Diffusion Module (DICTRA) Quick Start Guide - Graphical Mode

Thermo-Calc Version 2025b

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Introduction to the Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to the Thermo-Calc software package. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulations are both time- and space-dependent.

The Diffusion Module (DICTRA) is suitable for solving diffusion problems that include a moving boundary (so-called *Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. The concentration fields only vary along one spatial coordinate, but the geometry may be either planar, cylindrical or spherical.

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About this Quick Start Guide

The following introduces you to the basic concepts, steps and theory to start using the Diffusion Module (DICTRA). An understanding of this information is necessary to ensure accurate calculations.

More details about the use of DICTRA can be found in [2002And] and [2000Bor].

If you are not familiar with Graphical Mode, it is recommended you review the documentation and additional resources available on our website.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

References

[2000Bor] A. Borgenstam, L. Höglund, J. Ågren, A. Engström, DICTRA, a tool for simulation of diffusional transformations in alloys. J. Phase Equilibria 21, 269–280 (2000).

[2002And] J.-O. Andersson, T. Helander, L. Höglund, P. Shi, B. Sundman, Thermo-Calc & DICTRA, computational tools for materials science. Calphad 26, 273–312 (2002).

Diffusion Module Terminology in Graphical Mode

The following definitions are useful to help you understand the examples in this guide. For more detailed information search or browse the online help (press F1 or from the main menu select **Help → Online Help**).

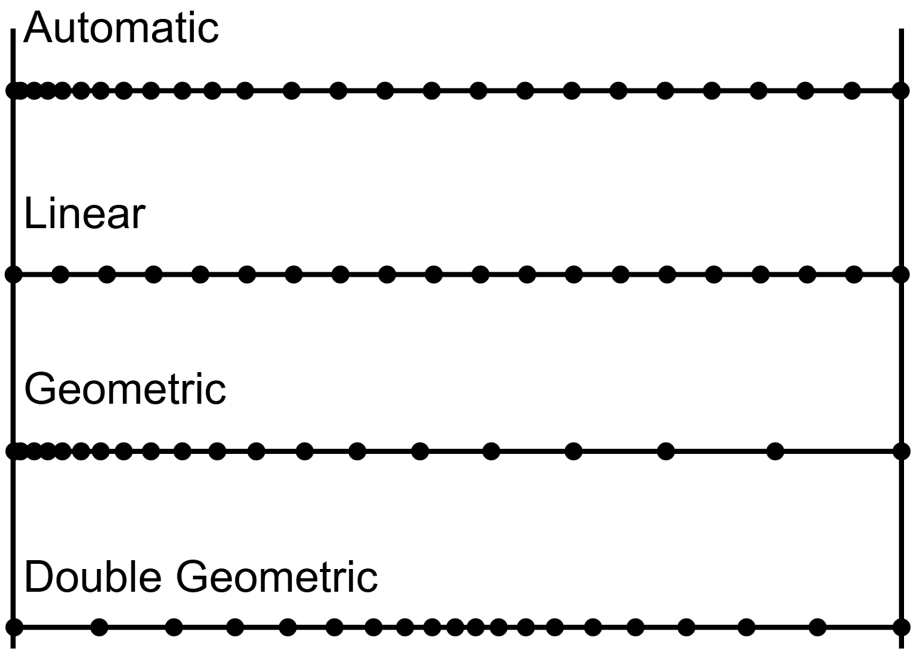
These terms are specific to working in Graphical Mode. The overall simulation in Console Mode is comparable but there are some differences in terminology and functionality.

Region

In Graphical Mode, a system consists of one *cell* with one or multiple *regions* in which the diffusion problem is to be solved.

Grid Types

These grid types are used in diffusion simulations: automatic, linear, geometric, and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Phases

Each region must contain at least one *phase*. The so-called *homogenization model* is used if multiple phases are added inside a region, then the average properties of the local phase mixture is used. Phase(s) can also be added to interphases of region(s) and then only participate in the simulation if the driving force for precipitation of the phase exceeds a predefined value. A new region is then created where the name of the region is set to the name of the phase but with `R_` added as a prefix.

Composition

These types of composition variables are used in the configuration of the Diffusion Calculator: *mass (weight) fraction*, *mass (weight) percent*, *mole fraction*, or *mole percent*.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$\mu_k = \frac{x_k}{\sum_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume. Weight fraction, mole fraction or u-fraction can be used when plotting the results from a simulation.

Geometry and Coordinates

The Diffusion Module (DICTRA) can only handle diffusion problems where compositions vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical*, or *spherical*.

The *planar* geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Setting up a Diffusion Simulation in Graphical Mode

When you are using the Graphical Mode version of the Diffusion Module (DICTRA), the steps to set up a simulation are a combination of adding *Activity* nodes (the System Definer, Diffusion Calculator, and Plot Renderer) and then defining the applicable settings for each of these nodes in a Configuration window.

The following is a general overview of the steps to set up the simulation.

1. Use the **Diffusion** template to add the System Definer, Diffusion Calculator, and Plot Renderer activity nodes.
2. On the **System Definer**, you select the thermodynamic and kinetic databases, add elements and phases, and generally define the system.
3. On the **Diffusion Calculator**, you set the geometry (by default the geometry is planar), add region(s) and enter grid(s) and phase(s) in the region(s). You then enter composition(s) of phase(s).
4. On the **Plot Renderer** or **Table Renderer**, you choose how to visualize your diagrams, and then run the simulation, i.e. you **Perform** the sequence of nodes you have defined in the tree to produce the output simulation.

Single Phase Simulations

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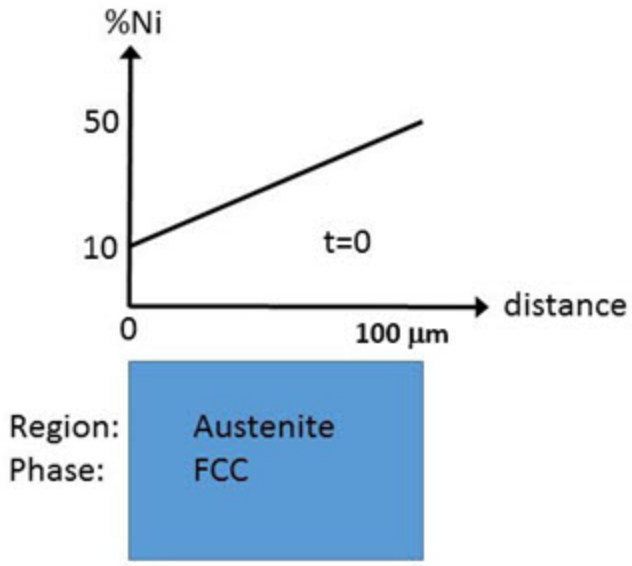
About the Single Phase Simulation

In a 100 µm wide planar domain, the single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase (in Thermo-Calc the name of this phase is FCC_A1). Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.

The simulation time is slightly different between the modes. For Console Mode it is 10^5 s and for Graphical Mode it is 30 hours.

By default the boundaries are closed. The plot generated shows the initial and final Ni profile.



Schematic view of the initial state of Single Phase Diffusion example. The width of the domain is 100 µm and there is a linear gradient in composition going from 10 to 50 mass-% Ni. There is a single region named Austenite that consists of an fcc phase.

Theory for the Single Phase Simulation

The flux of a component k in the z-direction in an isobarothermal system is in general given by

$$J_k = \sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z}$$

where L_{ki} is a matrix of kinetic coefficients and μ_i is the chemical potential of component i. The correlation effects, i.e. the coupling of the flux of k component to the chemical potential gradients of the other elements, are normally neglected

$$(L_{ki} = 0, k \neq i)$$

and thus

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

where c_k is the concentration and M_k the mobility of component k.

The equation for the flux is combined with the equation of continuity, which takes the following form in a planar domain,

$$\frac{\partial c_k}{\partial t} = \frac{\partial}{\partial z}(-J_k)$$

which relates the local evolution of the concentration of k to the divergence of the flux.

The expression for the flux can be expanded in terms of concentration gradients

$$J_k = -\sum_{i=1}^{n} M_k c_k \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z} = -\sum_{i=1}^{n} D_{kj} \frac{\partial c_j}{\partial z}$$

where the diffusion coefficient of component k with respect to the concentration gradient of component j has been introduced.

$$D_{kj} = M_k c_k \frac{\partial \mu_k}{\partial c_j}$$

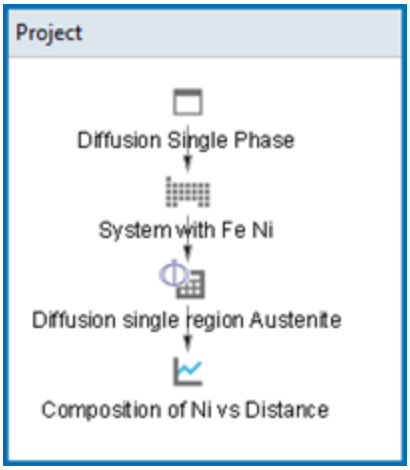
The flux expressions above are given in the so-called lattice-fixed frame of reference. In practical calculations it is more common to use a volume-fixed frame of reference. For a discussion of these concepts, see Andersson and Ågren [1992And].

"References" on page 50

Setting Up the Single Phase Simulation

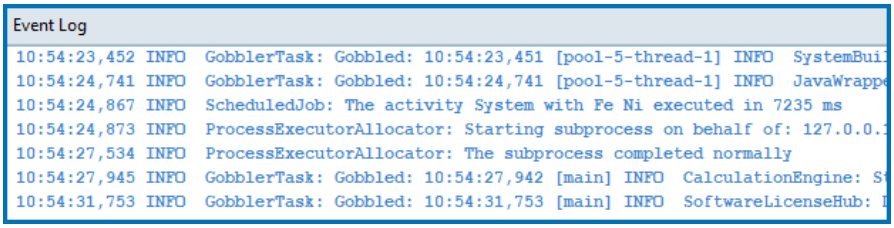
For the single phase example, you can open the example project file included with your installation to first see how it is set up:

1. Open Thermo-Calc.
2. There are different ways to access the examples.
   - From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
   - Click the **My Project** node and on the **Configuration** window under **Getting Started**, click **Example Files**.
3. Click to open the **Diffusion Module - DICTRA** folder and locate the **D_01_Diffusion_Single_Phase.tcu** file. Double-click to open it.
4. The project opens in Thermo-Calc and adds this tree structure:



5. Click the top Project node (renamed to *Diffusion Single Phase*). At the bottom of the **Configuration** window click **Perform Tree**. You can also right-click the node and select **Perform Now**.

   The **Event Log** shows the progress of the calculations:

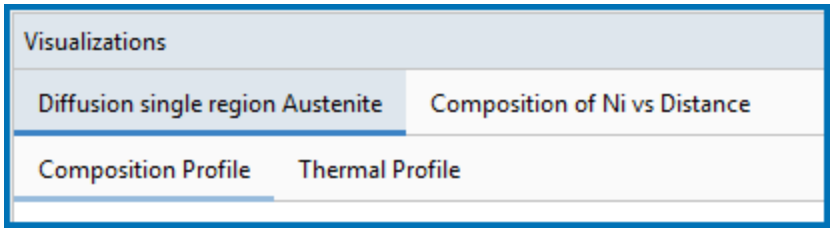


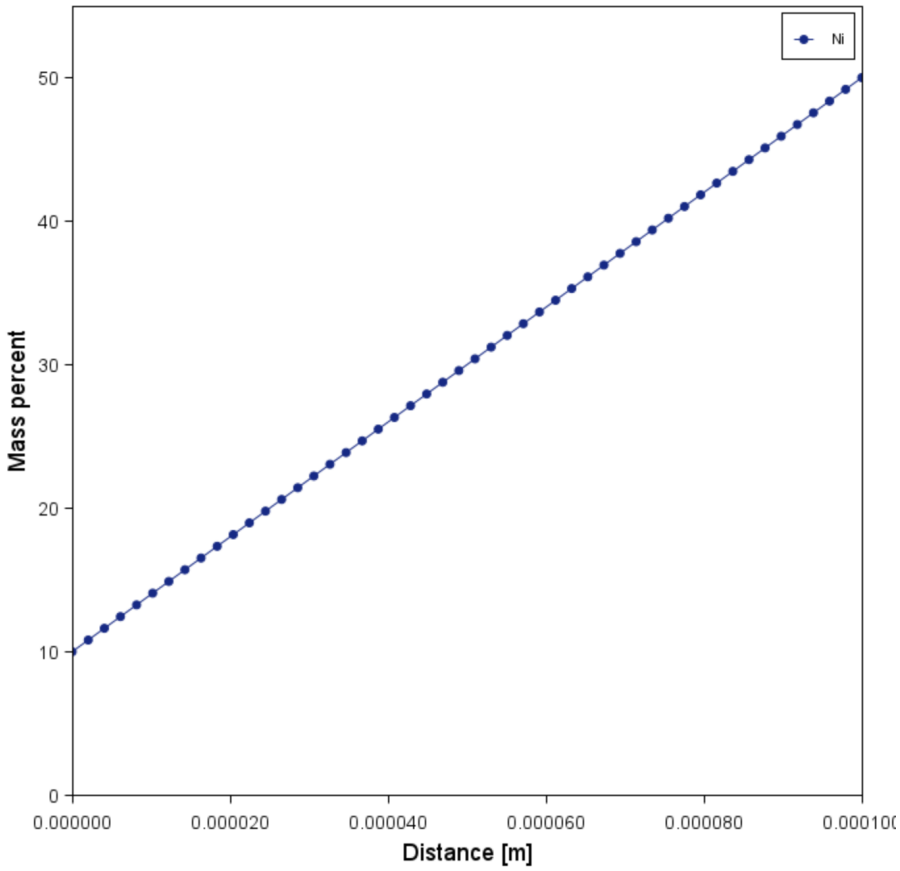
When completed, the results are plotted in the **Visualizations** window as shown below.

Visualizations

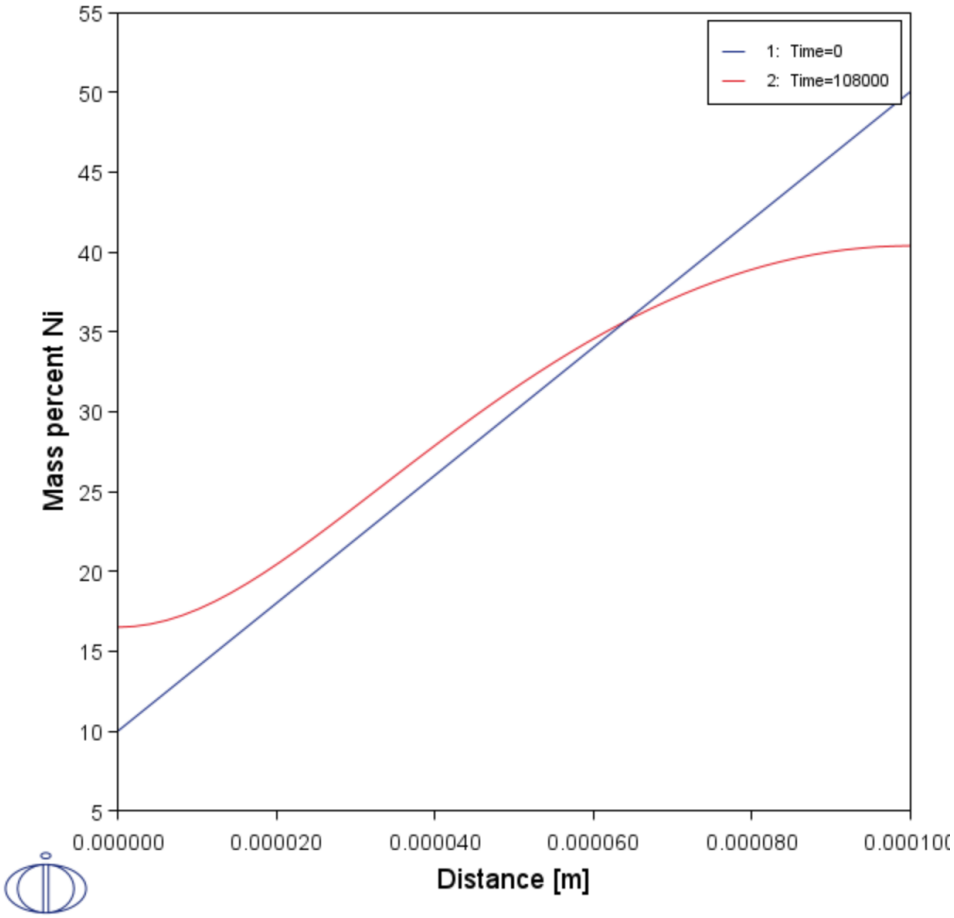
There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.





During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.



After performing the calculation, you can view the final Plot Renderer result on the Composition of Ni vs Distance tab, which shows the initial and final Ni profile. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

For the rest of the exercise, you will learn how to build this example step-by-step.

System Definer Settings

The following describes how to set up the *D_01_Diffusion_Single_Phase.tcu* example from the beginning.

> To learn more about the activity nodes and tree structure see 'Project Activities and the Tree Structure' in the *Thermo-Calc User Guide*.

Add a System Definer Node

1. Open Thermo-Calc.
2. In the **Project** window, right-click **My Project** and select **Create New Activity → System Definer**.
3. In the **System Definer Configuration** window, you select the thermodynamic and kinetic databases to use and select the elements.

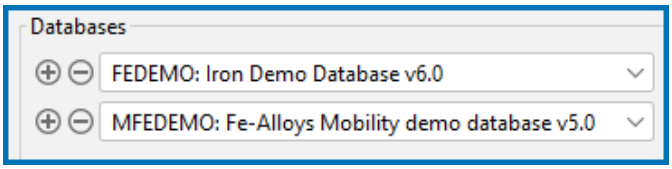
Tip: The Diffusion Template

For this first example the activity nodes are added one at a time. A faster way to add all the nodes you need is to use the **Diffusion** template (click **My Project** node then under **Non-Equilibrium** click **Diffusion**).

Choose the Databases

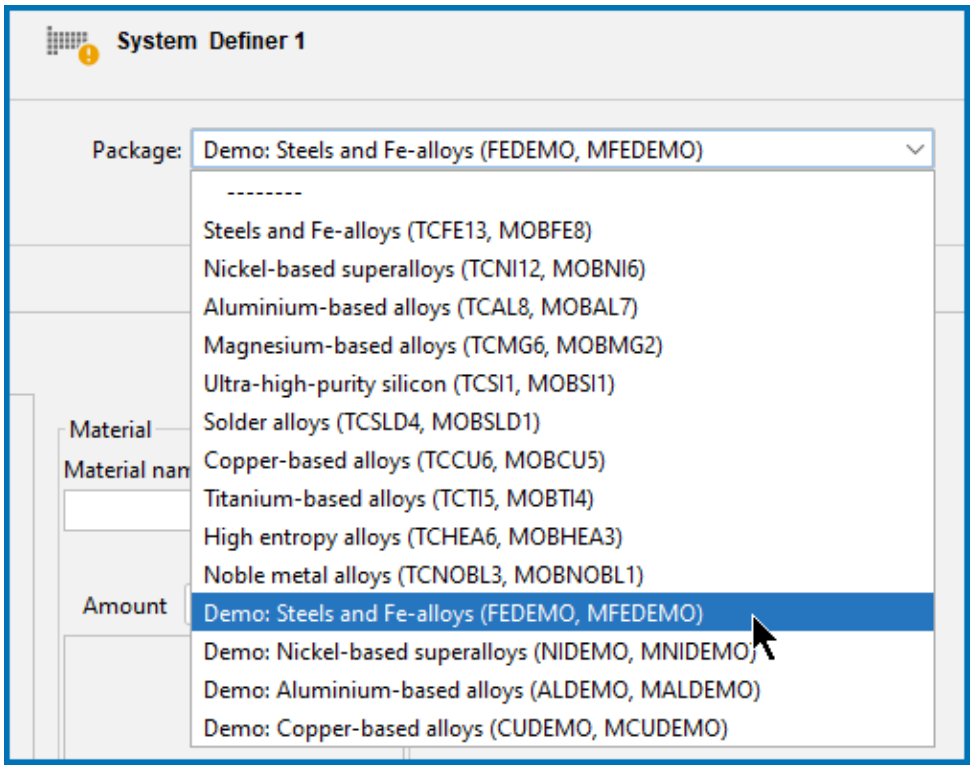
There are databases for different purposes and material types. This example uses two demonstration databases: **FEDEMO** (the thermodynamic steels/Fe-alloys database) and **MFEDEMO** (the kinetic/mobility steels/Fe-alloys database).

1. In the System Definer **Configuration** window click the **Databases** list and select the **FEDEMO** database.
2. Click the **Add a database** button.
3. Select the **MFEDEMO** database.



Tip: Database Packages

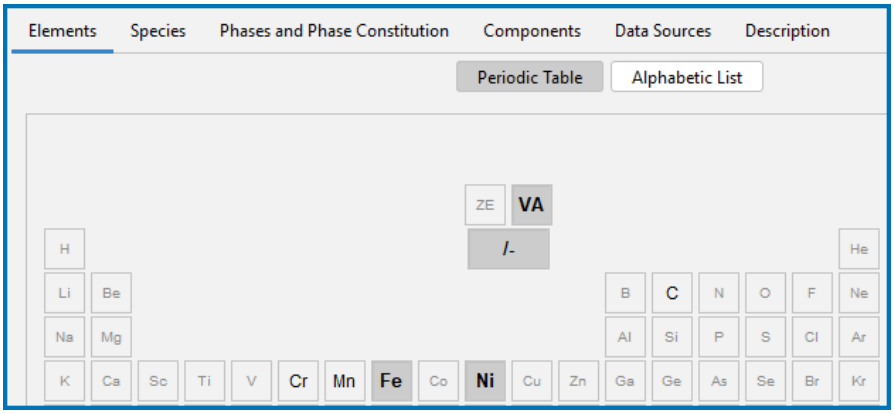
For this first example the databases are added one at a time. A faster way to add both the databases is to add a predefined database **Package**.



Choose the Elements

On the **Elements** tab, and based on the databases selected, you can select and review elements using a **Periodic Table** or **Alphabetic List** format. The demonstration databases have only a small number of elements to choose from.

1. In the **Periodic Table**, click **Fe**.
2. Click **Ni**.



When using the System Definer with the Diffusion Calculator, you can keep all phases selected on the **Phases and Phase Constitution** tab.

Diffusion Calculator Settings

After you have completed the settings for the System Definer you start defining the diffusion parameters on the Diffusion Calculator.

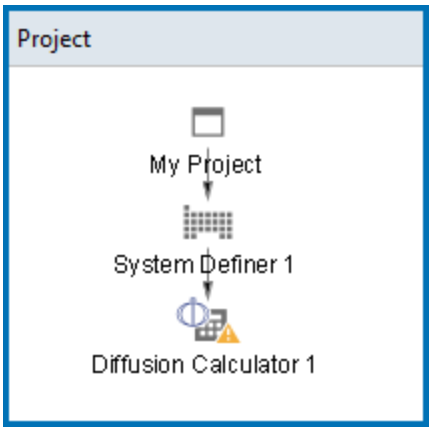
In any simulation at least one *region* must be defined. This is a named container that designates a certain part of the domain. In this case it is the whole domain. The name of a region is arbitrary and specified by you.

> The use of regions becomes clearer in the context of moving phase boundary simulations.

A region must contain a numerical *grid* specified by width and type. In this example, a 10^{-4} m (1e-4 m) wide, linear (i.e. equidistant) grid is used with 50 grid points.

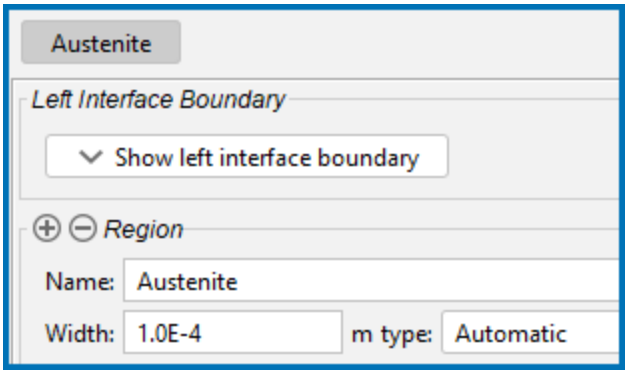
Define the Region and Composition Profiles

1. In the **Project** window, right click the **System Definer** node and select **Create New Successor → Diffusion Calculator**. A Diffusion Calculator node is added to the tree structure.



> If you used the **Diffusion** template, then this activity node is already there. Click the **Diffusion Calculator** node to access the **Configuration** window settings.

2. You are now going to add the settings to the Configuration window on the **Conditions** tab. Keep the defaults for *Composition unit* (**Mass percent**) and *Length unit* (**Meter**). A **Planar** *Geometry* is used for all the examples.
3. In the *Region* **Name** field, enter `Austenite`. This name is automatically updated on the tab.

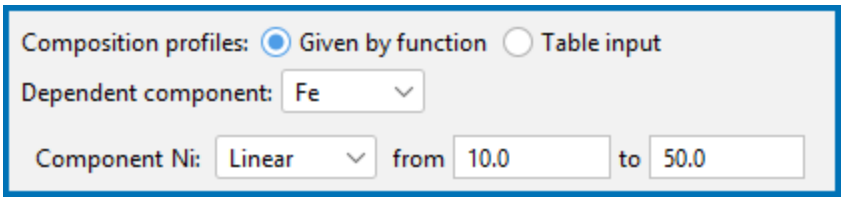


4. In the **Width** field replace the default with `1e-4`. Keep the defaults for number of points (`50`) and type of grid (`Automatic`).
5. From the **Phase** list, select **FCC_A1**.

   In the **Visualizations** window, the **Composition Profile** tab displays a preview. The initial composition profile must be specified for all regions. Since there are only two elements, Fe and Ni, the initial composition profile must only be given for one of them.

6. Next to **Composition profiles** the default selected is **Given by function**. Choose **Fe** as the **Dependent component**.

   There are many ways to specify the composition profile, e.g. an arbitrary position dependent function. In this example, the default *Linear* type is used. The initial profile for Ni is a **Linear** variation. In the **from** field enter `10` and in the **to** field enter `50`. These settings mean that the profile goes from 10 (mass-%) on the lower/left hand side of the system to 50 (mass-%) on the upper/right hand side of the system.

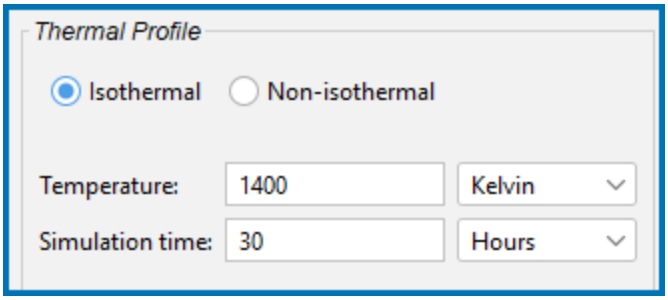


Watch as the **Composition Profile** changes on the **Visualizations** window to match these values.

Define the Thermal Profile

The default **Isothermal** profile is used for this example. A constant temperature of 1400 K is used during the simulation, which is run for 30 hours. Enter these values in the fields:

1. In the **Temperature** field, enter `1400`. Keep **Kelvin** as the default unit.
2. In the **Simulation time** field, enter `30`. Select **Hours** from the list.



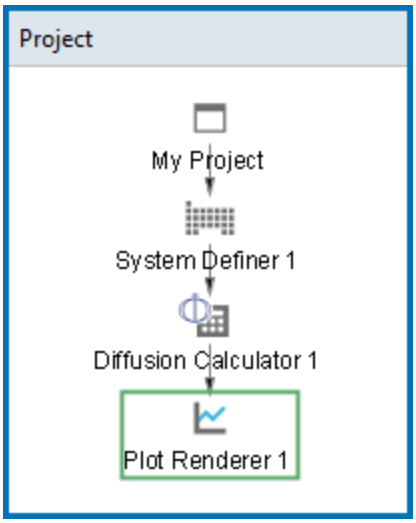
Watch as the **Thermal Profile** tab on the **Visualizations** window updates to match these values.

There are no changes to the default settings on the **Options** tab. You can click the tab to see what settings are available and then search the Online Help (press F1) for more information.

Plot Renderer Settings

After you have completed the settings for the System Definer and Diffusion Calculator you define the plot parameters and run (perform) the simulation.

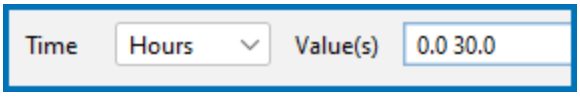
1. In the **Project** window, right click the **Diffusion Calculator** node and select **Create New Successor → Plot Renderer**. A Plot Renderer node is added to the tree structure.



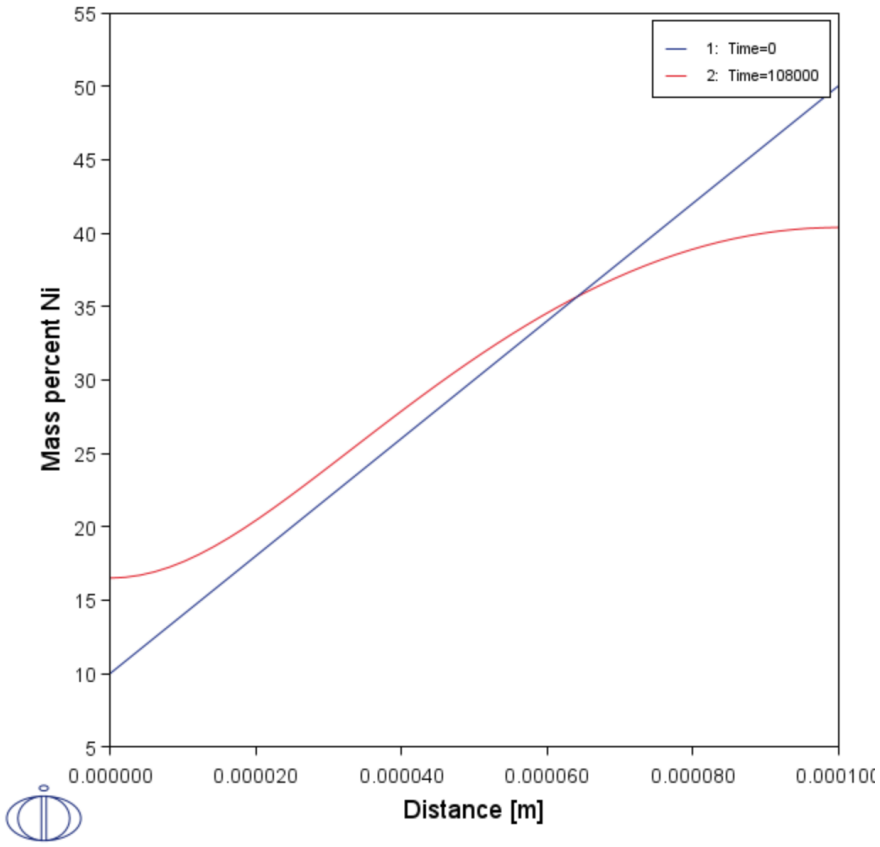
> If you used the **Diffusion** template, then this activity node is already there. Click the **Plot Renderer** node to access the **Configuration** window settings.

For this first example, some of the defaults are kept and there are only two settings to add. In most cases, either a specific position in the domain or one or more specific times must be specified depending on whether time or spatial position is chosen as independent (*X-axis*) variable.

2. In the *Axes* section for *Y* and next to **Composition**, choose **Ni**.
3. In the **Value(s)** field, enter `0.0` before the `30.0`, which is automatically taken from the Diffusion Calculator setting.



4. Click **Perform**. If you have entered everything correctly, you will get this plot showing the composition profile of Ni at the initial (0 hours) and final time (30 hours or 108,000 seconds).



Renaming the Nodes and Saving the Project

You can rename the nodes in the tree at any time during the creation of a project. For this first example it was left until the end so you could become familiar with the System Definer, Diffusion Calculator and Plot Renderer settings. It is also important at this point to save the project. You can do this at any time and it is good practice to save your project often.

The following renaming can be done to match the example file included with your installation:

When you rename a node, associated tabs are also renamed automatically. For example, when the Plot Renderer is renamed, so is the tab in the **Visualizations** window.

1. Right-click the **My Project** node and select **Rename**.
2. In the **New name** field enter `Diffusion Single Phase`. Click **OK**. Continue renaming the other nodes.
3. Right-click the **System Definer**, select **Rename** and enter `System with Fe Ni`.
4. Right-click the **Diffusion Calculator**, select **Rename** and enter `Diffusion single region Austenite`.
5. Right-click the **Plot Renderer**, select **Rename** and enter `Composition of Ni vs Distance`.
6. Save the project. To do this, click the **Save** button and navigate to a location on your computer where you can easily find this project file.

Moving Phase Boundary Simulations

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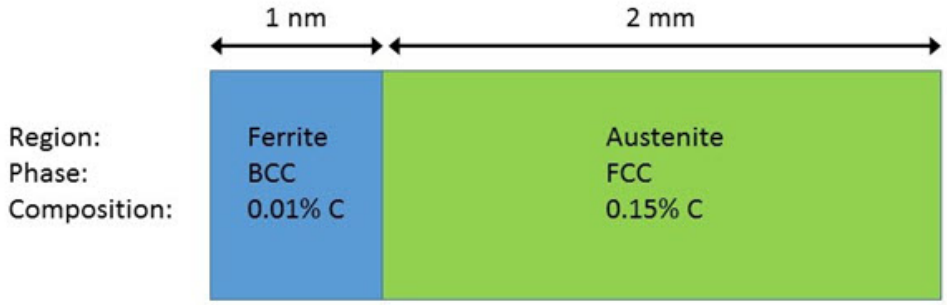
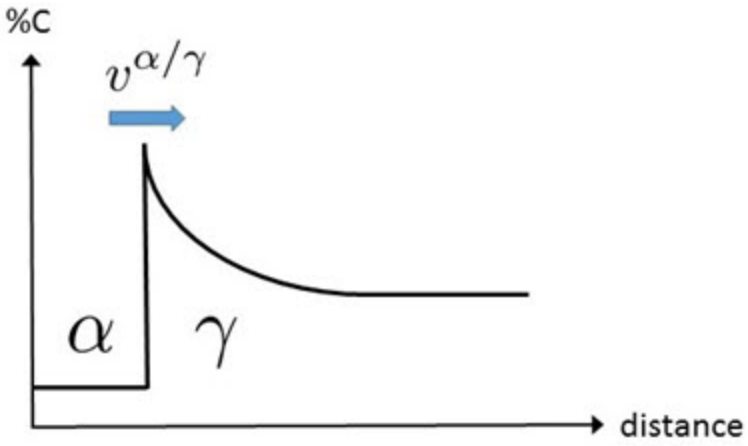
About the Moving Phase Boundary Simulation

The growth of ferrite (bcc) into austenite (fcc) is simulated in this example. The austenite is assumed to be initially homogeneous with the composition Fe - 0.15 mass-% C and the transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation. The initial state is as below.



The set-up of the Moving Boundary example. There are two regions, Ferrite and Austenite, consisting of bcc and fcc, respectively.

A schematic graph of the carbon profile during the transformation is shown in the image below. Crusius et al. [1992Cru-1] is recommended as further reading.



Schematic view of the carbon profile during the transformation from austenite (γ) to ferrite (α) in the Moving Boundary example.

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Theory for the Moving Phase Boundary Simulation

It is assumed that local equilibrium holds at the phase interface, i.e. the chemical potentials of all elements are continuous across the boundary, but the chemical potential gradients are in general discontinuous.

In order to maintain mass balance a set of flux balance equations must be satisfied at the phase interface:

$$v^{\alpha/\gamma}(c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma \qquad k = 1, \ldots, n-1$$

where v is the interfacial velocity. The concentrations and the fluxes c and J are those at the interface on the α and γ sides, respectively.

In the present case there are no degrees of freedom at the interface and the concentrations can be taken directly from a phase diagram. There is only one flux balance equation and the interface velocity can be evaluated once the fluxes at the interface are known. However, for ternary and higher systems the state at the interface must be found by some iterative procedure.

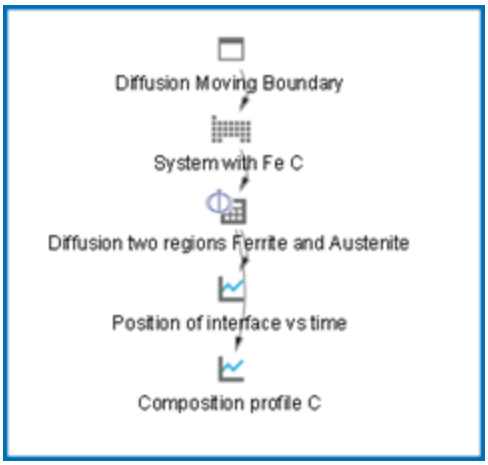
For more information on moving phase boundary problems, see, for example, [1982Ågr], [1992Cru-2], and [1997Hög].

"References" on page 50

Moving Phase Boundary Example Project

For the moving phase boundary simulation, you can open the example project file included with your installation to see how it is set up.

1. Open Thermo-Calc.
2. There are different ways to access the examples.
   - From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
   - Click the **My Project** node and on the **Configuration** window under **Getting Started**, click **Example Files**.
3. Click to open the **Diffusion Module - DICTRA** folder and locate the file **D_02_ Diffusion_Moving_Boundary.tcu**. Double-click to open it.
4. The project opens in Thermo-Calc. Click the top Project node (renamed to *Diffusion Moving Boundary*). At the bottom of the **Configuration** window click **Perform Tree**. You can also right-click the node and select **Perform Now**.



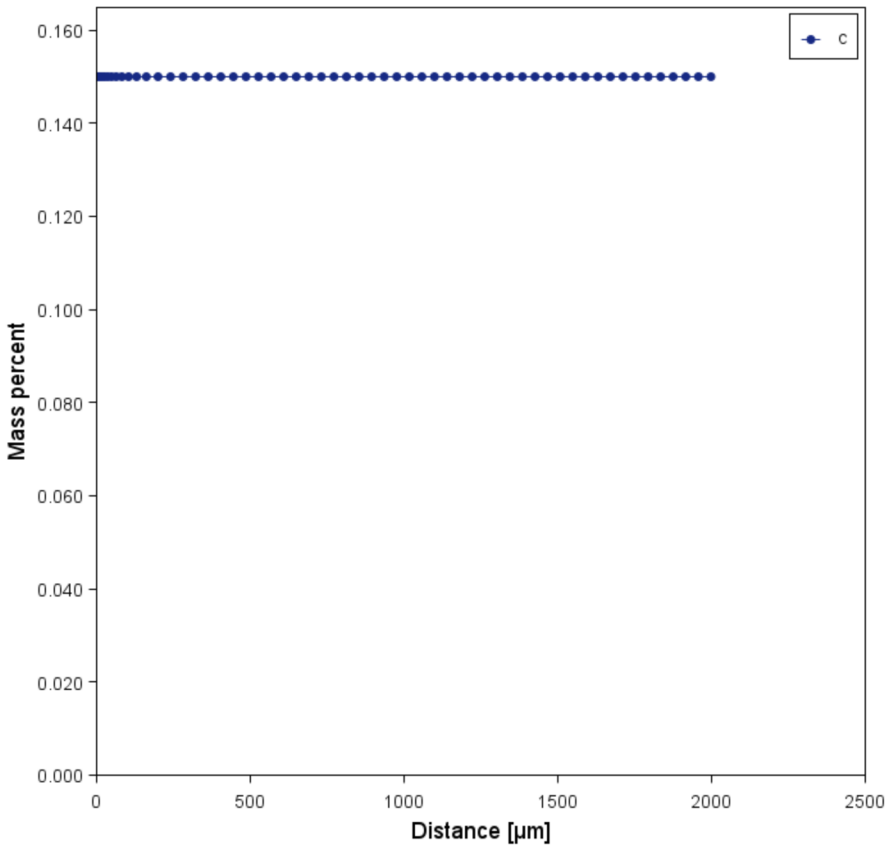
When completed, the results are plotted in the **Visualizations** window.

Visualizations

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

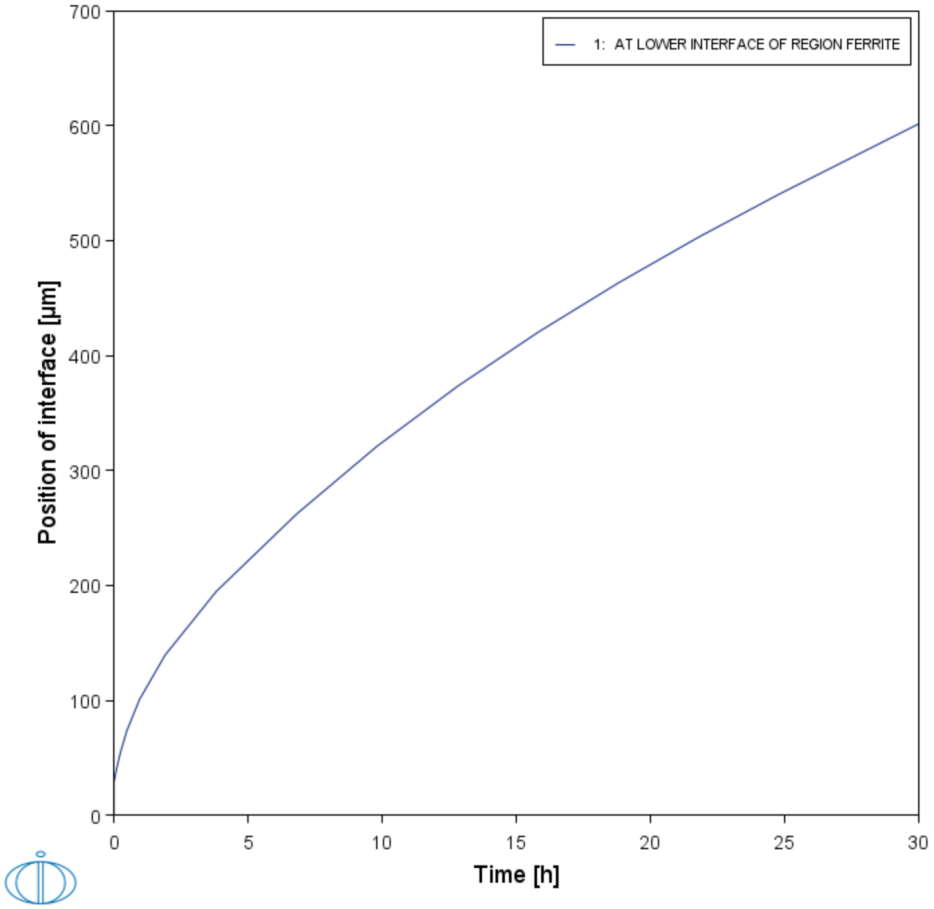
- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

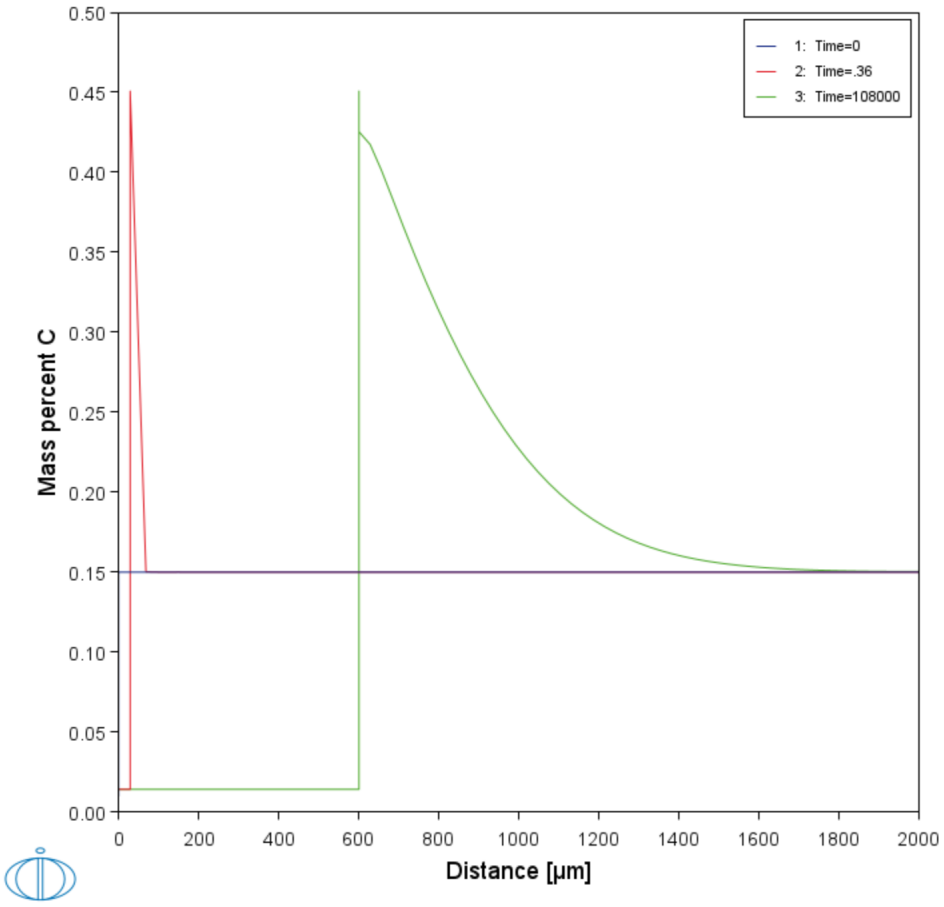


During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

There are two plot nodes, which creates two plots: The ferrite/austenite phase interface position as a function of time and the composition profile for Carbon.



After performing the calculation, you can view the final Plot Renderer result on the Position of interface vs time tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.



After performing the calculation, you can view the final Plot Renderer result on the Composition profile C tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

System Definer Settings

This is a continuation from the Single Phase simulation and it describes how to set up the example file *D_02_Diffusion_Moving_Boundary.tcu*. In this example, the shortcuts explained for the Single Phase System Definerare used.

Add the Databases and the Elements

1. Open a new instance of Thermo-Calc.
2. Click the **My Project** node and on the **Configuration** window under **Non-Equilibrium**, click the **Diffusion** template icon.
3. In the System Definer **Configuration** window click the **Package** list and choose **Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)**.
4. In the **Periodic Table**, click **Fe** then **C**.
5. Rename the nodes. Right-click **System Definer** and rename it to **System with Fe C**.
6. Right-click **My Project** and give it the same name as the project e.g. *Diffusion Moving Boundary*.
7. Save the project file with a new name, such as *Diffusion_Moving_Boundary*.

Diffusion Calculator Settings

After you have completed the settings for the System Definer you define the diffusion calculation parameters.

The phase interface between ferrite and austenite is created by introducing an austenite region that is attached to the ferrite region. Regions are always separated by phase interfaces and must therefore always contain different phases.

In this simulation both the FCC_A1 and BCC_A2 phases are included. Both phases are assumed to be initially homogeneous, the BCC phase having 0.01 mass-% C and the FCC phase 0.15 mass-% C. These settings are entered on the Diffusion Calculator.

As with the single phase example, the **Options** tab keeps all the defaults.

Add a Ferrite Region

1. In the **Project** window, click the **Diffusion Calculator** node.
2. Keep the default for **Composition unit** (**Mass percent**). Choose **Micrometer** for the **Length unit**. A **Planar** geometry is used for all the examples.
3. Under *Region* in the **Name** field enter `Ferrite` (replace the default text **Region 1**). Press <Enter>.
4. In the **Width** field enter `0.001` µm and change the default number of points to `10`. Keep the default **Automatic** grid type.

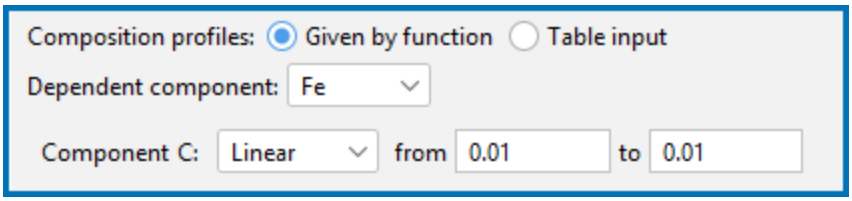
   The grid type for the ferrite region is the same as in the single-phase simulation example, i.e. equidistant.

5. From the **Phase** list select **BCC_A2**.

   In the **Visualizations** window, the **Composition Profile** tab displays a preview. The initial composition profile must be specified for all regions. Since there are only two elements, Fe and C, the initial composition profile must only be given for one of them.

6. Next to **Composition profiles** the default selected is **Given by function**. **Fe** is chosen as the **Dependent component** and the initial profile for **Component C** is a **Linear** variation.

7. Enter `0.01` in both fields to represent C going from 0.01 (mass-%) on the lower, left-hand side of the system to 0.01 (mass-%) on the upper, right-hand side of the system.



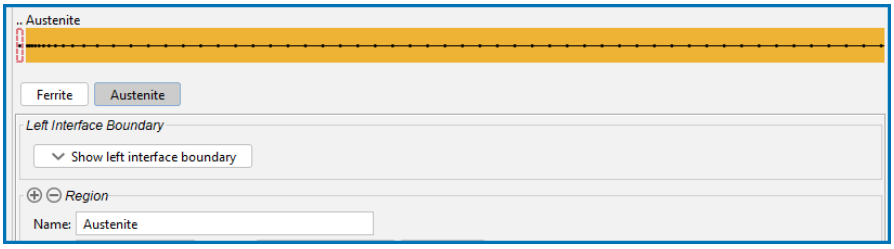
Watch as the **Composition Profile** changes on the **Visualizations** window to match these values.

Add an Austenite Region

1. Next to *Region*, click the add button ⊕. A new tab called **Region 1** is added.

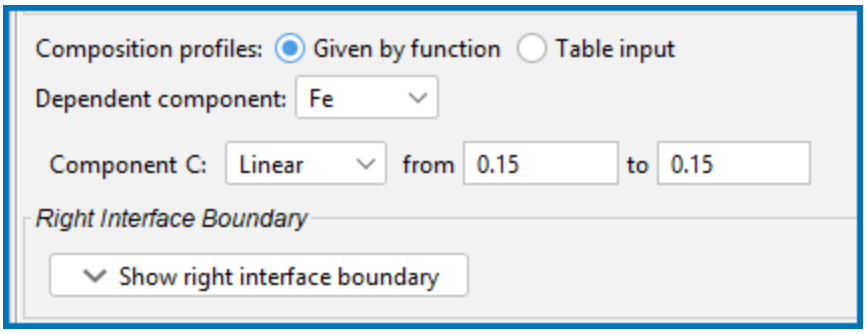
> If you add a region and then need to change the order, right-click the applicable tab and choose **Move left** or **Move right**.

2. In the *Region* **Name** field, enter `Austenite`. This name is automatically updated on the tab and above the grid points in a new section for the second region.



3. In the **Width** field enter `2000` µm.
4. Select a **Automatic** type of grid and choose **Medium**.
5. From the **Phase** list, select **FCC_A1**.
6. Next to **Composition profiles** the default selected is **Given by function** and **Fe** is the **Dependent component**. Enter `0.15` in both the **from** and **to** fields to represent **Component C** going from 0.15 (mass-%) on the lower, left-hand side of the system to 0.15 (mass-%) on the upper, right-hand side of the system. The Austenite grid shows the points and the **Composition Profile** changes on the **Visualizations** window to

match these values.

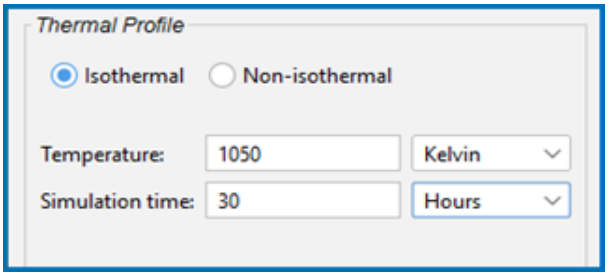


The domain now consists of two regions: Ferrite and Austenite.

Define the Thermal Profile

The default **Isothermal** profile is used.

1. In the **Temperature** field, enter `1050`. Keep the default unit, **Kelvin**.
2. In the **Simulation time** field, enter `30`. Choose **Hours** from the list.
3. Right-click **Diffusion Calculator** and rename it to `Diffusion two regions Ferrite and Austenite`.

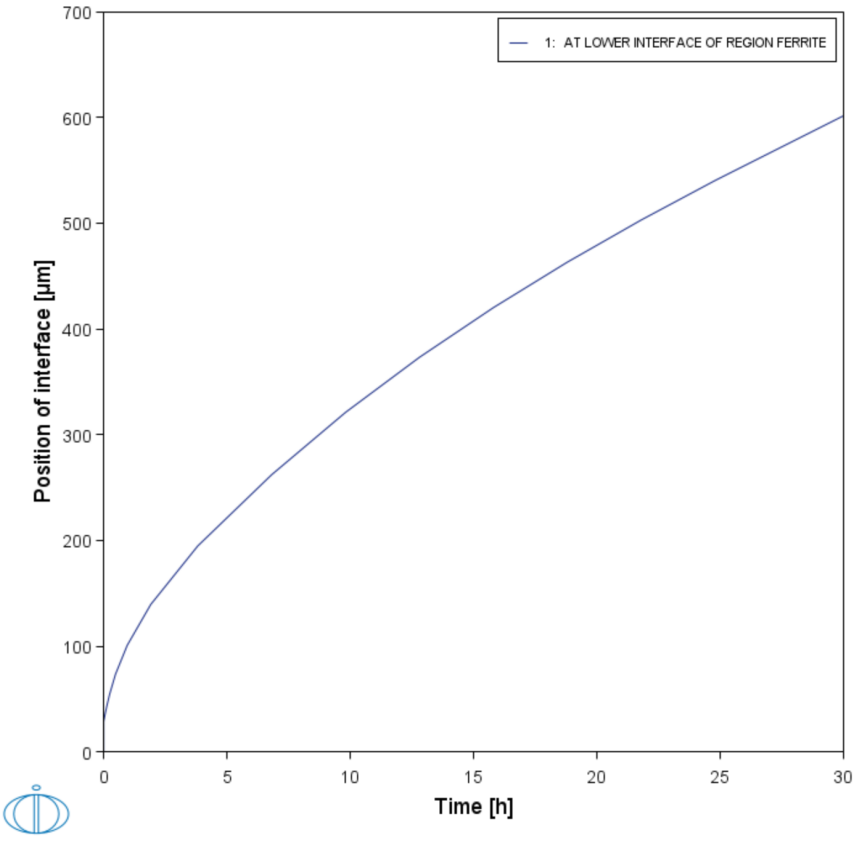


Plot Renderer Settings

After you have completed the settings for the System Definer and Diffusion Calculator you define the plot parameters.

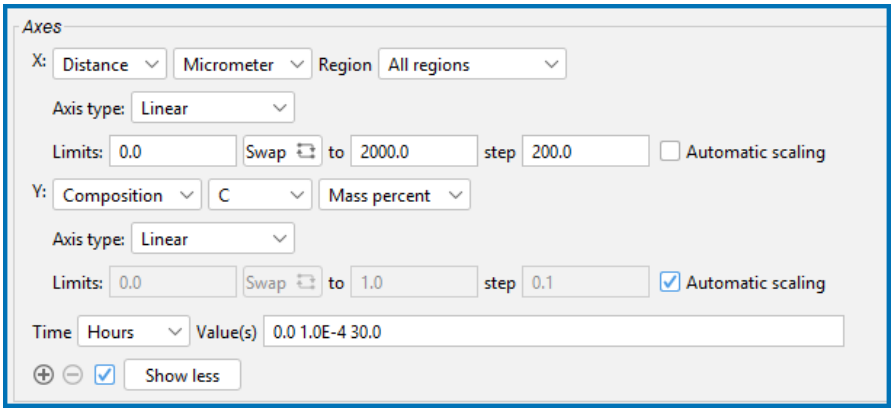
1. In the **Project** window, click the **Plot Renderer** node.
2. In the *Axes* section, choose **Time** for *X* and select **Hours**.
3. Choose **Position of interface** for *Y*. After you click **Perform**, the **Interface** list is populated.
4. Right-click the **Plot Renderer** and rename it to `Position of interface vs time`.
5. Click **Perform**. If you have entered the same settings the plot shows the ferrite/austenite phase interface position as a function of time. The plot has the parabolic appearance characteristic for many types of diffusion simulations.

   Plot result from the example showing the phase interface position as a function of time.



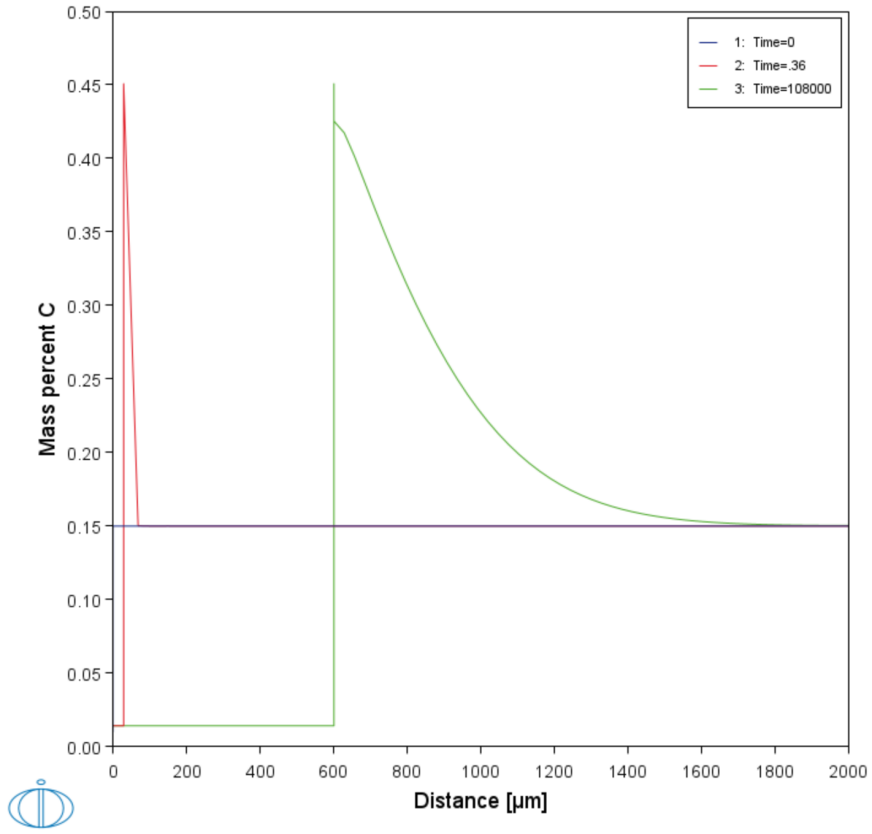
Add a Second Plot

1. Right-click the **Diffusion Calculator** node. Remember it is renamed to *Diffusion two regions Ferrite and Austenite*.
2. From the **Create New Successor** list, click **Plot Renderer**.
3. In the new Plot Renderer node **Configuration** window *Axes* section, for *X*, change the **Distance** units to **Micrometer**.
4. Click **Show more**, then click to clear the **Automatic scaling** checkbox.
5. In the **Limits** fields, keep `0.0` as the lower limit, enter `2000` for the upper limit and `200` for **step**.
6. For *Y*, keep the default **Composition** and choose **C** from the list.
7. Choose **Hours** as the **Time** unit and enter `0.0 1.0E-4 30.0` in the field.



8. Right-click **Plot Renderer** and rename it to `Composition profile C`.

9. Click **Perform** If you have entered the same settings the plot shows the composition profile of C.



Multiphase Simulations

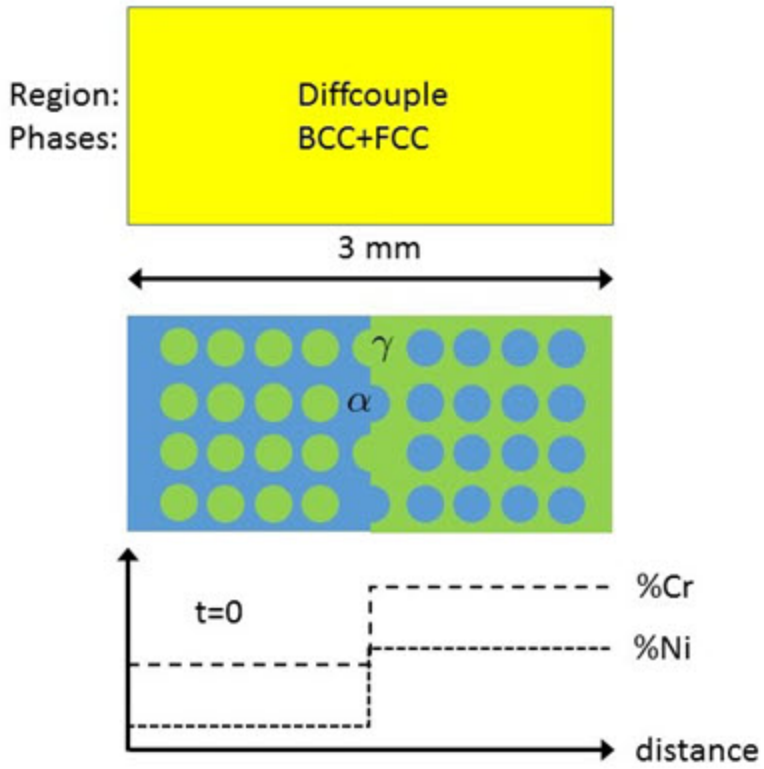
In this section:

About the Multiphase Simulation 39
Theory for the Multiphase Simulation 40
Multiphase Example Project 41
System Definer Settings 44
Diffusion Calculator Settings 45
Plot Renderer Settings 48

About the Multiphase Simulation

This example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.



Schematic view of the initial state of the Multiphase example. Two ternary Fe-Cr-Ni alloys form a diffusion couple. There is a single region (diffcouple) where both the bcc and fcc phases are entered. Both alloys are duplex bcc+fcc, but the majority phase is bcc (α) in the left-hand side alloy and fcc (γ) in the right.

Theory for the Multiphase Simulation

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström [2006Lar] and Larsson and Höglund [2009Lar]. As mentioned in the description of this simulation, it is assumed that the material is locally fully equilibrated and that the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition. From a numerical point of view the homogenization model treats the multiphase material as a single phase having the “average”, or “effective”, properties of the local phase mixture.

When estimating the effective kinetics of a multiphase mixture the product of solubility and mobility in each phase is considered. It is therefore convenient to define

$$\Gamma_k^\phi = M_k^\phi c_k^\phi$$

for each phase ϕ. The effective kinetics of the multiphase mixture is denoted and in this example it was evaluated using the lower Hashin-Shtrikman bound. The default method is a simple rule of mixtures

$$\Gamma^\star = \sum_\phi f^\phi \Gamma_k^\phi$$

where f^ϕ is the volume fraction of ϕ. The flux is obtained as

$$J_k = -\Gamma_k^\star \frac{\partial \mu_k}{\partial z}$$

which replaces the single-phase equation

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

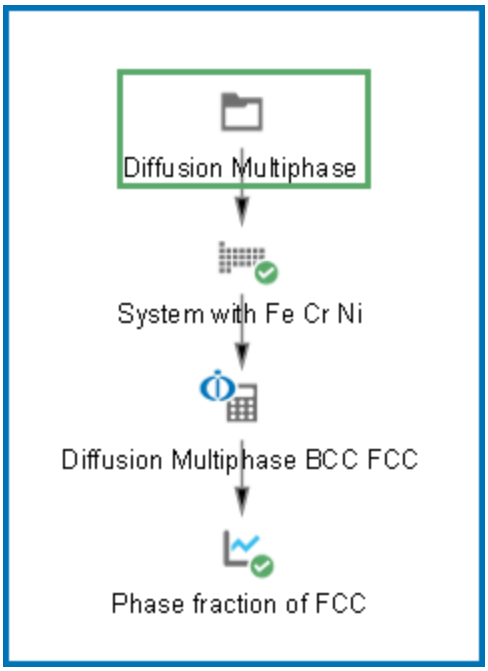
for multiphase simulations.

"References" on page 50

Multiphase Example Project

For the multiphase simulation, you can open the example project file included with your installation to see how it is set up.

1. Open Thermo-Calc.
2. There are different ways to access the examples.
   - From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
   - Click the **My Project** node and on the **Configuration** window under **Getting Started**, click **Example Files**
3. Click to open the **Diffusion Module - DICTRA** folder and locate the **D_03_Diffusion_Multiphase.tcu** file. Double-click to open it.
4. The project opens in Thermo-Calc. Click the top Project node (renamed to *Diffusion Multiphase*). At the bottom of the **Configuration** window click **Perform Tree**.

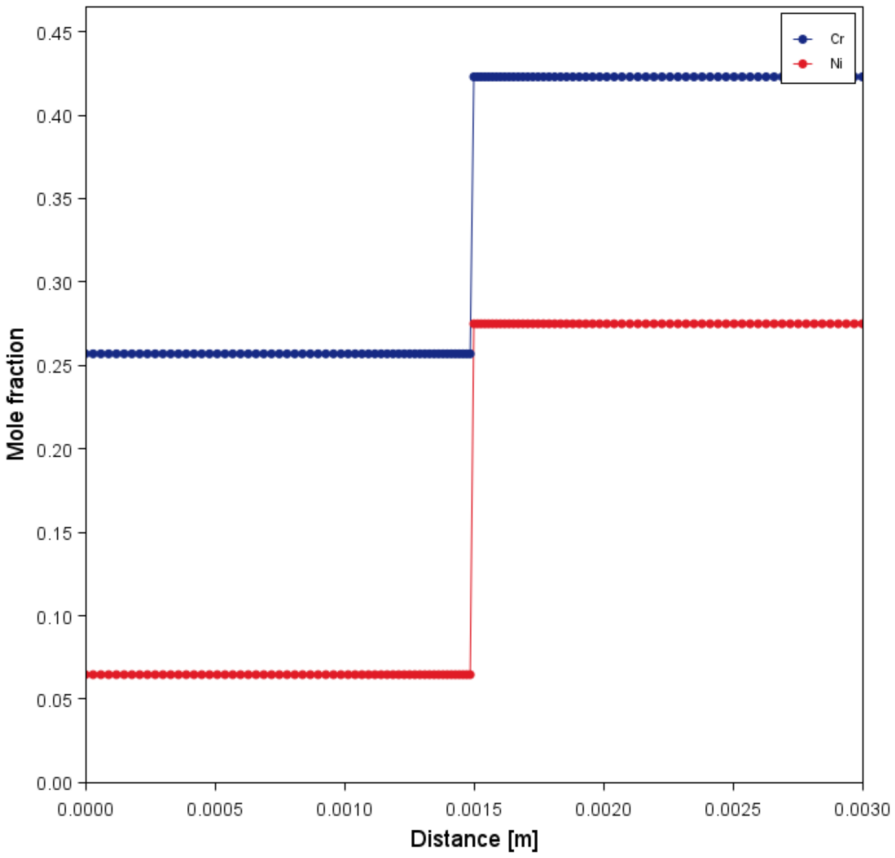


When completed, the results are plotted in the **Visualizations** window.

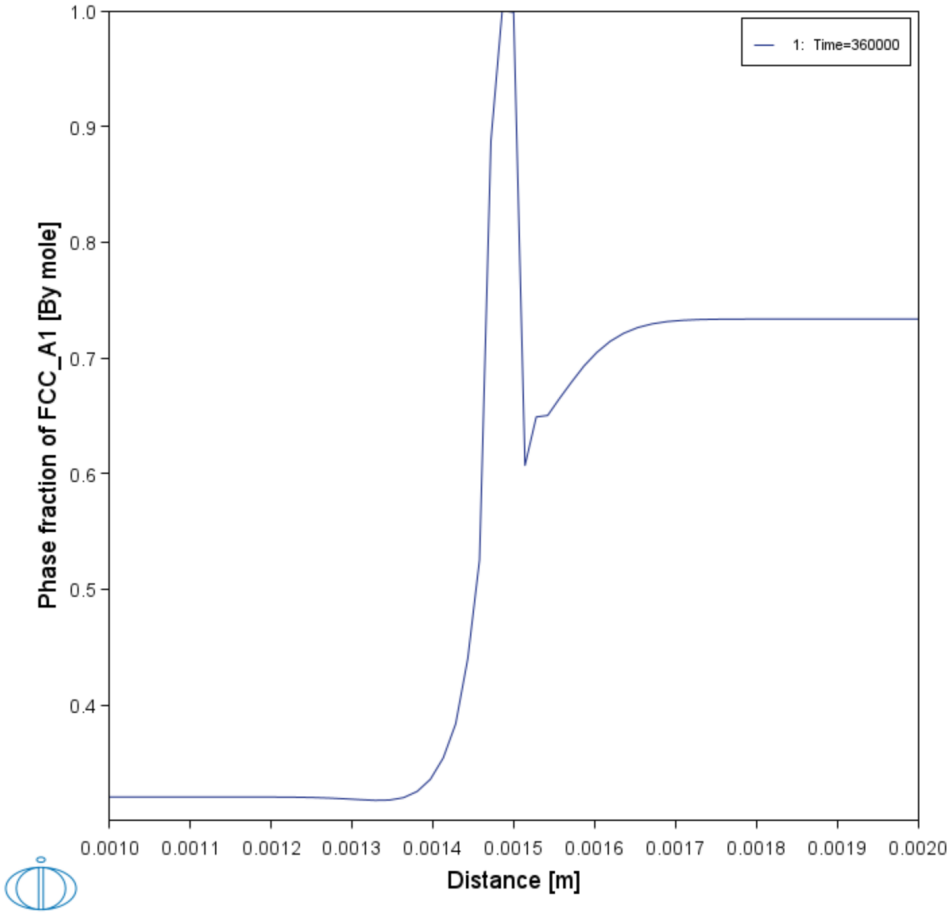
Visualizations

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.



During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.



After performing the calculation, you can view the final Plot Renderer result on the Phase fraction of FCC tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

System Definer Settings

This is a continuation from the previous examples and uses the short cuts already described. You can alternatively open a saved project and edit the settings.

Add the Databases and the Elements

1. Open a new instance of Thermo-Calc.
2. In the **My Project** window under **Non-Equilibrium**, click the **Diffusion** template icon.
3. In the System Definer **Configuration** window click the **Package** list and choose **Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)**.
4. In the **Periodic Table**, click **Fe**, then **Cr** and **Ni**.
5. Right-click **System Definer** and rename it to `System with Fe Cr Ni`.
6. Save the project file with a new name, e.g. *Diffusion_Multiphase*.

Diffusion Calculator Settings

After you have made the settings to the System Definer, you add the diffusion calculation parameters.

Define the Ferrite and Austenite Regions

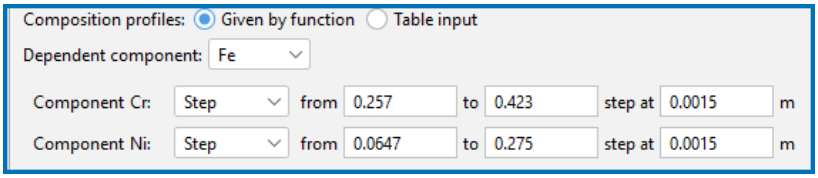
1. In the **Project** window, click the **Diffusion Calculator** node.
2. For **Composition unit** select **Mole fraction**.

   Keep the default **Length unit** as **Meter**. A **Planar** geometry is used for all the examples.

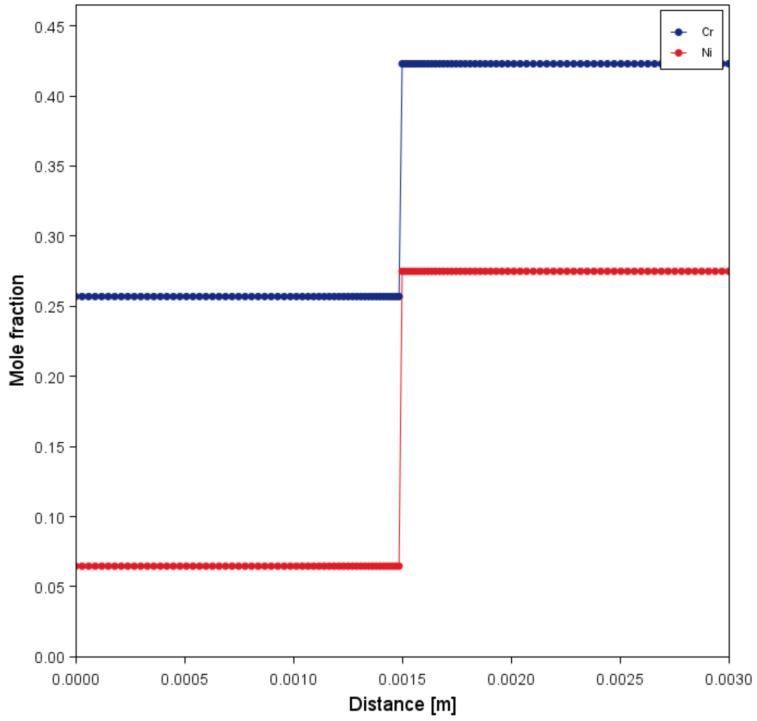
3. Under *Region* in the **Name** field enter `Diffcouple`.
4. In the **Width** field enter `0.003`.
5. Select **Automatic** as the grid type. Select **Fine**.
6. Choose **FCC_A1** from the **Phase** list.
7. Next to **Phase** click the **Add phase** button. From the **Phase** list select **BCC_A2**.

   In the **Visualizations** window, the **Composition Profile** tab displays a preview of these changes.

8. Next to **Composition profiles** the default selected is **Given by function**. **Fe** is chosen as the **Dependent component**.
   a. Define **Component Cr** and **Component Ni**. Choose **Step** for both the Cr and Ni elements.
   b. In each of the fields for Cr (**from**, **to**, **step at**) enter `0.257`, `0.423` and `0.0015`, respectively.
   c. In each of the fields for Ni (**from**, **to**, **step at**) enter `0.0647`, `0.275` and `0.0015`, respectively.



   In the **Visualizations** window, the **Composition Profile** tab displays a preview of these changes.



During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

The resulting Cr profile is thus 0.257 on the left half of the domain and 0.423 on the right with a sharp step at the center (as shown in "About the Multiphase Simulation" on page 39).

Define the Thermal Profile

The default **Isothermal** profile is used for this example.

1. In the **Temperature** field, enter `1100` and choose **Celsius** as the unit from the list.
2. In the **Simulation time** field, enter `100` and choose **Hours** from the list.
3. Right-click **Diffusion Calculator** and rename it to `Diffusion Multiphase BCC FCC`.

Choose the Homogenization Function

The local kinetics of the multiphase mixture must be estimated by means of some function that may depend on the local phase fractions, phase compositions, and the mobilities of the individual phases.

There are many such homogenization functions to choose from. In this particular example the **General lower Hashin–Shtrikman bound** is a good choice [1962Has].

1. To choose this homogenization function, click the **Diffusion Calculator** and then click the **Options** tab.
2. Under *Simulation Conditions*, select **Homogenization** as the **Default solver**.
3. Under *Homogenization Model Specific*, from the **Homogenization function** list, select **General lower Hashin–Shtrikman bound**.

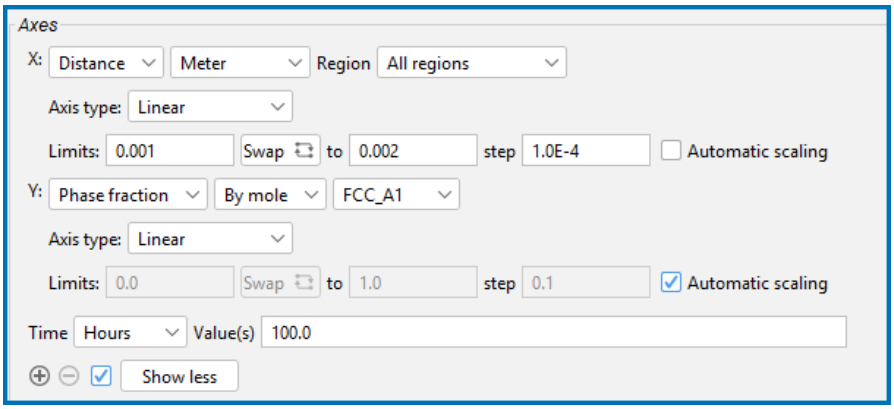
"References" on page 50

Plot Renderer Settings

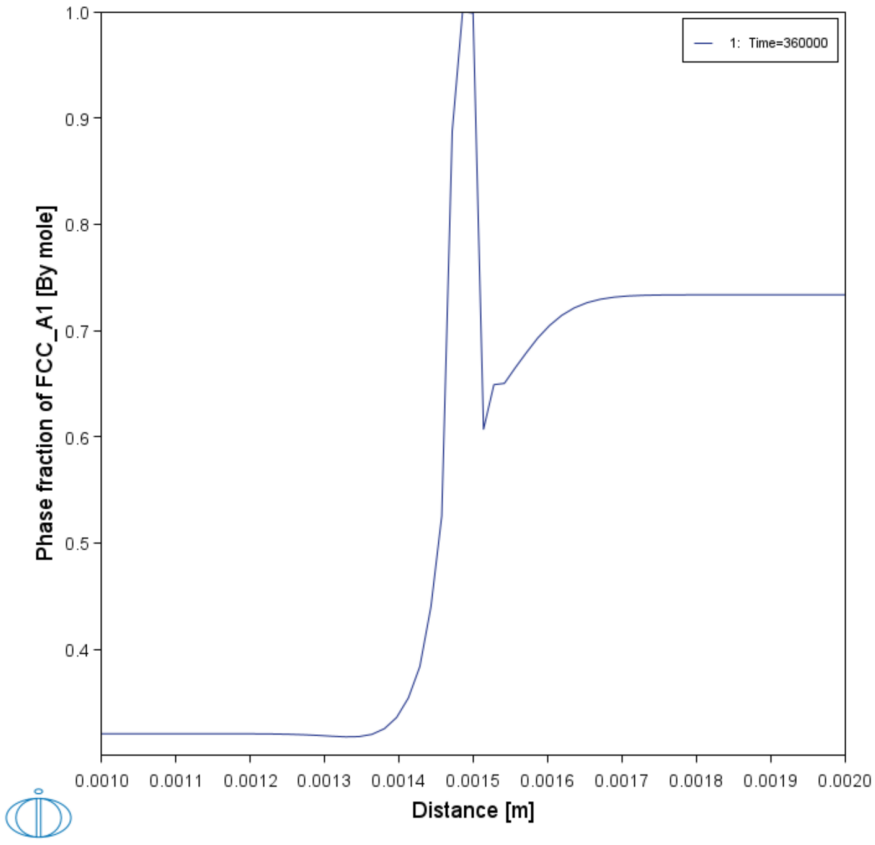
After you enter the settings for the System Definer and Diffusion Calculator, you define the plot parameters. For this example you want to plot the mole fraction fcc phase as a function of distance at the end of the heat treatment.

The plot of phase fraction vs distance shows that a single phase fcc zone has formed and this was also observed experimentally, see [1995Eng].

1. Click the **Plot Renderer** node.
2. Click **Show more**. Then under *Axes* for *X*, click to clear the **Automatic scaling** checkbox.
3. Enter the **Limits**: `0.001` **to** `0.002` **step** `1.0E-4`.
4. For *Y*, choose **Phase fraction** and **FCC_A1**.



5. Click **Perform** If you have entered the same settings you will get this plot result.



6. Right-click **Plot Renderer** and rename it to `Phase fraction of FCC`.

"References" on page 50

References

[1962Has] Z. Hashin, S. Shtrikman, A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials. J. Appl. Phys. 33, 3125–3131 (1962).

[1982Ågr] J. Ågren, Numerical treatment of diffusional reactions in multicomponent alloys. J. Phys. Chem. Solids 43, 385–391 (1982).

[1992And] J.-O. Andersson, J. Ågren, Models for numerical treatment of multicomponent diffusion in simple phases. J. Appl. Phys. 72, 1350–1355 (1992).

[1992Cru-1] S. Crusius, L. Höglund, U. Knoop, G. Inden, J. Ägren, On the Growth of Ferrite Allotriomorphs in Fe - C Alloys / Das Wachstum von allotriomorphem Ferrit in Fe — C-Legierungen. Int. J. Mater. Res. (Zeitschrift für Met. 83, 729–738 (1992).

[1992Cru-2] S. Crusius, G. Inden, U. Knoop, L. Höglund, J. Ägren, On the Numerical Treatment of Moving Boundary Problems. Int. J. Mater. Res. (Zeitschrift für Met. 83, 673–678 (1992).

[1995Eng] A. Engström, Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples. Scand. J. Metall. 24, 12–20 (1995).

[1997Hög] L. Höglund, “Computer simulation of diffusion controlled transformations in multicomponent alloys,” PhD Thesis, KTH Royal Institute of Technology, Stockholm, Sweden (1997).

[2000Bor] A. Borgenstam, L. Höglund, J. Ågren, A. Engström, DICTRA, a tool for simulation of diffusional transformations in alloys. J. Phase Equilibria 21, 269–280 (2000).

[2002And] J.-O. Andersson, T. Helander, L. Höglund, P. Shi, B. Sundman, Thermo-Calc & DICTRA, computational tools for materials science. Calphad 26, 273–312 (2002).

[2006Lar] H. Larsson, A. Engström, A homogenization approach to diffusion simulations applied to α+γ Fe–Cr–Ni diffusion couples. Acta Mater. 54, 2431–2439 (2006).

[2009Lar] H. Larsson, L. Höglund, Multiphase diffusion simulations in 1D using the DICTRA homogenization model. Calphad 33, 495–501 (2009).

Next Steps

Below are suggestions for you to learn more about using the Diffusion Module (DICTRA).

- Browse the Online Help (press F1) or open one of the available PDFs included with your installation (**Help → Manuals Folder**).
- You have been working within Graphical Mode. You might also want to try the *Diffusion Module Console Mode Quick Start Guide* (**Help → Manuals Folder**). This further prepares you to work with the Console Mode examples (**Help → Examples Files**), which contain some simulation types and advanced functionality not yet available in Graphical Mode.
- You can also go to the Thermo-Calc website to see if there are other options suited to you, such as a course or video tutorials. To go to the web page, in the **Project** window, click the top **My Project** node and then click **Video Tutorials**. Or from the main menu, select **Help → Video Tutorials**.

There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.