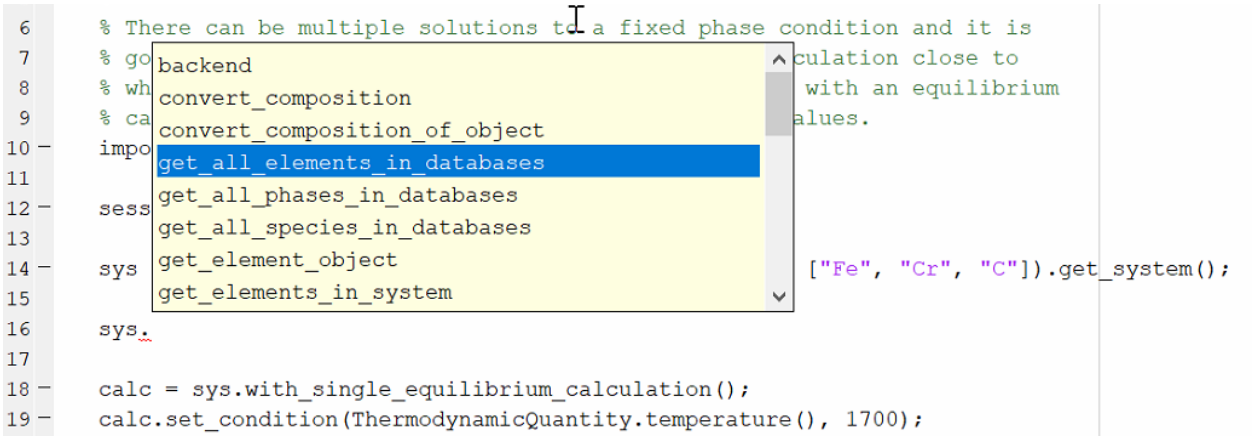
## 3.1 Using Tab-Completion and the Integrated documentation

TC-Toolbox contains over 1000 functions and more than 200 classes. These functions are available for use in different contexts, as described in the *Architecture overview*.

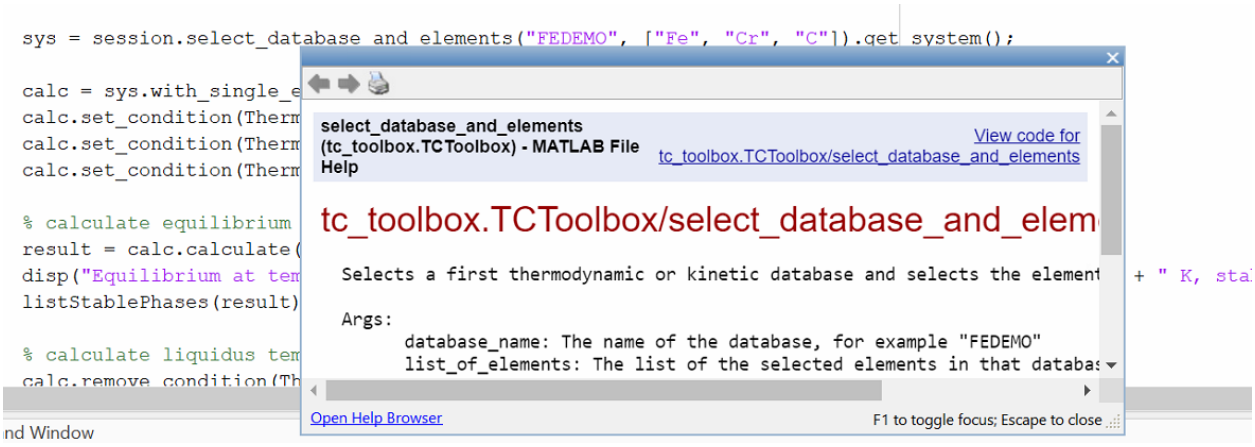
In order to know which functions and classes are available for you at a given time and how they can be used, we encourage you to use MATLAB® tab completion and the MATLAB® help.

This is a feature of MATLAB® and the exact functionality can vary depending on the version of MATLAB® and if you use MATLAB® live scripts, classic MATLAB® scripts or the interactive console.

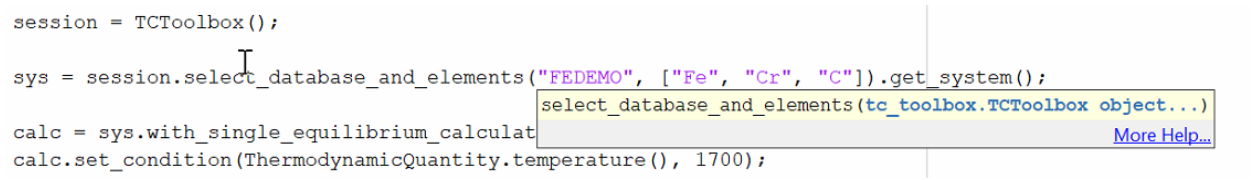
To access tab completion, press the **dot (.)** key then **Tab**. Use the **up/down arrow** keys to scroll through the list.




To open the help for a specific function or class, click to place the cursor on the function or object and press the **F1** key.




The built-in help for parameters of a specific function can be reached by placing the cursor within the parentheses of the function and pressing **CTRL + F1**.




Click **More Help...** to view the corresponding help text.

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**Note:** The MATLAB® script first needs to be run before you can view help text when **More Help...** is clicked. Once the script is run, the respective object is present in the workspace and the help is available.

---

## 3.2 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, etc.). This is 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 has already been calculated. "Similar" refers here primarily to composition, temperature, and entered phase set. This case can occur, for example, with the Thermo-Calc nickel-based superalloys database, TCNi.
- Convenient and fast switching between states that have changed a lot (for example regarding suspended phases, numerical settings, etc.)

The mechanism of saving and restoring the state is called bookmarking and is controlled with the two methods `bookmark_state()` and `set_state_to_bookmark()`. The following short example shows how to switch between two different states:

```
import tc_toolbox.*
session = TCToolbox();

calc = session...
        .select_database_and_elements("FEDEMO", ["Fe", "C"])...
        .get_system()...
```

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```
        .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);
disp("Conditions do contain temperature:")
disp(result_temp.get_conditions())
% this calculation had already been performed
disp("Stable phases (do not contain BCC):")
disp(result_temp.get_stable_phases())

result_fixed_phase = calc.set_state_to_bookmark(bookmark_fixed_phase_condition);
disp("Conditions do not contain temperature:")
disp(result_fixed_phase.get_conditions())
% this calculation had **not yet** been performed
disp("Stable phases (do contain BCC):")
disp(calc.calculate().get_stable_phases())
```

## 3.3 Re-use and Saving Results

Before a calculation is run in MATLAB®, 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 MATLAB®, but you can make it work the same way when re-running a script, or even when running a completely different script.

You can set up a folder location to re-use results from saved calculations. This folder can be a network folder and shared by many users. This is done using the method `set_cache_folder()`.

```
import tc_toolbox.*

session = TCToolbox();
session.set_cache_folder("cache")
```

The calculation is not re-run if there is a previous MATLAB® 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:

```
import tc_toolbox.*

session = TCToolbox();
% ... 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, for example:

```
import tc_toolbox.*

session = TCToolbox();
result = session.load_result_from_disk().diffusion("./result_dir")
[x, frac] = result.get_mole_fraction_of_component_at_time("Cr", 1000.0)
```

## 3.4 Using the TCToolbox class efficiently

Normally you should only create *one* `TCToolbox()` variable.

---

**Note:** When a `TCToolbox()` variable is deleted, the Java backend engine process is stopped and all temporary data is deleted. When creating a new `TCToolbox()` variable, a new Java process is started. This can take several seconds.

---

If appropriate, it is safe to create a `TCToolbox()` variable 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 creating a `TCToolbox()` variable multiple times, you can use the following pattern.

**Example**:

```
import tc_toolbox.*

session = tc_toolbox.TCToolbox();
system = session.select_database_and_elements("FEDEMO", ["Fe", "Cr"]).get_system();
calculation = system.with_single_equilibrium_calculation();
calculation.set_condition("T", 1000);

for i = 0:50
    calculate(calculation)
end

function calculate(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
end
```

## 3.5 Parallel Calculations

It is possible to perform parallel calculations with TC-Toolbox using the Parallel Computing Toolbox™ of MATLAB®. This is a separate toolbox that can be purchased for MATLAB®, it is not part of the standard configuration of MATLAB®.

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.

**Example**:

```
num_processes = 2;
min_cr = 10;  % in wt-%
max_cr = 19;  % in wt-%
delta_cr = 1;  % in wt-%
chunk_size = 5;  % this simple code expects that the Cr-range can be exactly divided␣
↪into such chunks

if (isempty(gcp('nocreate')))
    parpool("local", num_processes);
end

num_points = 1 + (max_cr - min_cr) / delta_cr;
total_cr_range = linspace(min_cr, max_cr, num_points);
chunked_cr_ranges = num2cell(reshape(total_cr_range, chunk_size, []), 1);

% this requires the Parallel Computing Toolbox(TM), can be run with "for" instead␣
↪without parallelization
num_chunks = ceil(num_points / chunk_size);
bcc_fraction_results = cell(num_chunks, 1);
parfor chunk_index = 1 : num_chunks
    bcc_fraction_results{chunk_index} = do_perform(chunked_cr_ranges{chunk_index});
end

bcc_phase_fraction = cell2mat(bcc_fraction_results);
% ... use the result in `bcc_phase_fraction`, for example for plotting


function phase_fractions = do_perform(cr_range)
    % this function is running in a subprocess
    import tc_toolbox.step_or_map_diagrams.*
    import tc_toolbox.*

    elements = ["Fe", "Cr", "Ni", "C"];

    session = TCToolbox();

    sys = session.select_database_and_elements("FEDEMO", elements).get_system();

    calc = sys.with_single_equilibrium_calculation();
    calc.set_condition(ThermodynamicQuantity.temperature(), 1100.0); % in K
    calc.set_condition(ThermodynamicQuantity.mass_fraction_of_a_component("C"), 0.1 /␣
↪100);
    calc.set_condition(ThermodynamicQuantity.mass_fraction_of_a_component("Ni"), 2.0 /
↪ 100);

    phase_fractions = zeros(size(cr_range, 1));
    for cr_index = 1 : size(cr_range, 1)
        cr = cr_range(cr_index);
        calc.set_condition("W(Cr)", cr / 100);
        result = calc.calculate();
        phase_fractions(cr_index) = result.get_value_of("NPM(BCC_A2)");
    end
end
```

## 3.6 Handling Calculation Engine Crashes

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 error you can use: `UnrecoverableCalculationException()`.

That error is raised if the calculation server enters a state where no further calculations are possible. You should catch that exception and create a new instance of `TCToolbox()`, which you use from that point.

**Example**:

```
import tc_toolbox.*
import tc_toolbox.diffusion.*

temperatures = linspace(900,1100,10);
session = TCToolbox();
for i = 1:length(temperatures)
    temperature = temperatures(i);
    try
        diffusion_result = session...
                .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);
        disp("Succeeded!")

    catch e
        if contains(e.message, 'UnrecoverableCalculationException')
            disp('Could not calculate. Creating a new TCToolbox and continuing with␣
↪next calculation...')
            session = TCToolbox();
        else
            disp('Could not calculate. Using the previous TCToolbox and continuing␣
↪with next calculation...')
        end
    end
end
```

## 3.7 Process Metallurgy Calculations

### 3.7.1 Equilibrium calculations with changing elements between calculations

It is possible to add, change or remove additions after performing an equilibrium calculation using *+tc_toolbox.+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)**:

```
import tc_toolbox.process_metallurgy.base.*;
import tc_toolbox.process_metallurgy.equilibrium.*;
import tc_toolbox.*

session = tc_toolbox.TCToolbox();

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

% add the element Al with zero-fraction already
steel = EquilibriumAddition(containers.Map(["Fe", "C", "Al"]), {NaN, 4.5, 0.0}), 100.
↪0e3, 1700 + 273.15);
slag = EquilibriumAddition(containers.Map(["CaO", "SiO2"], {70.0, 30.0}), 3.0e3, 1700␣
↪+ 273.15);

al_addition = EquilibriumAddition(containers.Map(["Al"], {100}), 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**:

```
import tc_toolbox.process_metallurgy.base.*;
import tc_toolbox.process_metallurgy.equilibrium.*;
import tc_toolbox.*

session = tc_toolbox.TCToolbox();

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

steel = EquilibriumAddition(containers.Map(["Fe", "C"]), {NaN, 4.5}), 100.0e3, 1700 +␣
↪273.15);
slag = EquilibriumAddition(containers.Map(["CaO", "SiO2"], {70.0, 30.0}), 3.0e3, 1700␣
↪+ 273.15);
```

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```
% add the addition for now with zero-amount
al_addition = EquilibriumAddition(containers.Map(["Al"], {100}), 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 ...
```

### 3.7.2 Zones

TC-Toolbox 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.

### 3.7.3 Applications

While this approach can in principle be extended to any number of zones, in the current release TC-Toolbox 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_toolbox.+process_metallurgy.+process.Zone.add_power()*)
- cooling (*+tc_toolbox.+process_metallurgy.+process.Zone.add_power()*)
- heat transfer between bulk zones (*+tc_toolbox.+process_metallurgy.+process.ReactionZone.add_heat_transfer()*)
- inclusion formation
- inclusion flotation and other transfer of phase groups between bulk zones (*+tc_toolbox.+process_metallurgy.+process.ReactionZone.add_transfer_of_phase_group()*)
- addition of material and gas at any time in any zone (*+tc_toolbox.+process_metallurgy.+process.Zone.add_addition()* / *+tc_toolbox.+process_metallurgy.+process.Zone.add_continuous_addition()*)
- an exhaust gas zone collecting all formed gas (*+tc_toolbox.+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.

### 3.7.4 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-Toolbox 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

FOUR

# API REFERENCE

## 4.1 Calculations

### 4.1.1 Package "single_equilibrium"

**class** +tc_toolbox.+single_equilibrium.**AbstractSingleEquilibriumCalculation**(*back*)

Abstract configuration required for a single equilibrium calculation.

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

**AbstractSingleEquilibriumCalculation**(*back*)

Call base constructor: tc_toolbox.AbstractCalculation.

**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**()

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

**Returns** The components

**get_configuration_as_string**()

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_gibbs_energy_addition_for**(*phase*)

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**()
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.

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

---

**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 Thermo-Calc Console Mode command

**Returns** This *SingleEquilibriumCalculation* object

**set_component_to_entered**(*component*)
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*, *reset_conditions*)
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*, *gibbs_energy*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *SingleEquilibriumCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)

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_toolbox.+single_equilibrium.**SingleEquilibriumCalculation**(*back*)

Configuration for a single equilibrium calculation.

---

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

---

**SingleEquilibriumCalculation**(*back*)

Call base constructor: `tc_toolbox.single_equilibrium.AbstractSingleEquilibriumCalculation`.

**bookmark_state**(*bookmark_id*)

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**()

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.

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

**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.

**calculate_with_state**(*timeout_in_minutes*)

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**()

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

**Returns** The components

**get_configuration_as_string**()

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_gibbs_energy_addition_for**(*phase*)

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*, *precipitate_phases*, *zero_volume_elements*)
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**()
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.

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

**Returns** This *SingleEquilibriumCalculation* object

**remove_condition**(*quantity*)
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*)
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

**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 Thermo-Calc Console Mode command

**Returns** This *SingleEquilibriumCalculation* object

**set_component_to_entered**(*component*)
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*, *reset_conditions*)
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*, *value*)
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*, *gibbs_energy*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
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*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *SingleEquilibriumCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)
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_toolbox.+single_equilibrium.**SingleEquilibriumOptions**
General simulation conditions for the thermodynamic calculations.

**SingleEquilibriumOptions**()
General simulation conditions for thermodynamic calculations. Constructs an instance of *SingleEquilibriumOptions*.

**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.

---

**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.

---

**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*)
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*)
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*)
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*)
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_toolbox.+single_equilibrium.**SingleEquilibriumResult**(*back*)
Result of a single equilibrium calculation, it can be evaluated using a Quantity or Console Mode syntax.

**SingleEquilibriumResult**(*back*)
Call base constructor: tc_toolbox.AbstractResult.

**change_pressure**(*pressure*)
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*)
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**()
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**()
Returns the conditions.

**Returns** The selected conditions

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

**Returns** The names of the stable phases

**get_value_of**(*quantity*)
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

**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.

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

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

**Returns** This *SingleEquilibriumCalculation* object

**save_to_disk**(*path*)
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_toolbox.+single_equilibrium.**SingleEquilibriumTempResult**(*back*)
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.

**SingleEquilibriumTempResult**(*back*)
Call base constructor: `tc_toolbox.AbstractResult`.

**change_pressure**(*pressure*)
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*)
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**()
Returns the names of the components selected in the system (including any components auto-selected by the database(s)).

**Returns** If something has been changed in the state of the calculation since that result object has been created

**get_conditions**()
Returns the conditions.

**Returns** If something has been changed in the state of the calculation since that result object has been created

**get_phases**()
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** If something has been changed in the state of the calculation since that result object has been created

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

**Returns** If something has been changed in the state of the calculation since that result object has been created

**get_value_of**(*quantity*)
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** If something has been changed in the state of the calculation since that result object has been created

**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.

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

---

**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 Thermo-Calc Console Mode command

**Returns** This *SingleEquilibriumCalculation* object

### 4.1.2 Package "batch_equilibrium"

**class** +tc_toolbox.+batch_equilibrium.**BatchEquilibriumCalculation**(*back*)
Configuration for a series of single equilibrium calculations performed in a vectorized fashion.

---

**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).

---

---

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

---

**BatchEquilibriumCalculation**(*back*)
Call base constructor: `tc_toolbox.AbstractCalculation`.

**calculate**(*quantities*, *logging_frequency*, *timeout_in_minutes*)
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**()
Returns a list of components in the system (including all components auto-selected by the database(s)).

**Returns** The components

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

**Returns** This *BatchEquilibriumCalculation* object

**remove_condition**(*quantity*)
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*)
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

---

**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 Thermo-Calc Console Mode command

**Returns** This *BatchEquilibriumCalculation* object

**set_component_to_entered**(*component*)
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*, *reset_conditions*)
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*, *value*)
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*)
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:

- A Console Mode syntax string or a `ThermodynamicQuantity` instance,
- 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*, *gibbs_energy*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *BatchEquilibriumCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)
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_toolbox.+batch_equilibrium.**BatchEquilibriumResult**(*back*)
Result of a batch equilibrium calculation. This can be used to query for specific values.

**BatchEquilibriumResult**(*back*)
Constructs an instance of *BatchEquilibriumResult*.

**get_values_of**(*quantity*)
Returns values from a batch equilibrium calculation.

Example:

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

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

**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.

### 4.1.3 Package "precipitation"

**class** +tc_toolbox.+precipitation.**FixedGrainSize**(*grain_radius*)
Factory class providing objects representing a grain growth model.

**FixedGrainSize**(*grain_radius*)
Fixed grain radius size. **Default**: 1.0E-4 m

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

**static fixed_grain_size**(*grain_radius*)
Fixed grain radius size. **Default**: 1.0E-4 m

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

**static grain_growth**(*grain_size_distribution*)
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

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

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

**class** +tc_toolbox.+precipitation.**GrainGrowth**(*grain_size_distribution*)
Factory class providing objects representing a grain growth model.

**GrainGrowth**(*grain_size_distribution*)
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

**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

**static fixed_grain_size**(*grain_radius*)
Fixed grain radius size. **Default**: 1.0E-4 m

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

**static grain_growth**(*grain_size_distribution*)
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

**set_grain_boundary_energy**(*energy*)
Set the energy of the grain bounday.

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

**Returns** This *GrainSizeDistribution* object

**set_grain_boundary_mobility_activation_energy**(*activation_energy*)
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*)
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_toolbox.+precipitation.**GrainGrowthModel**
Factory class providing objects representing a grain growth model.

**static fixed_grain_size**(*grain_radius*)
Fixed grain radius size. **Default**: 1.0E-4 m

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

**static grain_growth**(*grain_size_distribution*)
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_toolbox.+precipitation.**GrainSizeDistribution**
Represents the grain size distribution at a certain time.

**GrainSizeDistribution**()
Constructs an instance of *GrainSizeDistribution*.

**add_radius_and_number_density**(*radius*, *number_density*)
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_toolbox.+precipitation.**GrowthRateModel**
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.

**class** +tc_toolbox.+precipitation.**MatrixPhase**(*matrix_phase_name*)
The matrix phase in a precipitation calculation

**MatrixPhase**(*matrix_phase_name*)

**add_precipitate_phase**(*precipitate_phase*)
Adds a precipitate phase.

**Parameters** **precipitate_phase** – The precipitate phase

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

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

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

---

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

---

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

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

---

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

---

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

**set_mobility_enhancement_activation_energy**(*mobility_enhancement_activation_energy*)
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*)
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*)
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*, *c12*, *c44*)
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*, *poisson_ratio*)
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*)
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_toolbox.+precipitation.**NumericalParameters**
Numerical parameters

**NumericalParameters**()
Constructs an instance of *NumericalParameters*.

**set_max_overall_volume_change**(*max_overall_volume_change*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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_toolbox.+precipitation.**ParticleSizeDistribution**
Represents the state of a microstructure evolution at a certain time including its particle size distribution, composition and overall phase fraction.

**ParticleSizeDistribution**()
Constructs an instance of *ParticleSizeDistribution*.

**add_radius_and_number_density**(*radius*, *number_density*)
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*, *composition_value*)
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*)
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*)
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_toolbox.+precipitation.**PrecipitateElasticProperties**
Represents the elastic transformation strain of a certain precipitate class.

---

**Note:** This class is only relevant if the option `TransformationStrainCalculationOption.USER_DEFINED` has been chosen using *PrecipitatePhase.set_transformation_strain_calculation_opti*
The elastic strain can only be considered for non-spherical precipitates.

---

**PrecipitateElasticProperties**()
Constructs an instance of *PrecipitateElasticProperties*.

**set_e11**(*e11*)
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*)
Sets the strain tensor component e12. **Default**: 0.0

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

**Returns** This *PrecipitateElasticProperties* object

**set_e13**(*e13*)
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*)
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*)
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*)
Sets the elastic strain tensor component e33. **Default**: 0.0

**Parameters** **e33** – The elastic strain tensor component e33

**Returns** This *PrecipitateElasticProperties* object

**class** +tc_toolbox.+precipitation.**PrecipitateMorphology**
Available precipitate morphologies.

**class** +tc_toolbox.+precipitation.**PrecipitatePhase**(*precipitate_phase_name*)
Represents a certain precipitate class (i.e. a group of precipitates with the same phase and settings).

**PrecipitatePhase**(*precipitate_phase_name*)

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

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

---

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

---

**Returns** This *PrecipitatePhase* object

**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.

---

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

---

**Returns** This *PrecipitatePhase* object

**set_alias**(*alias*)
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.

---

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

---

**Parameters** **alias** – The alias string for this class of precipitates

**Returns** This *PrecipitatePhase* object

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

---

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

---

**Parameters** **aspect_ratio_value** – The aspect ratio value

**Returns** This *PrecipitatePhase* object

**set_gibbs_energy_addition**(*gibbs_energy_addition*)
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*)
Sets the interfacial energy. **Default**: If the interfacial energy is not set, it is automatically calculated using a broken-bond model.

---

**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.

---

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

**Returns** This *PrecipitatePhase* object

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

---

**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

---

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

**Returns** This *PrecipitatePhase* object

**set_molar_volume**(*volume*)
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*)
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*, *number_density*)
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*, *number_density*)
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*, *number_density*)
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*)
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*)
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*)
Sets the precipitate morphology. **Default**: `PrecipitateMorphology.SPHERE`

**Parameters** **precipitate_morphology_enum** – The precipitate morphology

**Returns** This *PrecipitatePhase* object

**set_transformation_strain_calculation_option**(*transformation_strain_calculation_option_enum*)
Sets the transformation strain calculation option. **Default**: `TransformationStrainCalculationOption.DISREGARD`.

**Parameters** **transformation_strain_calculation_option_enum** – The chosen option

**Returns** This *PrecipitatePhase* object

**with_elastic_properties**(*elastic_properties*)
Sets the elastic properties. **Default**: The elastic transformation strain is disregarded by default.

---

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

---

**Parameters** **elastic_properties** – The elastic properties object

**Returns** This *PrecipitatePhase* object

**with_growth_rate_model**(*growth_rate_model_enum*)
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*)
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.

---

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

---

**Parameters** **particle_size_distribution** – The initial particle size distribution object

**Returns** This *PrecipitatePhase* object

**class** +tc_toolbox.+precipitation.**PrecipitationCCTCalculation**(*back*)
Configuration for a Continuous-Cooling-Time (CCT) precipitation calculation.

**PrecipitationCCTCalculation**(*back*)
Call base constructor: `tc_toolbox.AbstractCalculation`.

**calculate**(*timeout_in_minutes*)
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_configuration_as_string**()
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**()
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.

**set_composition**(*element_name*, *value*)
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*)
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*)
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*)
Sets maximum temperature of the CCT diagram.

**Parameters** **max_temperature** – the maximum temperature [K]

**Returns** This *PrecipitationCCTCalculation* object

**set_min_temperature**(*min_temperature*)
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*)
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*)
Sets the matrix phase.

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

**Returns** This *PrecipitationCCTCalculation* object

**with_numerical_parameters**(*numerical_parameters*)
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*)
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_toolbox.+precipitation.**PrecipitationCalculationResult**(*back*)
Result of a precipitation calculation. This can be used to query for specific values.

**PrecipitationCalculationResult**(*back*)
Call base constructor: `tc_toolbox.AbstractResult`.

**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.

**save_to_disk**(*path*)
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_toolbox.+precipitation.**PrecipitationCalculationSingleResult**(*back*)
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*.

**PrecipitationCalculationSingleResult**(*back*)
Call base constructor: `tc_toolbox.precipitation.PrecipitationCalculationResult`.

**get_aspect_ratio_distribution_for_particle_length_of**(*precipitate_id*, *time*)
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*, *time*)
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*)
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*, *time*)
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*, *time*)
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*)
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**()
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**()
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**()
Returns the grain number density in dependency of the time.

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

**get_grain_number_density_distribution_for_length**(*time*)
Returns the number density distribution of grains in dependency of its mean particle length at a certain time.

**Parameters** **time** – The time [s]

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

**get_grain_number_density_distribution_for_radius**(*time*)
Returns the number density distribution of a grains in dependency of its mean radius at a certain time.

**Parameters** **time** – The time [s]

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

**get_grain_size_distribution**(*time*)
Returns the size distribution of the matrix phase in dependency of its grain radius length at a certain time.

**Parameters** **time** – The time [s]

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

**get_matrix_composition_in_mole_fraction_of**(*element_name*)
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*)
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*)
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*)
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*)
Returns the mean particle length of a precipitate in dependency of the time.

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

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

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

**get_mean_radius_of** (*precipitate_id*)
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*)
Returns the normalized number density distribution of a grains at a certain time.

**Parameters** **time** – The time [s]

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

**get_normalized_number_density_distribution_of** (*precipitate_id*, *time*)
Returns the normalized number density distribution of a precipitate at a certain time.

**Parameters**

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

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

**get_nucleation_rate_of** (*precipitate_id*)
Returns the nucleation rate of a precipitate in dependency of the time.

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

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

**get_number_density_distribution_for_particle_length_of** (*precipitate_id*, *time*)
Returns the number density distribution of a precipitate in dependency of its mean particle length at a certain time.

**Parameters**

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

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

**get_number_density_distribution_for_radius_of** (*precipitate_id*, *time*)
Returns the number density distribution of a precipitate in dependency of its mean radius at a certain time.

**Parameters**

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

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

**get_number_density_of**(*precipitate_id*)
Returns the particle number density of a precipitate in dependency of the time.

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

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

**get_precipitate_composition_in_mole_fraction_of**(*precipitate_id*, *element_name*)
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*, *element_name*)
Returns the precipitate composition (as weight fraction) of a certain element in dependency of the time.

**Parameters**

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

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

**get_size_distribution_for_particle_length_of**(*precipitate_id*, *time*)
Returns the size distribution of a precipitate in dependency of its mean particle length at a certain time.

**Parameters**

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

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

**get_size_distribution_for_radius_of**(*precipitate_id*, *time*)
Returns the size distribution of a precipitate in dependency of its mean radius at a certain time.

**Parameters**

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

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

**get_volume_fraction_of**(*precipitate_id*)
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)

**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.

**save_to_disk**(*path*)
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_toolbox.+precipitation.**PrecipitationCalculationTTTorCCTResult**(*back*)
Result of a TTT or CCT precipitation calculation.

**PrecipitationCalculationTTTorCCTResult**(*back*)
Call base constructor: `tc_toolbox.precipitation.PrecipitationCalculationResult`.

**get_result_for_precipitate**(*precipitate_id*)
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])

**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.

**save_to_disk**(*path*)
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_toolbox.+precipitation.**PrecipitationIsoThermalCalculation**(*back*)
Configuration for an isothermal precipitation calculation.

**PrecipitationIsoThermalCalculation**(*back*)
Call base constructor: `tc_toolbox.AbstractCalculation`.

**calculate**(*timeout_in_minutes*)
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_configuration_as_string**()
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**()
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.

**set_composition**(*element_name*, *value*)
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*)
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*)
Sets the simulation time.

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

**Returns** This *PrecipitationIsoThermalCalculation* object

**set_temperature**(*temperature*)
Sets the temperature for the isothermal simulation.

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

**Returns** This *PrecipitationIsoThermalCalculation* object

**with_matrix_phase**(*matrix_phase*)
Sets the matrix phase.

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

**Returns** This *PrecipitationIsoThermalCalculation* object

**with_numerical_parameters**(*numerical_parameters*)
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*)
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_toolbox.+precipitation.**PrecipitationNonIsoThermalCalculation**(*back*)

Configuration for a non-isothermal precipitation calculation.

**PrecipitationNonIsoThermalCalculation**(*back*)

Call base constructor: `tc_toolbox.AbstractCalculation`.

**calculate**(*timeout_in_minutes*)

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_configuration_as_string**()

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**()

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.

**set_composition**(*element_name*, *value*)

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*)
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*)
Sets the simulation time.

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

**Returns** This `PrecipitationNonThermalCalculation` object

**with_matrix_phase**(*matrix_phase*)
Sets the matrix phase.

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

**Returns** This *PrecipitationIsoThermalCalculation* object

**with_numerical_parameters**(*numerical_parameters*)
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*)
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*)
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_toolbox.+precipitation.`**PrecipitationTTTCalculation**(*back*)
Configuration for a TTT (Time-Temperature-Transformation) precipitation calculation.

**PrecipitationTTTCalculation**(*back*)
Call base constructor: `tc_toolbox.AbstractCalculation`.

**calculate**(*timeout_in_minutes*)
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_configuration_as_string**()
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**()
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.

**set_composition**(*element_name*, *value*)
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*)
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*)
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*)
Sets the maximum temperature for the TTT diagram.

**Parameters** **max_temperature** – the maximum temperature [K]

**Returns** This *PrecipitationTTTCalculation* object

**set_min_temperature**(*min_temperature*)
Sets the minimum temperature for the TTT diagram.

**Parameters** **min_temperature** – the minimum temperature [K]

**Returns** This *PrecipitationTTTCalculation* object

**set_temperature_step** (*temperature_step*)
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*)
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*)
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*)
Sets the matrix phase.

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

**Returns** This *PrecipitationTTTCalculation* object

**with_numerical_parameters** (*numerical_parameters*)
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*)
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_toolbox.+precipitation.**TransformationStrainCalculationOption**
Options for calculating the transformation strain.

**class** +tc_toolbox.+precipitation.**VolumeFractionOfPhaseType**
Unit of the volume fraction of a phase.

### 4.1.4 Package "scheil"

**class** +tc_toolbox.+scheil.**CalculateSecondaryDendriteArmSpacing**

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.

**CalculateSecondaryDendriteArmSpacing**()

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. Constructs an instance of *CalculateSecondaryDendriteArmSpacing*.

**static 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*

**static constant_secondary_dendrite_arm_spacing**(*secondary_dendrite_arm_spacing*)

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*

**static 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*

**static scheil_classic**()

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

**static 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*

**set_c**(*c*)

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*)

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*)
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*)
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*)
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_toolbox.+scheil.**ConstantSecondaryDendriteArmSpacing**(*secondary_dendrite_arm_spacing*)
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.

**ConstantSecondaryDendriteArmSpacing**(*secondary_dendrite_arm_spacing*)
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.

**Default**: 50 µm

**Parameters** **secondary_dendrite_arm_spacing** – The dendrite arm spacing [m]

**static 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*

**static constant_secondary_dendrite_arm_spacing**(*secondary_dendrite_arm_spacing*)
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*

**static 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*

**static scheil_classic**()
Configuration for Classic Scheil with fast diffusers. :return: A *ScheilClassic*

**static 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*

**set_cooling_rate**(*cooling_rate*)
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*)
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*)
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_toolbox.+scheil.**ScheilBackDiffusion**
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.

**static 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*

**static constant_secondary_dendrite_arm_spacing**(*secondary_dendrite_arm_spacing*)
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*

**static 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*

**static scheil_classic**()
Configuration for Classic Scheil with fast diffusers. :return: A *ScheilClassic*

**static 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_toolbox.+scheil.**ScheilCalculation**(*back*)
Configuration for a Scheil solidification calculation.

---

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

---

**ScheilCalculation**(*back*)
Call base constructor: tc_toolbox.AbstractCalculation.

**calculate**(*timeout_in_minutes*)
Runs the Scheil calculation.

> **Warning:** Scheil calculations do not support the GAS phase being selected, this means the *GAS phase must always be deselected in the system* if it is present in the database

**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_configuration_as_string**()
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**()
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.

**set_composition**(*component_name*, *value*)
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*)
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*)
Sets the start temperature.

**Default**: 2500.0 K

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

**Parameters** **temperature_in_kelvin** – The temperature [K]

**Returns** This *ScheilCalculation* object

**with_calculation_type**(*scheil_calculation_type*)
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*)
Sets the Scheil simulation options.

**Parameters** **options** – The Scheil simulation options

**Returns** This *ScheilCalculation* object

**with_system_modifications**(*system_modifications*)
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_toolbox.+scheil.**ScheilCalculationResult**(*back*)
Result of a Scheil calculation.

**ScheilCalculationResult**(*back*)
Call base constructor: `tc_toolbox.AbstractResult`.

**get_values_grouped_by_quantity_of**(*x_quantity*, *y_quantity*, *sort_and_merge*)
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*, *y_quantity*, *sort_and_merge*)

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*, *y_quantity*)

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

**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.

**save_to_disk**(*path*)
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_toolbox.+scheil.**ScheilCalculationType**
Specific configuration for the different Scheil calculation types

**static 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*

**static scheil_classic**()
Configuration for Classic Scheil with fast diffusers. :return: A *ScheilClassic*

**static 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_toolbox.+scheil.**ScheilClassic**
Configuration for Classic Scheil with fast diffusers.

**ScheilClassic**()
Configuration for Classic Scheil when fast diffusers are included. Constructs an instance of *ScheilClassic*.

**static 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*

**static scheil_classic**()
Configuration for Classic Scheil with fast diffusers. :return: A *ScheilClassic*

**static 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*

**set_fast_diffusing_elements**(*element_names*)
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_toolbox.+scheil.**ScheilOptions**

Options for the Scheil simulation.

**ScheilOptions**()

Options for the Scheil simulation. Constructs an instance of *ScheilOptions*.

**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

**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.

---

**Returns** This *ScheilOptions* object

**disable_control_step_size_during_minimization**()

Disables stepsize control during minimization (non-global).

**Default**: Enabled

**Returns** This *ScheilOptions* object

**disable_equilibrium_solidification_calculation**()

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

In general it is not necessary to perform this calculation.

**Default**: Disabled. The equilibrium solidification calculation is skipped.

**Returns** This *ScheilOptions* object

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

**Default**: Enabled

**Returns** This *ScheilOptions* object

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

**Default**: Enabled

---

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

---

**Returns** This *ScheilOptions* object

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

**Default**: Enabled

**Returns** This *ScheilOptions* object

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

In general it is not necessary to perform this calculation.

**Default**: Disabled. The equilibrium solidification calculation is skipped.

**Returns** This *ScheilOptions* object

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

**Default**: Enabled

**Returns** This *ScheilOptions* object

**set_gas_phase**(*phase_name*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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_toolbox.+scheil.**ScheilSoluteTrapping**
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.

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

**static 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*

**static scheil_classic**()
Configuration for Classic Scheil with fast diffusers. :return: A *ScheilClassic*

**static 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*

**set_angle**(*alpha*)
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*)
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*)
Sets the scanning speed.

**Default**: 1 m/s

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

**Returns** This *ScheilSoluteTrapping* object

### 4.1.5 Package "step_or_map_diagrams"

**class** +tc_toolbox.+step_or_map_diagrams.**AbstractAxisType**
The abstract base class for all axis types.

**class** +tc_toolbox.+step_or_map_diagrams.**AbstractPhaseDiagramCalculation**(*back*)
Abstract configuration required for a property diagram calculation.

---

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

---

**AbstractPhaseDiagramCalculation**(*back*)
Call base constructor: tc_toolbox.AbstractCalculation.

**add_initial_equilibrium**(*initial_equilibrium*)
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*, *timeout_in_minutes*)

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

**Returns** The component names

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

---

**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 Thermo-Calc Console Mode command

**Returns** This *PhaseDiagramCalculation* object

**set_gibbs_energy_addition_for**(*phase*, *gibbs_energy*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *PhaseDiagramCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)
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_toolbox.+step_or_map_diagrams.**AbstractPropertyDiagramCalculation**(*back*)
Abstract configuration required for a property diagram calculation.

---

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

---

**AbstractPropertyDiagramCalculation**(*back*)
Call base constructor: `tc_toolbox.AbstractCalculation`.

**calculate**(*keep_previous_results*, *timeout_in_minutes*)

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

**Returns** The component names

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

---

**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 Thermo-Calc Console Mode command

**Returns** This *PropertyDiagramCalculation* object

**set_gibbs_energy_addition_for**(*phase*, *gibbs_energy*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *PropertyDiagramCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)

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_toolbox.+step_or_map_diagrams.**AxisType**

Factory class providing objects for configuring a logarithmic or linear axis by using *AxisType.linear()* or *AxisType.logarithmic()*.

**static 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

**static 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_toolbox.+step_or_map_diagrams.**CalculationAxis**(*quantity*)

A calculation axis used for property and phase diagram calculations.

**Default**: A *Linear* axis with a *minimum number of 40 steps*

**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*.

**CalculationAxis**(*quantity*)

**Default**: A *Linear* axis with a minimum number of 40 steps

**Parameters** **quantity** – The `ThermodynamicQuantity` to set as axis variable; a Console Mode syntax string can be used as an alternative (for example "X(Cr)")

**set_max**(*max*)

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*)

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*)

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*)

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_toolbox.+step_or_map_diagrams.**Direction**

An enumeration.

**class** +tc_toolbox.+step_or_map_diagrams.**InitialEquilibrium**(*first_axis*, *second_axis*)

**InitialEquilibrium**(*first_axis*, *second_axis*)

**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*)
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_toolbox.+step_or_map_diagrams.**Linear**
Represents a linear axis.

**Linear**()
Creates an object representing a linear axis. Constructs an instance of *Linear*.

**get_type**()
Convenience method for getting axis type.

**Returns** The type

**static 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

**static 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

**set_max_step_size**(*max_step_size*)
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*)
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_toolbox.+step_or_map_diagrams.**Logarithmic**(*scale_factor*)
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.

**Logarithmic**(*scale_factor*)
Creates an object representing a logarithmic axis.

**Default**: 1.1

**Parameters** **scale_factor** – The scale factor setting the maximum factor between two calculated values, must be larger than 1.0.

**get_type**()
Convenience method for getting axis type.

**Returns** The type

**static 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

**static 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

**set_scale_factor**(*scale_factor*)
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_toolbox.+step_or_map_diagrams.**PhaseDiagramCalculation**(*back*)
Configuration for a phase diagram calculation.

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

**PhaseDiagramCalculation**(*back*)
Call base constructor: tc_toolbox.step_or_map_diagrams.AbstractPhaseDiagramCalculation.

**add_initial_equilibrium**(*initial_equilibrium*)
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*, *timeout_in_minutes*)
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**()
Returns the names of the components in the system (including all components auto-selected by the database(s)).

**Returns** The component names

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

---

**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 Thermo-Calc Console Mode command

**Returns** This *PhaseDiagramCalculation* object

**set_condition**(*quantity*, *value*)
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*, *gibbs_energy*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
Sets the first calculation axis.

**Parameters** **axis** – The axis

**Returns** This *PhaseDiagramCalculation* object

**with_options**(*options*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *PhaseDiagramCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)
Sets the second calculation axis.

**Parameters** **axis** – The axis

**Returns** This *PhaseDiagramCalculation* object

**with_system_modifications**(*system_modifications*)
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_toolbox.+step_or_map_diagrams.**PhaseDiagramOptions**
Simulation options for phase diagram calculations.

**PhaseDiagramOptions**()
Simulation options for the phase diagram calculations. Constructs an instance of *PhaseDiagramOptions*.

**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.

**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.

**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*)
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*)
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*)
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*)
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*)
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*)
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_toolbox.+step_or_map_diagrams.**PhaseDiagramResult**(*back*)
Result of a phase diagram calculation, it can be evaluated using quantities or Console Mode syntax.

**PhaseDiagramResult**(*back*)
Call base constructor: tc_toolbox.AbstractResult.

**add_coordinate_for_phase_label**(*x*, *y*)
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*, *y_quantity*)
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 *'='*.

**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*, *y_quantity*)

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 *'='*.

---

**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

**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.

**remove_phase_labels**()

Erases all added coordinates for phase labels.

**Returns** This *PhaseDiagramResult* object

**save_to_disk**(*path*)

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*)

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_toolbox.+step_or_map_diagrams.**PhaseDiagramResultValues**(*back*)
Represents the data of a phase diagram.

**PhaseDiagramResultValues**(*back*)
Constructs an instance of *PhaseDiagramResultValues*.

**get_invariants**()
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**()
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**()
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**()
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_toolbox.+step_or_map_diagrams.**PhaseLabel**(*back*)
Represents a *phase label at a plot coordinate*, i.e. the stable phases that are present at that *plot* coordinate.

**PhaseLabel**(*back*)
Constructs an instance of *PhaseLabel*.

**get_text**()
Accessor for the phase label :return: the phase label

**get_x**()
Accessor for the x-value :return: the x value

**get_y**()
Accessor for the y-value :return: the y value

**class** +tc_toolbox.+step_or_map_diagrams.**PhaseNameStyle**
The style of the phase names used in the labels.

**class** +tc_toolbox.+step_or_map_diagrams.**PropertyDiagramCalculation**(*back*)
Abstract configuration required for a property diagram calculation.

---

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

---

**PropertyDiagramCalculation**(*back*)
Call base constructor: tc_toolbox.step_or_map_diagrams.AbstractPropertyDiagramCalculation.

**calculate**(*keep_previous_results*, *timeout_in_minutes*)
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**()
Returns the names of the components in the system (including all components auto-selected by the database(s)).

**Returns** The component names

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

**Returns** This *PropertyDiagramCalculation* object

**remove_condition**(*quantity*)
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*)
Runs a Thermo-Calc command from the Console Mode POLY module immediately in the engine.

---

**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 Thermo-Calc Console Mode command

**Returns** This *PropertyDiagramCalculation* object

**set_condition**(*quantity*, *value*)
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*, *gibbs_energy*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
Sets the calculation axis.

**Parameters** **axis** – The axis

**Returns** This *PropertyDiagramCalculation* object

**with_options**(*options*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *PropertyDiagramCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)
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_toolbox.+step_or_map_diagrams.**PropertyDiagramOptions**
Simulation options for the property diagram calculations.

**PropertyDiagramOptions**()
Simulation options for property diagram calculations. Constructs an instance of *PropertyDiagramOptions*.

**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.

---

**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.

---

**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*)
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*)
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*)
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*)
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*)
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_toolbox.+step_or_map_diagrams.**PropertyDiagramResult**(*back*)
Result of a property diagram. This can be used to query for specific values.

**PropertyDiagramResult**(*back*)
Call base constructor: tc_toolbox.AbstractResult.

**get_values_grouped_by_quantity_of**(*x_quantity*, *y_quantity*, *sort_and_merge*)
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 *'='*.

---

**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*, *y_quantity*, *sort_and_merge*)
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 *'='*.

**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*, *y_quantity*)

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 *'='*.

**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

**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.

**save_to_disk**(*path*)

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*)
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

### 4.1.6 Package "diffusion"

**class** +tc_toolbox.+diffusion.**AbstractBoundaryCondition**
The abstract base class for all boundary conditions.

**class** +tc_toolbox.+diffusion.**AbstractCalculatedGrid**
The abstract base class for calculated grids.

**class** +tc_toolbox.+diffusion.**AbstractElementProfile**
The abstract base class for all initial composition profile types.

**class** +tc_toolbox.+diffusion.**AbstractGrid**
The abstract base class for all grids.

**class** +tc_toolbox.+diffusion.**AbstractSolver**
Abstract base class for the solvers (Classic, Homogenization and Automatic).

**class** +tc_toolbox.+diffusion.**ActivityFluxFunction**
Contains factory methods for the the different boundary conditions available.

**ActivityFluxFunction**()
Represents a boundary having a activity flux function.

This types of boundary conditions 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).

---

Constructs an instance of *ActivityFluxFunction*.

**static 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

**static closed_system**()
Factory method that creates a **new** closed-system boundary condition.

**Returns** A new *ClosedSystem* object

**static 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

**static fixed_compositions**(*unit_enum*)
Factory method that creates a **new** fixed-composition boundary condition.

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

**Returns** A new *FixedCompositions* object

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

**Returns** The type

**static mixed_zero_flux_and_activity**()
Factory method that creates a **new** mixed zero-flux and activity boundary condition

**Returns** A new *MixedZeroFluxAndActivity* object

**set_flux_function**(*element_name*, *f*, *g*, *n*, *to_time*)
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_toolbox.+diffusion.**AutomaticSolver**

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.

---

**AutomaticSolver**()

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.

---

Constructs an instance of *AutomaticSolver*.

**static 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

**static 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_toolbox.diffusion.AutomaticSolver if necessary instead.

---

**Returns** A new *ClassicSolver* object

**get_type**()

The type of the solver.

**Returns** The type

**static 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_toolbox.diffusion.AutomaticSolver instead if you do not need that behavior.

---

**Returns** A new *HomogenizationSolver* object

**set_flux_balance_equation_accuracy**(*accuracy*)

**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_toolbox.+diffusion.**BoundaryCondition**
Contains factory methods for the the different boundary conditions available.

**static 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

**static closed_system**()
Factory method that creates a **new** closed-system boundary condition.

**Returns** A new *ClosedSystem* object

**static 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

**static fixed_compositions**(*unit_enum*)
Factory method that creates a **new** fixed-composition boundary condition.

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

**Returns** A new *FixedCompositions* object

**static 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_toolbox.+diffusion.**CalculatedGrid**
Factory class for grids generated by a mathematical series (linear, geometric, ...). Use +tc_toolbox.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.

---

**static double_geometric**(*no_of_points*, *lower_geometrical_factor*, *upper_geometrical_factor*)
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

**static geometric**(*no_of_points*, *geometrical_factor*)
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

**static linear**(*no_of_points*)
Factory method that creates a **new** equally spaced grid.

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

**Returns** A new *LinearGrid* object

**class** +tc_toolbox.+diffusion.**ClassicSolver**
Solver using the *Classic model*.

**Note:** This solver **never switches** to the homogenization model even if it fails to converge. Use the +tc_toolbox.diffusion.AutomaticSolver if necessary instead.

**ClassicSolver**()
Solver using the *Classic model*.

**Note:** This solver **never switches** to the homogenization model even though the solver fails to converge. Use the +tc_toolbox.diffusion.AutomaticSolver if necessary instead.

Constructs an instance of *ClassicSolver*.

**static 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

**static 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_toolbox.diffusion.AutomaticSolver if necessary instead.

**Returns** A new *ClassicSolver* object

**get_type**()
Convenience method for getting the type of the solver.

**Returns** The type of the solver

**static 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_toolbox.diffusion.AutomaticSolver instead if you do not need that behavior.

**Returns** A new *HomogenizationSolver* object

**set_flux_balance_equation_accuracy**(*accuracy*)
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_toolbox.+diffusion.**ClosedSystem**
Represents a boundary for a closed system.

**ClosedSystem**()
Represents a boundary for a closed system. Constructs an instance of *ClosedSystem*.

**static 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.

---

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**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

**static closed_system**()
Factory method that creates a **new** closed-system boundary condition.

**Returns** A new *ClosedSystem* object

**static 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

**static fixed_compositions**(*unit_enum*)
Factory method that creates a **new** fixed-composition boundary condition.

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

**Returns** A new *FixedCompositions* object

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

**Returns** The type of the boundary condition

**static 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_toolbox.+diffusion.**CompositionProfile**(*unit_enum*)
Contains initial concentration profiles for the elements.

**CompositionProfile**(*unit_enum*)
Contains initial concentration profiles for the elements.

**Parameters** **unit_enum** – The unit of the compositions

**add**(*element_name*, *profile*)
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_toolbox.+diffusion.**ConstantProfile**(*value*)
Represents a constant initial concentration profile.

**ConstantProfile**(*value*)
Represents a constant initial concentration profile.

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

**static constant**(*value*)
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

**static funct**(*dictra_console_mode_function*)
Factory method that creates a **new** 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_toolbox.diffusion.PointByPointGrid.

---

**Parameters** **dictra_console_mode_function** – The function, expressed in DICTRA Console Mode syntax.

**Returns** A new *FunctionProfile* object

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

**Returns** The type

**static linear**(*start_value*, *end_value*)
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

**static step**(*lower_boundary*, *upper_boundary*, *step_at*)
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_toolbox.+diffusion.**ContinuedDiffusionCalculation**(*back*)
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.

**ContinuedDiffusionCalculation**(*back*)
Call base constructor: tc_toolbox.AbstractCalculation.

**calculate**(*timeout_in_minutes*)
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_configuration_as_string**()
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**()
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.

**set_simulation_time**(*simulation_time*)
Sets the simulation time.

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

**Returns** This *DiffusionIsoThermalCalculation* object

**with_left_boundary_condition**(*boundary_condition*, *to*)
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.

### 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.

> **Note:** You can specify time-dependent boundary conditions by calling *with_left_boundary_condition()* many times, with different values of the "to" parameter.

**Parameters**

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns** This *DiffusionIsoThermalCalculation* object

**with_options**(*options*, *to*)
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*, *to*)
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.

### 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.

---

**Note:** You can specify time-dependent boundary conditions by calling *with_right_boundary_condition()* many times, with different values of the "to" parameter.

---

**Parameters**

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns** This *DiffusionIsoThermalCalculation* object

**with_solver**(*solver*, *to*)
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_system_modifications**(*system_modifications*)
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

**with_timestep_control**(*timestep_control*, *to*)
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_toolbox.+diffusion.**DiffusionCalculationResult**(*back*)
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.

**DiffusionCalculationResult**(*back*)
Call base constructor: `tc_toolbox.AbstractResult`.

**get_mass_fraction_at_lower_interface**(*region*, *component*)
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*, *component*)
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*, *time*)
Returns the mass fraction of the specified component at the specified time.

**Note:** Use the enum `+tc_toolbox.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*, *time*)
Returns the mass fraction of the specified phase.

**Note:** Use the enum `+tc_toolbox.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*, *component*)
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*, *component*)
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*, *time*)
Returns the mole fraction of the specified component at the specified time.

**Note:** Use the enum `+tc_toolbox.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*, *time*)
Returns the mole fraction of the specified phase.

**Note:** Use the enum `+tc_toolbox.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*)
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*)
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**()
Returns the regions of the diffusion simulation.

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

**Returns** The region names

**get_time_steps**()
Returns the timesteps of the diffusion simulation.

**Returns** The timesteps [s]

**get_total_mass_fraction_of_component**(*component*)
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*, *phase*)
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*)
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*)
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*, *phase*)
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*)
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*)
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*, *y_axis*, *plot_condition*, *independent_variable*)
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*)
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*)
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*)
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])

**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.

**save_to_disk**(*path*)
Saves the result to disk. The result can later be loaded using `+tc_toolbox.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_toolbox.+diffusion.**DiffusionIsoThermalCalculation**(*back*)
Configuration for an isothermal diffusion calculation.

**DiffusionIsoThermalCalculation**(*back*)
Call base constructor: `tc_toolbox.AbstractCalculation`.

**add_console_command**(*console_command*)
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_toolbox.diffusion.DiffusionIsoThermoCalculation.remove_all_console_commands`.

---

**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, ...).

**Parameters** **console_command** – The DICTRA Console Mode command

**Returns** This *DiffusionIsoThermalCalculation* object

**add_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*)
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_configuration_as_string**()
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**()
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.

**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*)
Sets the simulation time.

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

**Returns** This *DiffusionIsoThermalCalculation* object

**set_temperature**(*temperature*)
Sets the temperature for the isothermal simulation.

**Parameters** **temperature** – The temperature [K]

**Returns** This *DiffusionIsoThermalCalculation* object

**with_cylindrical_geometry**(*first_interface_position*)
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*, *to*)
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.

### 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.

---

**Note:** You can specify time-dependent boundary conditions by calling `with_left_boundary_condition()` many times, with different values of the "to" parameter.

---

**Parameters**

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns** This `DiffusionIsoThermalCalculation` object

**with_options**(*options*, *to*)
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*, *phase*, *temperature*, *pressure*)
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*, *to*)

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.

### 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.

---

**Note:** You can specify time-dependent boundary conditions by calling *with_right_boundary_condition()* many times, with different values of the "to" parameter.

---

**Parameters**

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns** This *DiffusionIsoThermalCalculation* object

**with_solver**(*solver*, *to*)

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*)
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*)
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*, *to*)
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_toolbox.+diffusion.**DiffusionNonIsoThermalCalculation**(*back*)
Configuration for a non-isothermal diffusion calculation.

**DiffusionNonIsoThermalCalculation**(*back*)
Call base constructor: `tc_toolbox.AbstractCalculation`.

**add_console_command**(*console_command*)

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_toolbox.diffusion.DiffusionNonIsoThermalCalculation.remove_all_console_commands`.

**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, ...).

**Parameters** **console_command** – The DICTRA Console Mode command

**Returns** This *DiffusionNonIsoThermalCalculation* object

**add_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*)

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_configuration_as_string**()

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**()

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.

**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*)
Sets the simulation time.

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

**Returns** This *DiffusionNonIsoThermalCalculation* object

**with_cylindrical_geometry**(*first_interface_position*)
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*, *to*)
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.

### 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.

**Note:** You can specify time-dependent boundary conditions by calling *with_left_boundary_condition()* many times, with different values of the "to" parameter.

**Parameters**

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns** This *DiffusionNonIsoThermalCalculation* object

**with_options**(*options*, *to*)
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*, *phase*, *temperature*, *pressure*)
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*, *to*)
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.

### 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.

---

**Note:** You can specify time-dependent boundary conditions by calling *with_right_boundary_condition()* many times, with different values of the "to" parameter.

---

**Parameters**

- **boundary_condition** – The boundary condition
- **to** – The upper time-limit for boundary_condition.

**Returns** This *DiffusionNonIsoThermalCalculation* object

**with_solver** (*solver*, *to*)
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*)
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*)
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*)
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*, *to*)
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_toolbox.+diffusion.**DoubleGeometricGrid**(*no_of_points*, *lower_geometrical_factor*, *upper_geometrical_factor*)
Represents a double geometric grid.

**DoubleGeometricGrid**(*no_of_points*, *lower_geometrical_factor*, *upper_geometrical_factor*)
Creates a 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

**static double_geometric**(*no_of_points*, *lower_geometrical_factor*, *upper_geometrical_factor*)
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

**static geometric**(*no_of_points*, *geometrical_factor*)
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

**get_lower_geometrical_factor**()
Returns the lower geometrical factor (for the left half).

**Returns** The lower geometrical factor

**get_no_of_points**()
Returns number of grid points.

**Returns** The number of grid points

**get_type**()
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

**static linear**(*no_of_points*)
Factory method that creates a **new** equally spaced grid.

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

**Returns** A new *LinearGrid* object

**set_lower_geometrical_factor**(*geometrical_factor*)
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*)
Sets the number of grid points.

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

**Returns** This *DoubleGeometricGrid* object

**set_upper_geometrical_factor**(*geometrical_factor*)
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_toolbox.+diffusion.**ElementProfile**
Factory class providing objects for configuring a step, function or linear initial concentration profile.

**static constant**(*value*)
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

**static funct**(*dictra_console_mode_function*)
Factory method that creates a **new** 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_toolbox.diffusion.PointByPointGrid`.

**Parameters** **dictra_console_mode_function** – The function, expressed in DICTRA Console Mode syntax.

**Returns** A new *FunctionProfile* object

**static linear**(*start_value*, *end_value*)
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

**static step**(*lower_boundary*, *upper_boundary*, *step_at*)
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_toolbox.+diffusion.**FixFluxValue**
Contains factory methods for the the different boundary conditions available.

**FixFluxValue**()
Represents a boundary having a fixed flux value.

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)*. Constructs an instance of *FixFluxValue*.

**static 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.

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**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

**static closed_system**()
Factory method that creates a **new** closed-system boundary condition.

**Returns** A new *ClosedSystem* object

**static 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

**static fixed_compositions**(*unit_enum*)
Factory method that creates a **new** fixed-composition boundary condition.

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

**Returns** A new *FixedCompositions* object

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

**Returns** The type

**static mixed_zero_flux_and_activity**()
Factory method that creates a **new** mixed zero-flux and activity boundary condition

**Returns** A new *MixedZeroFluxAndActivity* object

**set_flux**(*element_name*, *J*, *to_time*)
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_toolbox.+diffusion.**FixedCompositions**(*unit_enum*)
Represents a boundary having fixed composition values.

**FixedCompositions**(*unit_enum*)
Represents a boundary having fixed composition values.

**Parameters** **unit_enum** – The composition unit for all compositions at the boundary

**static 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.

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**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

**static closed_system**()
Factory method that creates a **new** closed-system boundary condition.

**Returns** A new *ClosedSystem* object

**static 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

**static fixed_compositions**(*unit_enum*)
Factory method that creates a **new** fixed-composition boundary condition.

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

**Returns** A new *FixedCompositions* object

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

**Returns** The type

**static mixed_zero_flux_and_activity**()
Factory method that creates a **new** mixed zero-flux and activity boundary condition

**Returns** A new *MixedZeroFluxAndActivity* object

**set_composition**(*element_name*, *value*)
Sets the composition for the specified element.

---

**Note:** The boundary composition needs to be specified for each element.

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**Parameters**

- **element_name** – The name of the element
- **value** – The composition value [unit according to the constructor parameter]

**class** +tc_toolbox.+diffusion.**FunctionProfile**(*dictra_console_mode_function*)
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_toolbox.diffusion.PointByPointGrid`.

**FunctionProfile**(*dictra_console_mode_function*)
Creates a 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_toolbox.diffusion.PointByPointGrid`.

**Parameters** **dictra_console_mode_function** – The function, expressed in DICTRA Console Mode syntax.

**Returns** A new *StepProfile* object

**static constant**(*value*)
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

**static funct**(*dictra_console_mode_function*)
Factory method that creates a **new** 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_toolbox.diffusion.PointByPointGrid`.

**Parameters** **dictra_console_mode_function** – The function, expressed in DICTRA Console Mode syntax.

**Returns** A new *FunctionProfile* object

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

**Returns** The type

**static linear**(*start_value*, *end_value*)
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

**static step**(*lower_boundary*, *upper_boundary*, *step_at*)
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_toolbox.+diffusion.**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.

**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. Constructs an instance of *GeneralLowerHashinShtrikman*.

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**GeneralLowerHashinShtrikmanExcludedPhase**(*excluded_phases*)
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.

**GeneralLowerHashinShtrikmanExcludedPhase**(*excluded_phases*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**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.

**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. Constructs an instance of *GeneralUpperHashinShtrikman*.

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)

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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)

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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)

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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)

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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)

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_toolbox.+diffusion.**GeneralUpperHashinShtrikmanExcludedPhase**(*excluded_phases*)

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.

**GeneralUpperHashinShtrikmanExcludedPhase**(*excluded_phases*)

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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)

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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)

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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)

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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)

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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)

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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)

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_toolbox.+diffusion.**GeometricGrid**(*no_of_points*, *geometrical_factor*)

Represents a geometric grid.

**GeometricGrid**(*no_of_points*, *geometrical_factor*)

A grid that yields a varying density of grid points in the region.

---

**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**

- **no_of_points** – The number of points
- **geometrical_factor** – The geometrical factor

**static double_geometric**(*no_of_points*, *lower_geometrical_factor*, *upper_geometrical_factor*)

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

**static geometric**(*no_of_points*, *geometrical_factor*)

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

**get_geometrical_factor**()
Returns the geometrical factor.

**Returns** The geometrical factor

**get_no_of_points**()
Returns the number of grid points.

**Returns** The number of grid points

**get_type**()
Returns the type of grid.

**Returns** The type

**static linear**(*no_of_points*)
Factory method that creates a **new** equally spaced grid.

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

**Returns** A new *LinearGrid* object

**set_geometrical_factor**(*geometrical_factor*)
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*)
Sets the number of grid points.

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

**Returns** This *GeometricGrid* object

**class** +tc_toolbox.+diffusion.**GridPoint**(*distance*)
Represents a grid point, this is used in combination with grids of the type +tc_toolbox.diffusion.PointByPointGrid.

**GridPoint**(*distance*)
Creates a grid point, this is used in combination with grids of the type +tc_toolbox.diffusion.PointByPointGrid.

**Parameters** **distance** – Position (origin at the left side of the grid)

**add_composition**(*element*, *value*)
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_toolbox.+diffusion.**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.

**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. Constructs an instance of *HashinShtrikmanBoundMajority*.

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)
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

**static labyrinth_factor_f**(*matrix_phase*)
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

**static labyrinth_factor_f2**(*matrix_phase*)
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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**HashinShtrikmanBoundMajorityExcludedPhase**(*excluded_phases*)
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.

**HashinShtrikmanBoundMajorityExcludedPhase**(*excluded_phases*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)
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

**static labyrinth_factor_f**(*matrix_phase*)
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

**static labyrinth_factor_f2**(*matrix_phase*)
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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**HashinShtrikmanBoundPrescribed**(*matrix_phase*)
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.

**HashinShtrikmanBoundPrescribed**(*matrix_phase*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)
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

**static labyrinth_factor_f**(*matrix_phase*)
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

**static labyrinth_factor_f2**(*matrix_phase*)
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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**HashinShtrikmanBoundPrescribedExcludedPhase**(*matrix_phase*, *excluded_phases*)

**HashinShtrikmanBoundPrescribedExcludedPhase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)
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

**static labyrinth_factor_f**(*matrix_phase*)
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

**static labyrinth_factor_f2**(*matrix_phase*)
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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**HomogenizationFunction**
*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)

**class** +tc_toolbox.+diffusion.**HomogenizationFunctions**

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)
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

**static labyrinth_factor_f**(*matrix_phase*)
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

**static labyrinth_factor_f2**(*matrix_phase*)
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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**HomogenizationSolver**
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_toolbox.diffusion.AutomaticSolver` instead if you do not need that behavior.

---

**HomogenizationSolver**()
Creating a 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_toolbox.diffusion.AutomaticSolver` instead if you do not need that behavior.

---

Constructs an instance of *HomogenizationSolver*.

**static 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

**static 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_toolbox.diffusion.AutomaticSolver` if necessary instead.

**Returns** A new *ClassicSolver* object

**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**()
The type of solver.

**Returns** The type

**static 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_toolbox.diffusion.AutomaticSolver` instead if you do not need that behavior.

---

**Returns** A new *HomogenizationSolver* object

**set_fraction_of_free_memory_to_use** (*fraction*)
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*)
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*)
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*)
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*)
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_toolbox.+diffusion.**InverseRuleOfMixtures**
Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion.

**InverseRuleOfMixtures**()
Lower Wiener bounds: the geometrical interpretation are continuous layers of each phase orthogonal to the direction of diffusion. Constructs an instance of *InverseRuleOfMixtures*.

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)
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

**static labyrinth_factor_f**(*matrix_phase*)
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

**static labyrinth_factor_f2**(*matrix_phase*)
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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**InverseRuleOfMixturesExcludedPhase**(*excluded_phases*)
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.

**InverseRuleOfMixturesExcludedPhase**(*excluded_phases*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)

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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**LabyrinthFactorF**(*matrix_phase*)
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.

**LabyrinthFactorF**(*matrix_phase*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)

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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**LabyrinthFactorF2**(*matrix_phase*)
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.

**LabyrinthFactorF2**(*matrix_phase*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)

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_toolbox.+diffusion.**LinearGrid**(*no_of_points*)

Represents an equally spaced grid.

**LinearGrid**(*no_of_points*)

Creates an equally spaced grid.

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

**static double_geometric**(*no_of_points*, *lower_geometrical_factor*, *upper_geometrical_factor*)

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

**static geometric**(*no_of_points*, *geometrical_factor*)

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

**get_no_of_points**()

Returns the number of grid points.

**Returns** The number of grid points

**get_type**()

Type of the grid.

**Returns** The type

**static linear**(*no_of_points*)
Factory method that creates a **new** equally spaced grid.

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

**Returns** A new *LinearGrid* object

**set_no_of_points**(*no_of_points*)
Sets the number of grid points.

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

**Returns** This *LinearGrid* object

**class** +tc_toolbox.+diffusion.**LinearProfile**(*start_value*, *end_value*)
Represents a linear initial concentration profile.

**LinearProfile**(*start_value*, *end_value*)
Represents a 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*].

**static constant**(*value*)
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

**static funct**(*dictra_console_mode_function*)
Factory method that creates a **new** 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_toolbox.diffusion.PointByPointGrid.

---

**Parameters** **dictra_console_mode_function** – The function, expressed in DICTRA Console Mode syntax.

**Returns** A new *FunctionProfile* object

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

**Returns** The type

**static linear**(*start_value*, *end_value*)
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

**static step**(*lower_boundary*, *upper_boundary*, *step_at*)
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_toolbox.+diffusion.**MixedZeroFluxAndActivity**
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.

**MixedZeroFluxAndActivity**()
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. Constructs an instance of *MixedZeroFluxAndActivity*.

**static 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.

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**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

**static closed_system**()
Factory method that creates a **new** closed-system boundary condition.

**Returns** A new *ClosedSystem* object

**static 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

**static fixed_compositions**(*unit_enum*)
Factory method that creates a **new** fixed-composition boundary condition.

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

**Returns** A new *FixedCompositions* object

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

**Returns** The type

**static mixed_zero_flux_and_activity**()
Factory method that creates a **new** mixed zero-flux and activity boundary condition

**Returns** A new *MixedZeroFluxAndActivity* object

**set_activity_for_element**(*element_name*, *activity*, *to_time*)
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*)
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_toolbox.+diffusion.**Options**
General simulation conditions for the diffusion calculations.

**Options**()
General simulation conditions for diffusion calculations. Constructs an instance of *Options*.

**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*)
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*)
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_toolbox.+diffusion.**PointByPointGrid**(*unit_enum*)
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.

**PointByPointGrid**(*unit_enum*)
Represents a point-by-point grid.

**Parameters** **unit_enum** – The unit of the compositions

**add_point**(*grid_point*)
Adds a grid point to the grid.

**Parameters** **grid_point** – The grid point

**Returns** This *PointByPointGrid* object

**get_type**()
Type of the grid.

**Returns** The type

**class** +tc_toolbox.+diffusion.**Region**(*name*)
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.

**Region**(*name*)
A region of the simulation domain that can contain more than one phase.

**Note:** The first added phase represents the matrix phase, while all later added phases are *spheriod phases*, i.e. precipitate phases.

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

**add_phase**(*phase_name*, *is_matrix_phase*)
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*, *driving_force*)
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*, *driving_force*)
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*)
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*)
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*)
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*)
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_toolbox.+diffusion.**RuleOfMixtures**
Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion.

**RuleOfMixtures**()
Upper Wiener bounds: the geometrical interpretation are continuous layers of each phase parallel with the direction of diffusion. Constructs an instance of *RuleOfMixtures*.

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)
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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)
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

**static labyrinth_factor_f**(*matrix_phase*)
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

**static labyrinth_factor_f2**(*matrix_phase*)
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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**RuleOfMixturesExcludedPhase**(*excluded_phases*)
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.

**RuleOfMixturesExcludedPhase**(*excluded_phases*)
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

**static 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

**static general_lower_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static general_upper_hashin_shtrikman_excluded_phase**(*excluded_phases*)
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

**static 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

**static hashin_shtrikman_bound_majority_excluded_phase**(*excluded_phases*)
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

**static hashin_shtrikman_bound_prescribed**(*matrix_phase*)
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

**static hashin_shtrikman_bound_prescribed_excluded_phase**(*matrix_phase*, *excluded_phases*)

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

**static 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

**static inverse_rule_of_mixtures_excluded_phase**(*excluded_phases*)

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

**static labyrinth_factor_f**(*matrix_phase*)

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

**static labyrinth_factor_f2**(*matrix_phase*)

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

**static 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

**static rule_of_mixtures_excluded_phase**(*excluded_phases*)
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_toolbox.+diffusion.**SimulationTime**
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.

---

**class** +tc_toolbox.+diffusion.**Solver**
Factory class providing objects representing a solver.

**static 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

**static 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_toolbox.diffusion.AutomaticSolver if necessary instead.

---

**Returns** A new *ClassicSolver* object

**static 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_toolbox.diffusion.AutomaticSolver` instead if you do not need that behavior.

---

**Returns** A new *HomogenizationSolver* object

**class** +tc_toolbox.+diffusion.**StepProfile**(*lower_boundary*, *upper_boundary*, *step_at*)

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

**StepProfile**(*lower_boundary*, *upper_boundary*, *step_at*)

Creates an initial concentration profile with a step at the specified position, 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].

**static constant**(*value*)

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

**static funct**(*dictra_console_mode_function*)

Factory method that creates a **new** 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_toolbox.diffusion.PointByPointGrid`.

---

**Parameters** **dictra_console_mode_function** – The function, expressed in DICTRA Console Mode syntax.

**Returns** A new *FunctionProfile* object

**get_type**()

The type of the element profile.

**Returns** The type

**static linear**(*start_value*, *end_value*)

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

**static step**(*lower_boundary*, *upper_boundary*, *step_at*)
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_toolbox.+diffusion.**TimestepControl**
Settings that control the time steps in the simulation.

**TimestepControl**()
Settings that control the time steps in the simulation. Constructs an instance of *TimestepControl*.

**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*)
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*)
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*)
Sets the maximum relative error. **Default**: 0.05

**Parameters** **relative_error** – The maximum relative error

**Returns** This *TimestepControl* object

**set_max_timestep_allowed_as_percent_of_simulation_time**(*max_timestep_allowed_as_percent_of_simulat*
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*)
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*)
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_toolbox.+diffusion.**Unit**
Represents a composition unit.

### 4.1.7 Package "propertymodel"

**class** +tc_toolbox.+propertymodel.**PropertyModelCalculation**(*back*)
Configuration for a Property Model calculation.

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

**PropertyModelCalculation**(*back*)
Call base constructor: tc_toolbox.AbstractCalculation.

**add_poly_command**(*poly_command*)
Registers a POLY Console Mode command for execution. These commands are executed after all other configuration directly before the calculation starts to run. All commands are stored and used until explicitly deleted using *remove_all_poly_commands*.

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

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

**Parameters** **poly_command** – The POLY Console Mode command

**Returns** This *PropertyModelCalculation* object

**calculate**(*timeout_in_minutes*)
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*)
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*)
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**()
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_configuration_as_string**()
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_dynamic_arguments**()
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**()
Returns the description text of the current model.

**Returns** the description

**get_model_parameter_value**(*model_parameter_id*)
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**()
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**()
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.

**invoke_dynamic_argument**(*argument_id*)
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**()
Removes all previously added POLY Console Mode commands.

**Returns** This *PropertyModelCalculation* object

**remove_dependent_element**()
Removes a manually set dependent element. This method does not affect the automatic choice of the dependent element if *set_composition()* is used.

**Returns** This *PropertyModelCalculation* object

**set_argument**(*argument*, *value*)
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*, *value*)
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*)
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*, *value*)
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

---

**Note:** It should not be necessary for most users to use this method, try to use *set_composition()* instead.

---

**Warning:** It is not possible to mix POLY-commands and compositions using *set_composition()*.

**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*)
Sets the dependent element manually.

---

**Note:** It should not be necessary for most users to use this method. Setting the dependent element manually is only necessary and allowed if *set_condition()* is used.

---

**Parameters** **dependent_element_name** – The name of the dependent element

**Returns** This *PropertyModelCalculation* object

**set_model_parameter**(*model_parameter_id*, *value*)
Resets an optimizable model parameter. The id can be obtained with *get_model_parameters()*.

**Parameters**

- **model_parameter_id** – The model parameter id
- **value** – The new value of the parameter

**Returns** This *PropertyModelCalculation* object

**set_temperature**(*temperature*)
Sets the temperature.

**Default**: 1000 K

**Parameters** **temperature** – The temperature [K]

**Returns** This *PropertyModelCalculation* object

**with_system_modifications**(*system_modifications*)
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_toolbox.+propertymodel.**PropertyModelResult**(*back*)
The result of a Property Model calculation.

**PropertyModelResult**(*back*)
Call base constructor: `tc_toolbox.AbstractResult`.

**get_result_quantities**()
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*)
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*)
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*)
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.

**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.

**save_to_disk**(*path*)
Saves the result to disk. The result can later be loaded using `+tc_toolbox.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

### 4.1.8 Package "material_to_material"

**class** +tc_toolbox.+material_to_material.**AbstractConstantCondition**
The abstract base class for all constant conditions.

**class** +tc_toolbox.+material_to_material.**AbstractMaterialToMaterialCalculationAxis**
The abstract base class of all calculation axis.

**class** +tc_toolbox.+material_to_material.**ConstantCondition**
A constant condition.

**static fraction_of_material_b**(*fraction_of_material_b*)
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

**static temperature**(*temperature*)
Creates a constant temperature condition object.

**Parameters** **temperature** – The temperature [K]

**Returns** The condition object

**class** +tc_toolbox.+material_to_material.**FractionOfMaterialBAxis**(*from_fraction*, *to_fraction*, *start_fraction*)
A fraction of material B axis.

**FractionOfMaterialBAxis**(*from_fraction*, *to_fraction*, *start_fraction*)
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]

**static fraction_of_material_b**(*from_fraction*, *to_fraction*, *start_fraction*)
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

**static temperature**(*from_temperature*, *to_temperature*, *start_temperature*)
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_toolbox.+material_to_material.**FractionOfMaterialBCondition**(*fraction_of_material_b*)
A constant fraction of material B condition.

**FractionOfMaterialBCondition**(*fraction_of_material_b*)
Creates a constant fraction of material B condition object.

---

**Note:** The unit depends on the composition unit setting in the calculator.

---

**Parameters** **fraction_of_material_b** – The fraction of material B [weight-fraction or mole-fraction]

**static fraction_of_material_b**(*fraction_of_material_b*)
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

**static temperature**(*temperature*)
Creates a constant temperature condition object.

**Parameters** **temperature** – The temperature [K]

**Returns** The condition object

**class** +tc_toolbox.+material_to_material.**MaterialToMaterialCalculationAxis**
A calculation axis.

**static fraction_of_material_b**(*from_fraction*, *to_fraction*, *start_fraction*)
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

**static temperature**(*from_temperature*, *to_temperature*, *start_temperature*)
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_toolbox.+material_to_material.**MaterialToMaterialCalculationContainer**(*back*)
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.

**MaterialToMaterialCalculationContainer**(*back*)
Constructs an instance of *MaterialToMaterialCalculationContainer*.

**with_phase_diagram_calculation**(*default_conditions*, *components*)
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*, *components*)
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*, *components*)
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_toolbox.+material_to_material.**MaterialToMaterialPhaseDiagramCalculation**(*back*)
Configuration for a Material to Material phase diagram calculation.

---

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

---

**MaterialToMaterialPhaseDiagramCalculation**(*back*)
Call base constructor: tc_toolbox.step_or_map_diagrams.AbstractPhaseDiagramCalculation.

**add_initial_equilibrium**(*initial_equilibrium*)
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*, *timeout_in_minutes*)
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**()
Returns the names of the components in the system (including all components auto-selected by the database(s)).

**Returns** The component names

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

---

**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 Thermo-Calc Console Mode command

**Returns** This *MaterialToMaterialPhaseDiagramCalculation* object

**set_activities** (*activities*)
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*)
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*, *gibbs_energy*)
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*, *dependent_component*)
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*, *dependent_component*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
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*)
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*)
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*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This PhaseDiagramCalculation object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)
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*)
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_toolbox.+material_to_material.**MaterialToMaterialPhaseDiagramResult**(*back*)
Result of a Material to Material phase diagram calculation, it can be evaluated using quantities or Console Mode syntax.

**MaterialToMaterialPhaseDiagramResult**(*back*)
Call base constructor: `tc_toolbox.step_or_map_diagrams.PhaseDiagramResult`.

**add_coordinate_for_phase_label**(*x*, *y*)
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*, *y_quantity*)
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 *'='*.

---

**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*, *y_quantity*)

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 *'='*.

---

**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

**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.

**remove_phase_labels**()

Erases all added coordinates for phase labels.

**Returns** This *MaterialToMaterialPhaseDiagramResult* object

**save_to_disk**(*path*)

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*)

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_toolbox.+material_to_material.**MaterialToMaterialPropertyDiagramCalculation**(*back*)
Configuration for a Material to Material property diagram calculation.

---

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

---

**MaterialToMaterialPropertyDiagramCalculation**(*back*)
Call base constructor: tc_toolbox.step_or_map_diagrams.AbstractPropertyDiagramCalculation.

**calculate**(*keep_previous_results*, *timeout_in_minutes*)
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**()
Returns the names of the components in the system (including all components auto-selected by the database(s)).

**Returns** The component names

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

**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 Thermo-Calc Console Mode command

**Returns** This *MaterialToMaterialPropertyDiagramCalculation* object

**set_activities** (*activities*)
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*)
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*, *gibbs_energy*)
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*, *dependent_component*)
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*, *dependent_component*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
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*)
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*)
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*)
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*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This *MaterialToMaterialPropertyDiagramCalculation* object

**with_reference_state**(*component*, *phase*, *temperature*, *pressure*)
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*)
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_toolbox.+material_to_material.**MaterialToMaterialPropertyDiagramResult**(*back*)
Result of a Material to Material property diagram. It can be used to query for specific values.

**MaterialToMaterialPropertyDiagramResult**(*back*)
Call base constructor: `tc_toolbox.step_or_map_diagrams.PropertyDiagramResult`.

**get_values_grouped_by_quantity_of**(*x_quantity*, *y_quantity*, *sort_and_merge*)
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 *'='*.

---

**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*, *y_quantity*, *sort_and_merge*)
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 *'='*.

**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*, *y_quantity*)

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 *'='*.

**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

**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.

**save_to_disk**(*path*)

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*)
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_toolbox.+material_to_material.**MaterialToMaterialSingleEquilibriumCalculation**(*back*
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()*.

---

**MaterialToMaterialSingleEquilibriumCalculation**(*back*)
Call base constructor: tc_toolbox.single_equilibrium.AbstractSingleEquilibriumCalculation.

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

**Returns** The components

**get_configuration_as_string**()
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_gibbs_energy_addition_for**(*phase*)
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**()
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.

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

**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 Thermo-Calc Console Mode command

**Returns** This *MaterialToMaterialSingleEquilibriumCalculation* object

**set_activities**(*activities*)
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*)
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*, *reset_conditions*)
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*)
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*, *gibbs_energy*)
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*, *dependent_component*)
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*, *dependent_component*)
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*)
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*, *amount*)
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*, *amount*)
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*)
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*)
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*)
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*)
Sets the first constant condition (either temperature of fraction of material B).

**Parameters** **condition** – The condition

**Returns** This *MaterialToMaterialSingleEquilibriumCalculation* object

**with_options** (*options*)
Sets the simulation options.

**Parameters** **options** – The simulation options

**Returns** This SingleEquilibriumCalculation object

**with_reference_state** (*component*, *phase*, *temperature*, *pressure*)
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*)
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*)
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_toolbox.+material_to_material.**MaterialToMaterialSingleEquilibriumResult**(*back*)

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.

**MaterialToMaterialSingleEquilibriumResult**(*back*)

Call base constructor: `tc_toolbox.single_equilibrium.SingleEquilibriumResult`.

**change_pressure**(*pressure*)

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*)

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**()

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**()

Returns the conditions.

**Returns** The selected conditions

**get_phases**()

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**()

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

**Returns** The names of the stable phases

**get_value_of**(*quantity*)
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

**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.

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

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

**Returns** This *MaterialToMaterialSingleEquilibriumResult* object

**save_to_disk**(*path*)
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_toolbox.+material_to_material.**TemperatureAxis**(*from_temperature*, *to_temperature*, *start_temperature*)
A temperature calculation axis.

**TemperatureAxis**(*from_temperature*, *to_temperature*, *start_temperature*)
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]

**static fraction_of_material_b**(*from_fraction*, *to_fraction*, *start_fraction*)
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

**static temperature**(*from_temperature*, *to_temperature*, *start_temperature*)
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_toolbox.+material_to_material.**TemperatureCondition**(*temperature*)
A constant temperature condition.

**TemperatureCondition**(*temperature*)
Creates a constant temperature condition object.

**Parameters** **temperature** – The temperature [K]

**static fraction_of_material_b**(*fraction_of_material_b*)
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

**static temperature**(*temperature*)
Creates a constant temperature condition object.

**Parameters** **temperature** – The temperature [K]

**Returns** The condition object

### 4.1.9 Package "process_metallurgy"

#### 4.1.9.1 Package "base"

**class** +tc_toolbox.+process_metallurgy.+base.**AbstractAddition**
The base class for representing an addition to an equilibrium calculation or process simulation.

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+base.**ActivityReference**
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_toolbox.process_metallurgy.process.ProcessSimulationResult.get_formula_for_activity_of_slag() or +tc_toolbox.process_metallurgy.equilibrium.EquilibriumResult.get_formula_for_activity_of_slag().

**class** +tc_toolbox.+process_metallurgy.+base.**PhaseGroup**
The phase group, such a group is collecting all phases that belong to a certain type.

**class** +tc_toolbox.+process_metallurgy.+base.**ProcessDatabase**
The database used for a Process Metallurgy calculation.

**class** +tc_toolbox.+process_metallurgy.+base.**ProcessMetallurgyOptions**
The options for a process metallurgy calculation.

**ProcessMetallurgyOptions**()
The options for a process metallurgy calculation. Constructs an instance of *ProcessMetallurgyOptions*.

**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.

---

**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.

---

**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*)
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*)
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*)
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*)
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*)
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_toolbox.+process_metallurgy.+base.**ProcessMinimizationPolicy**
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.

**class** +tc_toolbox.+process_metallurgy.+base.**SlagProperty**
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_toolbox.process_metallurgy.process.ProcessSimulationResult.getFormulaForSlagProperty() or +tc_toolbox.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*.

**class** +tc_toolbox.+process_metallurgy.+base.**SlagType**
The type of slag considered for a slag property calculation.

#### 4.1.9.2 Package "equilibrium"

**class** +tc_toolbox.+process_metallurgy.+equilibrium.**AbstractEquilibriumAddition**
The base class for representing an addition to an equilibrium calculation.

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**set_amount**(*amount*)
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*, *content*)
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_toolbox.+process_metallurgy.+equilibrium.**AdiabaticEquilibriumCalculation**(*back*)

An *adiabatic* Process Metallurgy equilibrium calculation. Such calculations can for example be used to determine the global equilibrium state of a process.

**AdiabaticEquilibriumCalculation**(*back*)

Call base constructor: tc_toolbox.process_metallurgy.equilibrium.EquilibriumCalculation.

**add_addition**(*addition*)

Adds an addition to the calculation.

**Parameters** **addition** – A *EquilibriumAddition* or *EquilibriumGasAddition*

**Returns** This *AdiabaticEquilibriumCalculation* object

**add_poly_command**(*command*)

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*)

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*)

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*)
Sets the pressure.

**Parameters** **pressure** – The pressure [Pa]

**Returns** This *AdiabaticEquilibriumCalculation* object

**update_addition**(*addition*)
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

**with_options**(*options*)
Sets the options for the calculation.

**Parameters** **options** – The options

**Returns** This *AdiabaticEquilibriumCalculation* object

**class** +tc_toolbox.+process_metallurgy.+equilibrium.**EquilibriumAddition**(*composition*, *amount*, *temperature*, *composition_unit*, *do_scale*)
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

**EquilibriumAddition**(*composition*, *amount*, *temperature*, *composition_unit*, *do_scale*)
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**()
Returns the amount of this addition.

**Returns** The amount [kg]

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**set_amount**(*amount*)
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*, *content*)
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_toolbox.+process_metallurgy.+equilibrium.**EquilibriumCalculation**(*back*)
A Process Metallurgy equilibrium calculation. Such calculations can for example be used to determine the global equilibrium state of a process.

**EquilibriumCalculation**(*back*)
Constructs an instance of *EquilibriumCalculation*.

**add_addition**(*addition*)
Adds an addition to the calculation.

**Parameters** **addition** – The addition

**Returns** This *EquilibriumCalculation* object

**add_poly_command**(*command*)
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

**calculate**(*timeout_in_minutes*)
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*)
Removes an addition from the calculation.

**Parameters** **addition** – The addition to be removed

**Returns** This *EquilibriumCalculation* object

**remove_all_additions**()
Removes all additions from the calculation.

**Returns** This *EquilibriumCalculation* object

**set_pressure**(*pressure*)
Sets the pressure.

**Parameters** **pressure** – The pressure [Pa]

**Returns** This *EquilibriumCalculation* object

**update_addition**(*addition*)
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

**with_options**(*options*)
Sets the options for the calculation.

**Parameters** **options** – The options

**Returns** This *EquilibriumCalculation* object

**class** +tc_toolbox.+process_metallurgy.+equilibrium.**EquilibriumGasAddition**(*composition*, *amount*, *temperature*, *amount_unit*, *composition_unit*, *do_scale*)
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*.

---

**EquilibriumGasAddition**(*composition*, *amount*, *temperature*, *amount_unit*, *composition_unit*, *do_scale*)
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*.

---

**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**()
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**()
Returns the amount unit used in this addition.

**Returns** The amount unit

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**set_amount**(*amount*)
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*, *content*)
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_toolbox.+process_metallurgy.+equilibrium.**EquilibriumResult**(*back*)
The result of a Process Metallurgy equilibrium calculation.

**EquilibriumResult**(*back*)
Call base constructor: tc_toolbox.AbstractResult.

**get_activity_of_slag**(*component*, *reference*)
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**()
Returns the total amount.

**Returns** The total amount [kg]

**get_amount_of_elements**()
Returns the amount of each element.

**Returns** The amount of the elements [kg]

**get_amount_of_phase_groups**()
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**()
Returns the amount of each phase.

**Returns** The amount of the phases [kg]

**get_components**()
Returns all components defined for the elements present in this result.

**Returns** The components present in this result

**get_composition**(*composition_unit*)
Returns the composition of the result.

**Parameters** **composition_unit** – The composition unit, **default: mass percent**

**Returns** The composition

**get_composition_of_phase**(*phase*, *composition_unit*, *composition_type*)
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*, *composition_unit*, *composition_type*)
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**()
Returns all elements defined for the result.

**Returns** All elements present in this result

**get_formula_for_activity_of_slag**(*component*, *reference*)
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*, *slag_type*)
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*)
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*)
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**()
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**()
Returns the partial pressure of oxygen in the result.

**Returns** The partial pressure [Pa]

**get_pressure**()
Returns the pressure in the result.

**Returns** The pressure [Pa]

**get_slag_property**(*slag_property*, *slag_type*)
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**()
Returns the stable phases in the result.

**Returns** The stable phases

**get_stable_phases_in_phase_group**(*phase_group*)
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**()
Returns the temperature in the result.

**Returns** The temperature [K]

**get_value_of**(*classic_expression*)
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*)
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*)
Returns the kinematic viscosity of a phase in the result.

**Parameters** **phase** – The phase name

**Returns** The kinematic viscosity [m**2/s]

**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_toolbox.+process_metallurgy.+equilibrium.**IsoThermalEquilibriumCalculation**(*back*)
An *isothermal* Process Metallurgy equilibrium calculation. Such calculations can for example be used to determine the global equilibrium state of a process.

**IsoThermalEquilibriumCalculation**(*back*)
Call base constructor: tc_toolbox.process_metallurgy.equilibrium.EquilibriumCalculation.

**add_addition**(*addition*)
Adds an addition to the calculation.

**Parameters** **addition** – A *EquilibriumAddition* or *EquilibriumGasAddition*

**Returns** This *IsoThermalEquilibriumCalculation* object

**add_poly_command**(*command*)
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*)
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*)
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*)
Sets the pressure.

**Parameters** **pressure** – The pressure [Pa]

**Returns** This *IsoThermalEquilibriumCalculation* object

**set_temperature**(*temperature*)
Sets the temperature.

**Parameters** **temperature** – The temperature [K]

**Returns** This *IsoThermalEquilibriumCalculation* object

**update_addition**(*addition*)
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*)
Sets the options for the calculation.

**Parameters** **options** – The options

**Returns** This *IsoThermalEquilibriumCalculation* object

#### 4.1.9.3 Package "process"

**class** +tc_toolbox.+process_metallurgy.+process.**AbstractContinuousAddition**
The base class representing an addition in a process simulation that is added continuously over a period of time.

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+process.**AbstractProcessAddition**
The base class for representing an addition in a process simulation.

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+process.**AbstractSingleTimeAddition**
The base class representing an addition in a process simulation that is added at a distinct time point.

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+process.**BulkZone**(*density*, *phase_group_to_transfer*, *name*)

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*.

---

**BulkZone**(*density*, *phase_group_to_transfer*, *name*)

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*.

---

**Parameters**

- **density** – The density of the zone [kg/m**3]
- **phase_group_to_transfer** – The phase group that is transferred from the attached reaction zones back to this zone after each time step, usually this is *ALL_METAL* or *ALL_OXIDES*
- **name** – The unique name of the zone

**add_addition**(*addition*, *time*)

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*, *from_time*, *to_time*)

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*, *from_time*, *to_time*)

Adds a constant power during a specified time period to the zone (for example heating or cooling).

**Parameters**

- **power** – The power [MW]

- **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**()
Returns the density of the zone

**Returns** The density [kg/m**3]

**get_elements**()
Returns the elements present in the zone. The elements are determined by the additions.

**Returns** The elements

**get_id**()
Returns the unique id of the zone. :return: The zone id

**get_phase_group_to_transfer**()
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**()
Returns if degassing is enabled in the zone.

**Returns** If degassing is enabled

**class** +tc_toolbox.+process_metallurgy.+process.**ContinuousAddition**(*composition*, *rate*, *temperature*, *composition_unit*, *do_scale*)

---

**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

**ContinuousAddition**(*composition*, *rate*, *temperature*, *composition_unit*, *do_scale*)
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**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_rate**()
Returns the rate of addition.

**Returns** The addition rate [kg/s]

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+process.**ContinuousGasAddition**(*composition*, *rate*, *temperature*, *rate_unit*, *composition_unit*, *do_scale*)

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*.

---

**ContinuousGasAddition**(*composition*, *rate*, *temperature*, *rate_unit*, *composition_unit*, *do_scale*)

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*.

---

**Parameters**

- **composition** – The composition
- **rate** – The rate of addition [kg/s]
- **temperature** – The initial addition temperature (**default: 20 °C**) [K]
- **rate_unit** – The amount unit
- **composition_unit** – The composition unit
- **do_scale** – If the composition is scaled to 100% / fraction of 1

**get_composition**()

Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()

Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()

Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_rate**()
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**()
Returns the rate unit used in this addition.

**Returns** The rate unit

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+process.**ExhaustGasResult**(*back*)
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()*.

**ExhaustGasResult**(*back*)
Constructs an instance of *ExhaustGasResult*.

**get_amount**()
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**()
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*, *unit*)
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**()
Returns the pressure of the exhaust gas zone at each time point.

**Returns** The pressure [Pa]

**get_stable_phases**()
Returns the stable phases within the exhaust gas zone at each time point.

**Returns** The stable phases

**get_temperature**()
Returns the temperature of the exhaust gas at each time point.

**Returns** The temperature at each time point [K]

**class** +tc_toolbox.+process_metallurgy.+process.**MassTransferCoefficients**
The mass transfer coefficients between a reaction zone and a bulk zone vs. time.

**MassTransferCoefficients**()
The mass transfer coefficients between a reaction zone and a bulk zone vs. time. Constructs an instance of *MassTransferCoefficients*.

**add**(*mass_transfer_coefficient*, *time*)
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_toolbox.+process_metallurgy.+process.**MetalBulkZone**(*density*)
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.

**MetalBulkZone**(*density*)
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.

**Parameters** **density** – The density of the zone [kg/m**3]

**add_addition**(*addition*, *time*)
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*, *from_time*, *to_time*)
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*, *from_time*, *to_time*)
Adds a constant power during a specified time period to the zone (for example heating or cooling).

**Parameters**

- **power** – The power [MW]
- **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**()
Returns the density of the zone

**Returns** The density [kg/m**3]

**get_elements**()
Returns the elements present in the zone. The elements are determined by the additions.

**Returns** The elements

**get_id**()
Returns the unique name / id of the zone.

**Returns** The zone name / id

**get_phase_group_to_transfer**()
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**()
Returns if degassing is enabled in the zone.

**Returns** If degassing is enabled

**class** +tc_toolbox.+process_metallurgy.+process.**ProcessSimulationCalculation**(*back*)
A Process Metallurgy process simulation. Such calculations represent complete metallurgical processes with several zones and simulate their evolution over time.

**ProcessSimulationCalculation**(*back*)
Constructs an instance of *ProcessSimulationCalculation*.

**calculate**(*timeout_in_minutes*)
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*)
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*)
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*)
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*)
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*)
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*)
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*, *from_time*, *to_time*)
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*)
Sets the options for the process simulation.

**Parameters** **options** – The options

**Returns** This *ProcessSimulationCalculation* object

**with_reaction_zone**(*reaction_zone*)
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_toolbox.+process_metallurgy.+process.**ProcessSimulationResult**(*back*)
The result of a Process Metallurgy process simulation.

**ProcessSimulationResult**(*back*)
Call base constructor: tc_toolbox.AbstractResult.

**get_activity_of_slag**(*zone*, *component*, *reference*)
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*)
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**()
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*)
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*)
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**()
Returns all components defined in the simulation.

**Returns** The components

**get_composition**(*zone*, *composition_unit*)
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*, *phase*, *composition_unit*, *composition_type*)
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*, *phase_group*, *composition_unit*, *composition_type*)
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**()
Returns all elements present in the simulation.

**Returns** The elements

**get_enthalpy**()
Returns the total enthalpy of the process at each time point.

**Returns** The enthalpy at each time point [J]

**get_exhaust_gas**()
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*, *component*, *reference*)
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*, *slag_property*, *slag_type*)
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*, *unit*)
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*, *unit*)
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**()
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**()
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*)
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*)
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*, *slag_property*, *slag_type*)
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*)
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*, *phase_group*)
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*)
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**()
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*, *classic_expression*)
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*, *phase*)
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*, *phase*)
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]

**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_toolbox.+process_metallurgy.+process.**ReactionZone**(*area*, *left_zone*, *mass_transfer_coefficient_left*, *right_zone*, *mass_transfer_coefficient_right*)
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.

**ReactionZone**(*area*, *left_zone*, *mass_transfer_coefficient_left*, *right_zone*, *mass_transfer_coefficient_right*)
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.

**Parameters**

- **area** – The contact area between the bulk zones in contact [m**2]
- **left_zone** – The left bulk zone
- **mass_transfer_coefficient_left** – The mass transfer coefficient between the left bulk zone and the reaction zone, can be a constant value or time-dependent [m/s]
- **right_zone** – The right bulk zone
- **mass_transfer_coefficient_right** – The mass transfer coefficient between the right bulk zone and the reaction zone, can be a constant value or time-dependent [m/s]

**add_addition**(*addition*, *time*)
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*, *from_time*, *to_time*)
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*)
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*, *from_time*, *to_time*)
Adds a constant power during a specified time period to the zone (for example heating or cooling).

**Parameters**

- **power** – The power [MW]
- **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*)
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**()
Returns the elements present in the zone. The elements are determined by the additions.

**Returns** The elements

**get_id**()
Returns the unique id of the zone. :return: The zone id

**is_degassing_enabled**()
Returns if degassing is enabled in the zone.

**Returns** If degassing is enabled

**class** +tc_toolbox.+process_metallurgy.+process.**SingleTimeAddition**(*composition*, *amount*, *temperature*, *composition_unit*, *do_scale*)
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

**SingleTimeAddition**(*composition*, *amount*, *temperature*, *composition_unit*, *do_scale*)

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**()

Returns the amount of this addition.

**Returns** The amount [kg]

**get_composition**()

Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()

Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()

Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()

Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+process.**SingleTimeGasAddition**(*composition*, *amount*, *temperature*, *amount_unit*, *composition_unit*, *do_scale*)

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

**SingleTimeGasAddition**(*composition*, *amount*, *temperature*, *amount_unit*, *composition_unit*, *do_scale*)
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**()
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**()
Returns the amount unit used in this addition.

**Returns** The amount unit

**get_composition**()
Returns the composition of the addition - without containing a dependent component.

**Returns** The composition [in the unit provided by `getCompositionUnit()`]

**get_composition_unit**()
Returns the composition unit used in this addition.

**Returns** The composition unit

**get_dependent_component**()
Returns the dependent component.

**Returns** The dependent component or an empty string if no dependent component is defined

**get_elements**()
Returns all elements of the addition.

**Returns** The elements

**get_id**()
Returns the unique ID of the addition.

**Returns** The unique ID of the addition

**get_temperature**()
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**()
Returns if the composition of the addition is being scaled to 100% / 1 or not.

**Returns** If the composition is scaled

**is_empty**()
Returns if the addition is "empty", i.e., has zero amount.

**Returns** If the addition is empty

**class** +tc_toolbox.+process_metallurgy.+process.**SlagBulkZone**(*density*)
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.

**SlagBulkZone**(*density*)
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.

**Parameters** **density** – The density of the zone [kg/m**3]

**add_addition**(*addition*, *time*)
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*, *from_time*, *to_time*)
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*, *from_time*, *to_time*)
Adds a constant power during a specified time period to the zone (for example heating or cooling).

**Parameters**

- **power** – The power [MW]
- **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**()
Returns the density of the zone

**Returns** The density [kg/m**3]

**get_elements**()
Returns the elements present in the zone. The elements are determined by the additions.

**Returns** The elements

**get_id**()
Returns the unique id of the zone. :return: The zone id

**get_phase_group_to_transfer**()
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**()
Returns if degassing is enabled in the zone.

**Returns** If degassing is enabled

**class** +tc_toolbox.+process_metallurgy.+process.**TransferOfPhaseGroup**(*phase_group_to_transfer*, *source_zone*)
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.

**TransferOfPhaseGroup**(*phase_group_to_transfer*, *source_zone*)
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.

**Parameters**

- **phase_group_to_transfer** – The phase group to be transferred
- **source_zone** – The source zone of the transfer

**add**(*transfer_rate*, *time*)
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**()
Returns the phase group to be transferred

**Returns** The phase group

**get_transfer_source_zone_id**()
The id of the source zone of the transfer

**Returns** This source zone id

**class** +tc_toolbox.+process_metallurgy.+process.**Zone**
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*, *time*)
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*, *from_time*, *to_time*)
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*, *from_time*, *to_time*)
Adds a constant power during a specified time period to the zone (for example heating or cooling).

**Parameters**

- **power** – The power [MW]
- **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**()
Returns the elements present in the zone. The elements are determined by the additions.

**Returns** The elements

**get_id**()
Returns the unique id of the zone. :return: The zone id

**is_degassing_enabled**()
Returns if degassing is enabled in the zone.

**Returns** If degassing is enabled

## 4.2 Root Package

**class** +tc_toolbox.**AbstractCalculation**(*back*)
Abstract base class for calculations.

**AbstractCalculation**(*back*)
Constructs an instance of *AbstractCalculation*.

**get_configuration_as_string**()
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**()
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*)
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

**class** +tc_toolbox.**AbstractResult**(*back*)
Abstract base class for results. This can be used to query for specific values .

**AbstractResult**(*back*)
Constructs an instance of *AbstractResult*.

**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_toolbox.**CompositionType**
The type of composition.

**class** +tc_toolbox.**CompositionUnit**
The composition unit.

**class** +tc_toolbox.**Constants**

**ALL_COMPONENTS = '"*"'**

**ALL_PHASES = '"*"'**

**CURRENT_TEMPERATURE = '-1.0'**

**MATERIAL_B_FRACTION = '"material_b_fraction"'**

**SER = '"SER"'**

**class** +tc_toolbox.**ConversionUnit**
The composition unit used in a conversion.

**class** +tc_toolbox.**DiffusionQuantity**
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(*)").

---

**static activity_of_component**(*component*, *use_ser*)
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.

**static chemical_diffusion_coefficient**(*phase*, *diffusing_element*, *gradient_element*, *reference_element*)
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.

**static chemical_potential_of_component**(*component*, *use_ser*)
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.

**static distance**(*region*)
Creates a quantity representing the distance [m].

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

**static intrinsic_diffusion_coefficient**(*phase*, *diffusing_element*, *gradient_element*, *reference_element*)
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.

**static l_bis**(*phase*, *diffusing_element*, *gradient_element*, *reference_element*)
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.

**static mass_fraction_of_a_component**(*component*)
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.

**static mass_fraction_of_a_phase**(*phase*)
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.

**static mobility_of_component_in_phase**(*phase*, *component*)
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.

**static mole_fraction_of_a_component**(*component*)
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.

**static mole_fraction_of_a_phase**(*phase*)
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.

**static position_of_lower_boundary_of_region**(*region*)
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.

**static position_of_upper_boundary_of_region**(*region*)
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.

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

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

**static thermodynamic_factor**(*phase*, *diffusing_element*, *gradient_element*, *reference_element*)
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.

**static time**()
Creates a quantity representing the time [s].

**static total_mass_fraction_of_component**(*component*)
Creates a quantity representing the total mass fraction of a component.

**Parameters** **component** – The name of the component

**Returns** A new `TotalMassFractionOfComponent` object.

**static total_mass_fraction_of_component_in_phase**(*phase*, *component*)
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.

**static total_mass_fraction_of_phase**(*phase*)
Creates a quantity representing the total mass fraction of a phase.

**Parameters** **phase** – The name of the phase.

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

**static total_mole_fraction_of_component**(*component*)
Creates a quantity representing the total mole fraction of a component.

**Parameters** **component** – The name of the component

**Returns** A new `TotalMoleFractionOfComponent` object.

**static total_mole_fraction_of_component_in_phase**(*phase*, *component*)
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.

**static total_volume_fraction_of_phase**(*phase*)
Creates a quantity representing the total volume fraction of a phase.

**Parameters** **phase** – The name of the phase.

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

**static tracer_diffusion_coefficient**(*phase*, *diffusing_element*)
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.

**static u_fraction_of_a_component**(*component*)
Creates a quantity representing the u-fraction of a component.

**Parameters** **component** – The name of the component

**Returns** A new `UFractionOfAComponent` object.

**static user_defined_function**(*expression*)
Creates a quantity representing a user-defined function.

**Parameters** **expression** – The function expression

**Returns** A new `Function` object

**static velocity_of_lower_boundary_of_region**(*region*)
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.

**static velocity_of_upper_boundary_of_region**(*region*)
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.

**static width_of_region**(*region*)
Creates a quantity representing the width of a region [m].

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

**Returns** A new `WidthOfRegion` object.

**class** +tc_toolbox.**GasAmountUnit**
The amount of a gas.

**class** +tc_toolbox.**GasCompositionUnit**
The composition unit for a gas.

**class** +tc_toolbox.**GasRateUnit**
The rate of a gas flow.

**class** +tc_toolbox.**IndependentVariable**
Factory class providing quantities used for defining the independent variable in general diffusion result querying.

**static distance**(*region*)
Creates an independent variable representing the distance [m].

**Returns** A new *Distance* object

**static time**()
Creates an independent variable representing the time [s].

**Returns** A new *Time* object

**class** +tc_toolbox.**InterfacePosition**
The position of an interface relative to its region. Only used for diffusion simulations.

**class** +tc_toolbox.**MetallurgyCalculations**(*back*)
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.

**MetallurgyCalculations**(*back*)
Constructs an instance of *MetallurgyCalculations*.

**with_adiabatic_equilibrium_calculation**(*database*)
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*)
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*)
Creates an isothermal equilibrium calculation for Process Metallurgy.

**Parameters** **database** – The thermodynamic database used in the calculation

**Returns** A new `IsoThermalEquilibriumCalculation` object

**class** +tc_toolbox.**PhaseParameter**(*parameter_name*)
Database phase parameter expression used by `SystemModifications.set()`.

**Parameters** **parameter_name** – The phase parameter name

**PhaseParameter**(*parameter_name*)
Constructs an instance of *PhaseParameter*.

**get_intervals**()
Returns the list of all defined intervals.

**Returns** The defined temperature intervals

**get_lower_temperature_limit**()
Returns the lower temperature limit.

**Returns** The lower temperature limit in K

**get_name**()
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*)
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*, *upper_temperature_limit*)
Adds/overwrites a parameter expression for a temperature interval.

**Default value of the upper limit of the interval**: 6000 K

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**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.

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**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*)
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*)
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_toolbox.**PhaseUnit**
The units available for a phase fraction.

**class** +tc_toolbox.**PlotCondition**
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").

**static distance**(*distancepoint*, *region*)
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

**static integral**()
Creates an integral plot condition.

**Returns** A new *IntegralCondition* object

**static interface**(*region*, *interface_position*)
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

**static time**(*timepoint*)
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_toolbox.**ResultLoader**(*back*)
Contains methods for loading results from previously done calculations.

**ResultLoader**(*back*)
Constructs an instance of *ResultLoader*.

**diffusion**(*path*)
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*)
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*)
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*)
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*)
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*)
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*)
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*)
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_toolbox.**ResultValueGroup**(*back*)
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.

**Returns** list of floats representing the second quantity ("y-axis")

**ResultValueGroup**(*back*)
Constructs an instance of *ResultValueGroup*.

**get_label**()
Accessor for the line label :return the line label

**get_x**()
Accessor for the x-values :return the x values

**get_y**()
Accessor for the y-values :return the y values

**class** +tc_toolbox.**ScheilQuantity**
Factory class providing quantities used for defining a Scheil calculation result (`+tc_toolbox.scheil.ScheilCalculationResult`).

**static apparent_heat_capacity_per_gram**()
Creates a quantity representing the apparent heat capacity [J/g/K].

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

**static apparent_heat_capacity_per_mole**()
Creates a quantity representing the apparent heat capacity [J/mol/K].

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

**static apparent_volumetric_thermal_expansion_coefficient**()
Creates a quantity representing the apparent volumetric thermal expansion coefficient of the system [1/K].

**Returns** A new `ApparentVolumetricThermalExpansionCoefficient` object.

**static composition_of_phase_as_mole_fraction**(*phase*, *component*)
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.

**static composition_of_phase_as_weight_fraction**(*phase*, *component*)
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.

**static density_of_phase**(*phase*)
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.

**static density_of_solid_phase**(*phase*)
Creates a quantity representing the average density of a solid phase [g/cm^3].

---

**Note:** Deprecated in version 2022a: This quantity has been renamed to *density_of_phase()*. It will be removed in release 2023a.

---

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

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

**static density_of_system**()
Creates a quantity representing the average density of the system [g/cm^3].

**Returns** A new `DensityOfSystem` object.

**static distribution_of_component_of_phase**(*phase*, *component*)
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.

**static heat_per_gram**()
Creates a quantity representing the total heat release from the liquidus temperature down to the current temperature [J/g].

---

**Note:** The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*latent_heat_per_mole()* and *latent_heat_per_gram()*), and the other is the heat related to the specific heat of liquid and solid phases (*heat_per_mole()* and *heat_per_gram()*).

---

**Returns** A new `HeatPerGram` object.

**static heat_per_mole**()
Creates a quantity representing the total heat release from the liquidus temperature down to the current temperature [J/mol].

---

**Note:** The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*latent_heat_per_mole()* and *latent_heat_per_gram()*), and the other is the heat related to the specific heat of liquid and solid phases (*heat_per_mole()* and *heat_per_gram()*).

---

**Returns** A new `HeatPerMole` object.

**static latent_heat_per_gram**()
Creates a quantity representing the cumulated latent heat release from the liquidus temperature down to the current temperature [J/g].

---

**Note:** The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*latent_heat_per_mole()* and *latent_heat_per_gram()*), and the other is the heat related to the specific heat of liquid and solid phases (*heat_per_mole()* and *heat_per_gram()*).

---

**Returns** A new `LatentHeatPerGram` object.

**static latent_heat_per_mole**()
Creates a quantity representing the cumulated latent heat release from the liquidus temperature down to the current temperature [J/mol].

---

**Note:** The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid -> solid phase transformation (*latent_heat_per_mole()* and *latent_heat_per_gram()*), and the other is the heat related to the specific heat of liquid and solid phases (*heat_per_mole()* and *heat_per_gram()*).

---

**Returns** A new `LatentHeatPerMole` object.

**static mass_fraction_of_a_solid_phase**(*phase*)
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.

**static mass_fraction_of_all_liquid**()
Creates a quantity representing the total mass fraction of all the liquid phase.

**Returns** A new `MassFractionOfAllLiquid` object.

**static mass_fraction_of_all_solid_phases**()
Creates a quantity representing the total mass fraction of all solid phases.

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

**static molar_volume_of_phase**(*phase*)
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.

**static molar_volume_of_system**()
Creates a quantity representing the molar volume of the system [m^3/mol].

**Returns** A new `MolarVolumeOfSystem` object.

**static mole_fraction_of_a_solid_phase**(*phase*)
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.

**static mole_fraction_of_all_liquid**()
Creates a quantity representing the total molar fraction of all the liquid phase.

**Returns** A new `MoleFractionOfAllLiquid` object.

**static mole_fraction_of_all_solid_phases**()
Creates a quantity representing the total molar fraction of all solid phases.

**Returns** A new `MoleFractionOfAllSolidPhases` object.

**static site_fraction_of_component_in_phase**(*phase*, *component*, *sub_lattice_ordinal_no*)
Creates a quantity representing the site fractions [-].

---

**Note:** Detailed information about the sublattices can be obtained by getting the *Phase* object of a phase from the *System* object using `+tc_toolbox.system.System.get_phase_in_system`. For each phase the sublattices are obtained by using `+tc_toolbox.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**.

---

**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

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

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

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

**class** +tc_toolbox.**SystemData**(*back*)
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.

---

**SystemData**(*back*)
Constructs an instance of *SystemData*.

**get_phase_parameter**(*parameter*)
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**()
Returns all phase parameters present in the current system.

**Returns** The list of phase parameters

**get_system_function**(*f*)
Returns a system function.

Example:

*system_data.get_system_function('GHSERCR')*

---

**Note:** The parameter 'f' was previously called 'function' but was renamed.

---

---

**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**()
Returns all system functions present in the current system.

**Returns** The list of system functions

**class** +tc_toolbox.**SystemFunction**(*function_name*)
Database function expression used by `SystemModifications.set()`.

**Parameters** **function_name** – The function name

**SystemFunction** (*function_name*)
Constructs an instance of *SystemFunction*.

**get_intervals** ()
Returns the list of all defined intervals.

**Returns** The defined temperature intervals

**get_lower_temperature_limit** ()
Returns the lower temperature limit.

**Returns** The lower temperature limit in K

**get_name** ()
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*)
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*, *upper_temperature_limit*)
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*)
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*)
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_toolbox.**SystemModifications**
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_toolbox.abstract_base.AbstractCalculation.with_system_modifications()` on a calculator object.

**SystemModifications**()
Constructs an instance of *SystemModifications*.

**run_ges_command**(*ges_command*)
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

**class** +tc_toolbox.**TCToolbox**
TCToolbox Starting point for all calculations. This class exposes methods that have no precondition, it is used for choosing databases and elements.

**TCToolbox**()
TCToolbox Construct an instance of this class

**delete**()
TCToolbox Clears all resources used by the session Shuts down the API server and deletes all temporary files. The disk usage of temporary files might be significant.

**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*)
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*)
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**()
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*)
Lists the names of all Property Models in the specified directory.

If the directory is not specified, the Property Model folder used by the normal Thermo-Calc application is used.

**Parameters** **path_to_models** – The path where the Property Models are installed. If no value is entered, the Property Model folder used by the normal Thermo-Calc application is used.

**Returns** Set containing all Property Model names

**load_result_from_disk**()
Loads a previously calculated result from disk.

**Note:** This **only** works for results created by calling one of the `save_result()` methods on a *Result* class created from a calculation.

**Returns** A new *ResultLoader* object

**select_database_and_elements**(*database_name*, *list_of_elements*)
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*, *kinetic_db_name*, *list_of_elements*)
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*, *list_of_elements*)
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"])*

**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*, *precision_for_floats*)
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*)
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_metallurgy**()
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_toolbox.**TemperatureInterval**(*expression*, *upper_temperature_limit*)
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

**TemperatureInterval**(*expression*, *upper_temperature_limit*)
Constructs an instance of *TemperatureInterval*.

**get_expression**()
Returns the function expression of this temperature interval.

**Returns** The temperature function expression

**get_upper_temperature_limit**()
Returns the upper limit of this temperature interval.

**Returns** The upper temperature limit in K

**set_expression**(*expression*)
Sets the function expression of this temperature interval.

**Parameters** **expression** – The temperature function expression

**set_upper_temperature_limit**(*upper_temperature_limit*)
Sets the upper limit of this temperature interval.

**Parameters** **upper_temperature_limit** – The upper temperature limit in K

**class** +tc_toolbox.**TemperatureProfile**
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.

---

**TemperatureProfile**()
Constructor. Constructs an instance of *TemperatureProfile*.

**add_time_temperature**(*time*, *temperature*)
Adds a time-temperature point to the non-isothermal temperature profile.

**Parameters**

- **time** – The time [s]
- **temperature** – The temperature [K]

**Returns** This *TemperatureProfile* object

**class** +tc_toolbox.**ThermodynamicQuantity**
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(*)").

---

**static activity_of_component**(*component*, *use_ser*)
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.

**static chemical_diffusion_coefficient**(*phase*, *diffusing_element*, *gradient_element*, *reference_element*)
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.

**static chemical_potential_of_component**(*component*, *use_ser*)
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.

**static composition_of_phase_as_mole_fraction**(*phase*, *component*)
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.

**static composition_of_phase_as_weight_fraction**(*phase*, *component*)
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.

**static gibbs_energy_of_a_phase**(*phase*, *use_ser*)
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.

**static mass_fraction_of_a_component**(*component*)
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.

**static mass_fraction_of_a_phase**(*phase*)
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.

**static mole_fraction_of_a_component**(*component*)
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.

**static mole_fraction_of_a_phase**(*phase*)
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.

**static normalized_driving_force_of_a_phase**(*phase*)
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.

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

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

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

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

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

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

**static tracer_diffusion_coefficient**(*phase*, *diffusing_element*)
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.

**static u_fraction_of_a_component**(*component*)
Creates a quantity representing the u-fraction of a component.

**Parameters** **component** – The name of the component

**Returns** A new `UFractionOfAComponent` object.

**static user_defined_function**(*expression*)
Creates a quantity representing a user-defined function.

**Parameters** **expression** – The function expression

**Returns** A new `Function` object

**static volume_fraction_of_a_phase**(*phase*)
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.

## 4.3 Package "system"

**class** +tc_toolbox.+system.**CompositionSet**(*phase_name*)
Used by the method `+tc_toolbox.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

**CompositionSet**(*phase_name*)

**set_major_constituents_for_sublattice**(*sublattice_index*, *major_constituents*)
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_toolbox.+system.**Element**(*back*)
Represents an element, making detailed information about the element accessible.

**Element**(*back*)
Constructs an instance of *Element*.

**get_enthalpy**()
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**()
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**()
Returns the molar mass of the element.

**Returns** The molar mass [g/mol]

**get_name**()
Returns the name of the element.

**Returns** The element name

**get_stable_element_reference**()
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**()
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**()
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**()
Returns if the element is valid. Non-valid elements are represented by an empty name.

**Returns** If the element is valid

**class** +tc_toolbox.+system.**MultiDatabaseSystemBuilder**(*back*)
Used to select databases, elements, phases etc. and create a System object. The difference to the class SystemBuilder is that the operations are performed on all the previously selected databases. The system is then used to create calculations.

**MultiDatabaseSystemBuilder**(*back*)
Constructs an instance of *MultiDatabaseSystemBuilder*.

**create_and_select_species**(*stoichiometry*)
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*, *sublattice_no*, *constituent_name_to_deselect*)
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*)
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*)
Removes the species from the system.

**Parameters** **species_name** – The species

**Returns** This *MultiDatabaseSystemBuilder* object

**get_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*, *sublattice_no*, *constituent_name_to_select*)
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*)
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*)
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*)
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_toolbox.+system.**Phase**(*back*)
Represents a phase, making detailed information about the phase accessible.

**Phase**(*back*)
Constructs an instance of *Phase*.

**get_name**()
Returns the name of the phase.

**Returns** The phase name

**get_species**()
Returns the species of the phase.

**Returns** A set containing the species

**get_species_for_composition_profile**()
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**()
Returns the sublattices of the phase in a well-defined contiguous order.

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

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

**Returns** The type of a phase

**has_diffusion_data**()
Returns if diffusion data exists for the phase.

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

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

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

**is_dilute_diffusion_model**()
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**()
Returns if the phase is a gas phase.

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

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

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

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

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

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

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

**class** +tc_toolbox.+system.**PhaseType**
The type of a phase.

**class** +tc_toolbox.+system.**Species**(*back*)
Represents a species, making detailed information about the species accessible.

**Species**(*back*)
Constructs an instance of *Species*.

**get_all_elements**()
Returns all the elements that the species is composed of.

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

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

**Returns** The charge of the species

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

**Returns** The species name

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

**Returns** If the species represents an element

**is_interstitial**()
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**()
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**()
Returns if the species is valid. Non-valid species are represented by an empty name.

**Returns** If the species is valid

**to_element**()
Returns the *Element* representation of the species - if the species actually represents an element.

**Returns** The *Element* object

**class** +tc_toolbox.+system.**Sublattice**(*back*)
Represents a sublattice of a phase.

**Sublattice**(*back*)
Constructs an instance of *Sublattice*.

**get_constituents**()
Returns the constituents of the sublattice.

**Returns** A set containing the constituents

**get_nr_of_sites**()
Returns the number of sites in the sublattice.

**Returns** A float number

**class** +tc_toolbox.+system.**System**(*back*)
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.

---

**System**(*back*)
Constructs an instance of *System*.

**convert_composition**(*input_composition*, *input_unit*, *output_unit*, *dependent_component*)
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**()
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**()
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**()
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*)
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** object

**Return type** A *Element*

**get_elements_in_system**()
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*)
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** object

**Return type** A *Phase*

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

**Returns** A list of phase names

**get_references**()
Provides a dictionary with database references per database in the selected system.

**Returns** The database references

**get_species_in_system**()
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*)
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** object

**Return type** A *Species*

**get_system_data**()
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*, *components*)
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**()
Creates a CCT diagram calculation.

**Returns** A new `PrecipitationCCTCalculation` object

**with_isothermal_diffusion_calculation**()
Creates an isothermal diffusion calculation.

**Returns** A new `DiffusionIsoThermalCalculation` object

**with_isothermal_precipitation_calculation**()
Creates an isothermal precipitation calculation.

**Returns** A new `PrecipitationIsoThermalCalculation` object

**with_material_to_material**()
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**()
Creates a non-isothermal precipitation calculation.

**Returns** A new `PrecipitationNonIsoThermalCalculation` object

**with_non_isothermal_precipitation_calculation**()
Creates a non-isothermal precipitation calculation.

**Returns** A new `PrecipitationNonIsoThermalCalculation` object

**with_phase_diagram_calculation**(*default_conditions*, *components*)
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*, *components*)
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*, *path_to_models*, *debug_model*)
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**()
Creates a Scheil solidification calculation.

> **Warning:** Scheil calculations do not support the *GAS* phase being selected, this means the **`GAS`** **phase must always be deselected in the system** if it is present in the database

**Returns** A new `ScheilCalculation` object

**with_single_equilibrium_calculation**(*default_conditions*, *components*)
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**()
Creates a TTT diagram calculation.

**Returns** A new `PrecipitationTTTCalculation` object

**class** +tc_toolbox.+system.**SystemBuilder**(*back*)
Used to select databases, elements, phases etc. and create a System object. The system is then used to create calculations.

**SystemBuilder**(*back*)
Constructs an instance of *SystemBuilder*.

**create_and_select_species**(*stoichiometry*)
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*, *sublattice_no*, *constituent_name_to_deselect*)
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*)
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*)
Removes the species from the system.

**Parameters** **stoichiometry** – The species

**Returns** This *SystemBuilder* object

**get_system**()
Creates a new System object that is the basis for all calculation types. Several calculation types can be defined later from the object; these are independent.

**Returns** A new *System* object

**get_system_for_scheil_calculations**()
Creates a new System object **without gas phases being selected**, that is the basis for all calculation types, but its particularly useful for Scheil solidification calculations, where the model does not allow that a gas phase is selected in the system.

Several calculation types can be defined later from the object; these are independent.

---

**Note:** Deprecated in version 2022b: Use *get_system()* instead. There are no longer any special requirements from the Thermo-Calc program to deselect the gas phase for Scheil. It will be removed in release 2023b.

---

**Returns** A new *System* object

**select_constituent_on_sublattice**(*phase_name*, *sublattice_no*, *constituent_name_to_select*)
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*, *list_of_element_strings*)
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*)
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*)
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*, *list_of_element_strings*)
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"])*

---

---

**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*)
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

CHAPTER

FIVE

# TROUBLESHOOTING

This section provides an FAQ for common problems that occur when using the TC-Toolbox for MATLAB®.

## 5.1 Diagnostics Script

If you have problems running TC-Toolbox, run the diagnostics script below.

```
%{
    Run this script when troubleshooting TC-Toolbox

    It is important to run this script EXACTLY the same way as you run your MATLAB␣
↪script

%}

clc

toolbox_version = "2022b";


disp("Testing TC-Toolbox toolbox_version: " + toolbox_version)
disp('Please make sure that the variable "toolbox_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.

[matlab_version, matlab_release_data] = version;
fprintf("\n")
disp("MATLAB version: " + matlab_version)
fprintf("\n")


tc_env_variable = 'TC' + extractBetween(toolbox_version, 3, 5).upper() + '_HOME';
if isempty(getenv(tc_env_variable))
    fprintf(2, 'No Thermo-calc environment variable for ' + toolbox_version + ' was␣
↪found. (' + tc_env_variable + ')\n')
else
    disp(getenv(tc_env_variable))
end
fprintf("\n")

disp('Url of license server: (if license server is NO-NET, you need a local license␣
↪file)')
```

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```
if isempty(getenv("LSHOST"))
    disp('No Thermo-calc license server url was found. (LSHOST)')
else
    disp(getenv("LSHOST"))
end
fprintf("\n")

disp('Path to local license file: (only necessary if not using license server)')
if isempty(getenv("LSERVRC"))
    disp('No path to local license file was found. (LSERVRC)')
else
    disp(getenv("LSERVRC"))
end
fprintf("\n")

try
    session = tc_toolbox.TCToolbox();
catch e
    fprintf(2,'TC-Toolbox not properly installed !!!\n%s\n', e.message);
end

fprintf("\n")
disp('Lists the databases: (should be a complete list of the installed databases that␣
↪you have license for or do not require license)')
disp(transpose(session.get_databases()))

fprintf(1, 'Make sure no error messages were printed !\n\n')
```