

# **Additive Manufacturing (AM) Module User Guide**

**Thermo-Calc Version 2023b**



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# Introduction to the Additive Manufacturing (AM) Module

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# About the Additive Manufacturing (AM) Module



This guide is a supplement to the full Thermo-Calc documentation set. Access the help in Thermo-Calc by pressing F1, or choose **Help** → **Online help**, or click **Online Help** on the main **My Project Configuration** window. See "["Additive Manufacturing \(AM\) Module Help Resources"](#)" on page 12 to learn other ways to access information.

The Additive Manufacturing (AM) Module (also referred to as the AM Module) is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the **AM Calculator**. The aim of the Additive Manufacturing Module is to better understand the laser powder bed fusion (LPBF) process by predicting the temperature distribution and melt pool geometry as a function of process parameters and using material properties from the Thermo-Calc thermodynamic and properties databases. Special focus is to have a unified treatment of alloy-dependent material properties and process parameters when solving the multiphysics problem of a moving heat source that melts and solidifies metal powder. The multiphysics simulation involves thermal conduction, fluid flow, evaporation-, radiation-, and convective-heat loss. Furthermore, once you have the temperature distribution, for instance as a function of time and space, you can also use this information for other Thermo-Calc Add-on-Module simulations such as with the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA), or for input to other external finite element programs.

## Overview of the Content

There are "["Additive Manufacturing \(AM\) Module Help Resources"](#)" on page 12 and "["Network License Restrictions"](#)" on page 13 to consider and access.

Theory is covered in a summary of the "["Additive Manufacturing Simulation Types"](#)" on page 15 and then some basic equations pertaining to the logic behind the simulation and settings are discussed in "["Additive Manufacturing Module Theory"](#)" on page 17.

The workflow for the AM Module is outlined in "["Setting Up the Additive Manufacturing Simulation"](#)" on page 33 and there are two default "["Additive Manufacturing Templates"](#)" on page 37 you can use to start defining your project. You can also add nodes individually to build your own tree. There are two workflows, and in either workflow, defining the AM Calculator involves choosing one of the available simulation types: Steady-state, Transient, or Transient with heat source from Steady-state.

Then you can start building the simulation using the activity nodes and depending on which workflow you start with.

This involves the standard **System Definer** and **Scheil Calculator** settings, which are the same as what is used with a standard Thermo-Calc configuration. When you add an Additive Manufacturing Template (and need to generate some materials properties or do not have a material library to use), then some unique default settings for the Scheil Calculator and these particular types of simulations are already set by default. These are discussed in "Setting Up the Additive Manufacturing Simulation" on page 33.

This guide specifically includes details about the settings for the "AM Calculator" on page 40 and the specialized "AM Calculator Plot Renderer" on page 58.

Then finally you can visualize and examine your results using the "AM Visualizations Window Plot Toolbar" on page 62 and learn how to "Rotate, Zoom, and Pan 3D Plots: AM Calculations" on page 64.



Read more about the [Additive Manufacturing \(AM\) Module](#) on our website. You can also use the [Getting Started Guide](#) to learn about the key features available.

## Available Options

The Additive Manufacturing (AM) Module is an Add-on Module to the core Thermo-Calc software.



A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run three examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.

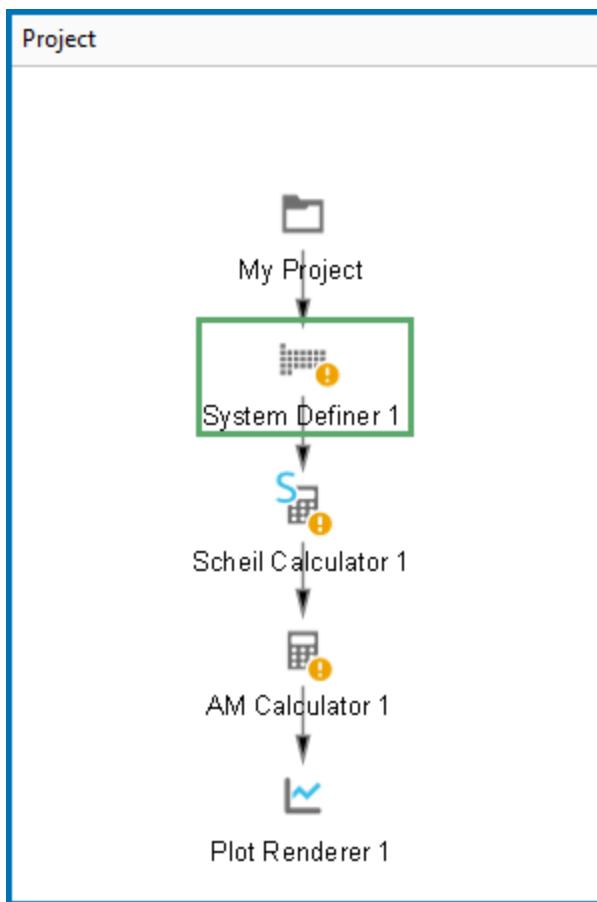
### Additive Manufacturing Templates

Two types of **Additive Manufacturing** templates are under **Applications** and these are available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO mode then this is indicated by the addition of **DEMO** text. See [Figure 1](#).

### Using the Templates

After opening Thermo-Calc in Graphical Mode, in the templates section under **Applications**, click the **Additive Manufacturing** button to add a *System Definer*, *Scheil Calculator*, *AM Calculator*, and *Plot Renderer* to the **Project** tree.

This template is used when you need to generate and use data from a Scheil calculation.



An alternate template is available when you already have data or can directly use or import a Material Library.

After opening Thermo-Calc in Graphical Mode, in the templates section under **Applications**, and to the right of **Additive Manufacturing**, click the **With Material Library** button to add an *AM Calculator* and *Plot Renderer* to the **Project** tree.

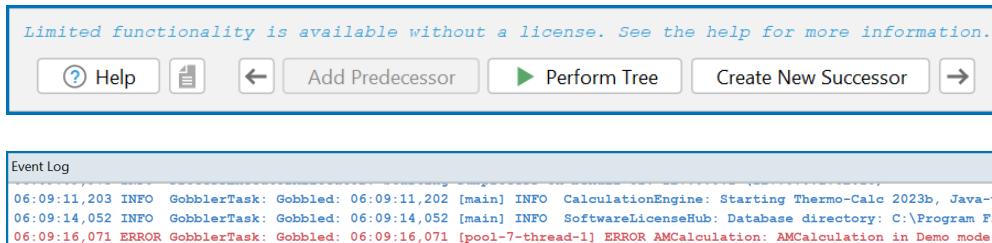
## Demonstration (Demo) Mode

The Additive Manufacturing (AM) Module is available in a demonstration (DEMO) mode without a license. It includes access to the templates, some examples, and some access to the embedded predefined material properties libraries. You also have access to the fluid flow settings and a steady-state calculation can be done. However, there are limitations such as the ability to change settings and to fully run calculations.

- Three examples (AM\_01, AM\_02, and AM\_03) use embedded and predefined Material Properties libraries that are included for all users. Although these examples can be run without a license, you cannot make any changes to the settings. If changes are made, the **Perform** button can still be clicked but the calculation will fail and a message displays above the **Perform Tree** button to inform you of the need for a license. In addition, the **Event Log** displays an error message, `ERROR AM Calculation: AMCalculation in Demo mode has limited functionality.` See [Figure 2](#).
- Generally, when in DEMO mode and using the **With Materials Library** template, you can perform a calculation with default values. You cannot change any setting, including the calculation types (i.e. Steady-state, Transient, or Transient with heat source from Steady-state) as well as the Material Properties library i.e. meaning only Steady-state with the IN625 library is available with the default setup is possible.
- All plot configurations are possible to perform in the above cases.
- Examples AM\_04 and AM\_05 require a full license to the Additive Manufacturing (AM) ModuleModule to run, plus these additional licenses.
  - AM\_04 also requires a license for TCS Ti/TiAl-based Alloys Database (TCTI5 and newer).
  - AM\_05 also requires a license for the Diffusion Module (DICTRA), plus additional database licenses for the TCS Steel and Fe-alloys Database (TCFE13 and newer), and the TCS Steels/Fe-Alloys Mobility Database (MOBFE8 and newer).
  - For those without the applicable licenses, you can still open the examples to review the settings and then refer to the documentation for discussions of what it is showing. In addition, AM\_04 is used in the Getting Started Guide on the website.



*Figure 1: The templates indicate that you are in DEMO mode and would need a license to fully use the templates or run AM\_04 and AM\_05.*



*Figure 2: When in DEMO mode and you click on the AM Calculator node, the above note is included at the bottom of the Configuration window to remind you that a license is needed for full functionality. The Perform Tree button is not always available and sometimes even if it is available to click, the calculation itself cannot complete due to lack of a license. There will also be an error message in the Event Log to indicate the need for a license.*

## Material Properties and Libraries

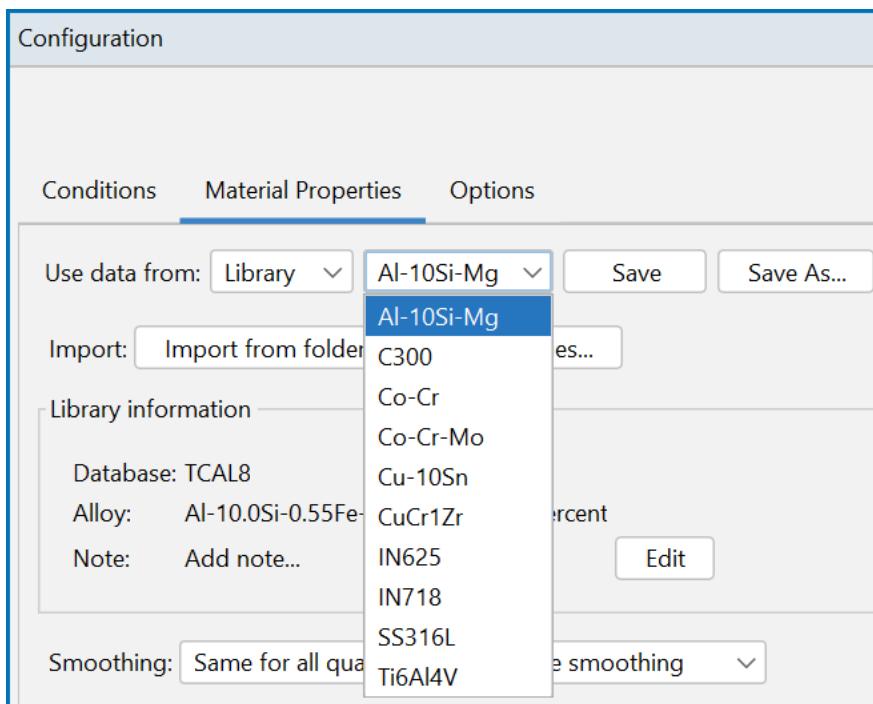


All predefined Material Properties libraries are available if you have a license for the Additive Manufacturing (AM) Module, even if you do not have the alloy database it is created with.

### Create or Import Your Own Material Library

The use of the Scheil Calculator with an AM Calculator provides you with a way to generate the data you need to feed into any AM calculation. When this Scheil calculation is completed, and if you have a full license, you can save the results to the Material Properties Library for later use. From the AM Calculator there is an option to use either Scheil data (when it is connected to the Scheil Calculator) or predefined library data (as long as you have a license to the Additive Manufacturing Module the calculations can be run fully). With the applicable license, you can also import your own material library for a particular alloy of interest and then you can just use the AM Calculator (i.e. the With Material Library template setup) without needing the additional Scheil calculation step.

Users with a full Additive Manufacturing license can access all the predefined libraries for use in calculations (and also can create and import their own libraries and save these for reuse).



## Using Data with other Add-on Modules



When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.



See "AM Calculator: Working with Probe Data" on page 56.

# Additive Manufacturing (AM) Module Help Resources

## 'Online' Help: No Internet Required

There are several ways to access online help in a browser. The content opens in a browser but uses local content so you do not need an Internet connection except for links to external websites.

First open Thermo-Calc, then choose one of these options:

- Press <F1> on the keyboard.
- Select **Help** →  **Online Help**.
- On the **My Project Configuration** window, click  **Online Help**.
- At the bottom of any **Configuration** window, click  **Help**.



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.



## Additive Manufacturing (AM) Module Specific Information



Read more about the [Additive Manufacturing \(AM\) Module](#) on our website. You can also use the [Getting Started Guide](#) to learn about the key features available.

## Network License Restrictions

The Additive Manufacturing (AM) Module requires a separate license. If you are using a network client installation of Thermo-Calc, then you may not be able to use it even if you have access to a license server with a valid network license file. The reason for this is because other clients who are part of your network installation may have checked out all instances of the network license allowed to run simultaneously.



For users with a network license, you must exit Thermo-Calc to release the license for other users. The license is checked out as soon as you add an AM Calculator and remains unavailable to other users until you exit the program.



With a network license, and if as per above you temporarily do not have access to a license, you are automatically put into *Demo Mode*. Then the AM Calculator is available.



Search the online help or see the *Thermo-Calc Installation Guide* for more about network licenses.

# General Theory and Background

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# Additive Manufacturing Simulation Types

Three simulation types are available on the "AM Calculator" on page 40 – *Steady-state*, *Transient*, and *Transient with heat source from Steady-state*.

## Steady-state

In the *Steady-state* mode it is assumed that the temperature distribution and the fluid flow around the heat source is in steady state and does not change with time. This is useful to get an estimation of the temperature distribution and size of the melt pool when you assume that the heat source is moving at a constant speed in a given path. In the single-track experiments, temperature distribution around the heat source and fluid flow inside the melt pool reach a steady state very quickly, and you should then perform steady state simulations to predict melt pool geometry and cooling rates around the melt pool. In a sense, Steady-state simulations give you an overall picture of the process but in order to get more precise details and predict temperature distribution in a multi-layer build, as a function of time, you should perform Transient simulations. The benefit of the steady state option is that these simulations are quick, and you get a solution typically within 1-5 minutes, depending on the process parameters and your computational resources. For the Steady-state simulations, you can include or exclude fluid flow inside the melt pool due to the Marangoni effect. For the given processing conditions, if convection is the dominant mode of heat transfer, inclusion of fluid flow is crucial to enhance the accuracy of the model by correctly capturing the underlying physical behavior of melting and solidification of material. Furthermore, you can also perform simulations with a powder layer on the top of the substrate having different material properties than the bulk material. The Steady-state simulations are performed on a symmetric domain where you specify only the height of the substrate and the thickness of the powder layer, if present. The length and width of the computational domain are determined automatically based on the process parameters. The temperature distribution is computed using the energy equation while the fluid flow is modeled using the Navier-Stokes equation.

## Transient

In the *Transient* mode, you can perform full-scale transient simulations in a 3D rectangular build part and have the possibility to specify a scanning strategy comprising multiple tracks and multiple layers. Here you can enter the height, width, and length of the entire build part or a representative segment of the build part and configure a scanning strategy either for a single track or for multiple tracks (bidirectional or unidirectional). You can also add multiple layers of powder and rotate the scanning pattern between layers.

Similar to the Steady-state mode, here you can also choose to include fluid flow inside the melt pool to correctly capture the underlying physical phenomena of melting and solidification of the material and thereby increasing the accuracy of the model. The inclusion of fluid flow requires coupling the Navier-Stokes equations together with the energy equation which comes at the cost of increased numerical complexity resulting in longer simulation times.

## Transient with Heat Source from Steady-state

In order to perform full scale 3D simulations in an efficient manner, with multitracks and multilayers, including fluid flow in the melt pool or with powder layer(s) having different properties than the solid material, you can use the *Transient with heat source from Steady-state* mode. This mode develops a novel approach where the effect of fluid flow due to Marangoni convection in the melt pool is incorporated without solving for Navier-Stokes equations in the full-scale 3D domain.

The concept here involves the assumption that the temperature distribution and fluid flow inside the melt pool instantly reach steady state. We first solve for temperature distribution, using the energy equation and fluid flow due to Marangoni convection, using the Navier-Stokes equations for the given process parameters in the Steady-state mode. Once we have the steady state solution, we use this solution inside the melt pool and map it as a “heat source” in the transient simulations. Using this approach, we do not have to solve for the complicated Navier-Stokes equations at each time step in the transient simulation, yet we still capture the effect of fluid flow on the shape of the melt pool. Furthermore, we also reduce the computational time by solving for the most non-linear region in the energy equation i.e., inside the melt pool, only once, and then reusing the solution as a boundary condition in the transient simulations. This approach has considerably decreased the numerical complexity of the full-scale transient simulations consequently reducing the simulation time without making a significant compromise on the accuracy of the solution.



"Additive Manufacturing Module Theory" on the next page

## Additive Manufacturing Module Theory

This section is an overview of the underlying fundamental theory used and applied to the calculations when you are setting up the "AM Calculator" on page 40 using one of the "Additive Manufacturing Simulation Types" on page 15.

### Energy Equation: The Enthalpy Formulation

The following formulation is based on a simple assumption that each volume element, which may contain several dendrites or a considerable part of a dendrite, is approximated as homogeneous, i.e., it is sufficient to characterize the whole volume with a single set of state variables. This assumption thus excludes the direct account of varying composition caused by microsegregation within the element.

The enthalpy formulation is based on the conservation of energy and is essentially equivalent with Fourier's second law:

$$[Eq. 1] \quad \dot{H}_V = -\operatorname{div}(J_Q) + \dot{Q}$$

$H_V$  is the enthalpy density and  $\dot{H}_V$  is its time derivative.

The enthalpy density is related to the molar enthalpy  $H_m$  and molar volume  $V_m$  by:

$$[Eq. 2] \quad H_V = \frac{H_m}{V_m}$$

$\operatorname{div}$  denotes the divergence operator and  $J_Q$  is the heat flux given by Fourier's law:

$$[Eq. 3] \quad J_Q = -\kappa \operatorname{grad}(T)$$

where  $\kappa$  is the heat conductivity,  $\operatorname{grad}$  denotes the gradient operator and  $T$  is the temperature.  $\dot{Q}$  is a source term and represents the heat added from the outside at a certain point. In modeling of a process like welding or additive manufacturing this is a key term and requires a lot of modeling.

As state functions the enthalpy and the molar volume depend on temperature, state of phase, and composition of the individual phases. In a volume element approximated as homogeneous, one thus has:

$$[Eq. 4] \quad H_m = \sum_{\beta} f^{\beta} H_m^{\beta} (T, x_k^{\beta})$$

$$V_m = \sum_{\beta} f^{\beta} V_m^{\beta} (T, x_k^{\beta})$$

[Eq. 5]

where  $f^{\beta}$  is the mole fraction of the phase  $\beta$  and  $x_k^{\beta}$  is the mole fraction of  $k$  in  $\beta$ . The time derivatives thus are:

$$\dot{H}_m = \sum_{\beta} \dot{f}^{\beta} H_m^{\beta} (T, x_k^{\beta}) + \sum_{\beta} f^{\beta} \left( c_P^{\beta} (T, x_k^{\beta}) + \sum_{k=1}^n \frac{\partial H_m^{\beta}}{\partial x_k^{\beta}} \frac{\partial x_k^{\beta}}{\partial T} \right) \dot{T}$$

[Eq. 6]

$$\dot{V}_m = \sum_{\beta} \dot{f}^{\beta} V_m^{\beta} (T, x_k^{\beta}) + \sum_{\beta} f^{\beta} \left( V_m^{\beta} \alpha^{\beta} (T, x_k^{\beta}) + \sum_{k=1}^n \frac{\partial V_m^{\beta}}{\partial x_k^{\beta}} \frac{\partial x_k^{\beta}}{\partial T} \right) \dot{T}$$

[Eq. 7]

Here  $c_P^{\beta}$  is the molar heat capacity of the  $\beta$  phase and  $\alpha^{\beta}$  its volumetric thermal expansion. For a given volume element the rates can be calculated from Thermo-Calc for the temperature, fraction of phases and their composition with the input of the rates  $\dot{f}^{\beta}$  and  $\dot{T}$ .

The rate of change of the enthalpy density, i.e., the left-hand side of Eq. 1 thus is obtained as:

$$\dot{H}_V = \frac{1}{V_m} \left( \dot{H}_m - H_m \frac{\dot{V}_m}{V_m} \right)$$

[Eq. 8]

The first term inside the brackets represents the change for a constant number of atoms due to a change in temperature or phase. The second term represents a change in volume for a constant number of atoms. However, the second term is balanced by a corresponding contribution in the heat flux, which we do not usually account for, and we should thus leave it out.

$$\dot{H}_V = \frac{\dot{H}_m}{H_m}$$

[Eq. 9]

The fraction of phases sums up to unity and in the case of only one solid phase:

$$\dot{f}^L = -\dot{f}^{\beta}$$

In most treatments the positive quantity

$$\Delta H_m = (H_m^L(T, x_k^L) - H_m^{\beta}(T, x_k^{\beta}))$$

treated as constant and referred to as the latent heat. It is also common to neglect the difference in heat capacity between solid and liquid and the variation of  $\Delta H_m$  with composition. Eq. 6 then is simplified into.

$$[Eq. 10] \quad \dot{H}_m = \dot{f}^L \Delta H_m + c_P \dot{T}$$

By the same token

$$\Delta V_m = \left( V_m^L(T, x_k^L) - V_m^\beta(T, x_k^\beta) \right)$$

is often approximated as constant and so Eq. 7 is simplified into

$$[Eq. 11] \quad \dot{V}_m = \dot{f}^L \Delta V_m + V_m \alpha \dot{T}$$

where  $V_m$  is given by Eq. 5 and yields

$$V_m = f^L V_m^L + (1 - f^L) V_m^\beta = V_m^\beta + f^L \Delta V_m$$

Eq. 9 now becomes:

$$[Eq. 12] \quad \dot{H}_V = \frac{1}{V_m} \left( \dot{f}^L \Delta H_m^L + c_P \dot{T} \right)$$

and Eq. 1 becomes:

$$[Eq. 13] \quad \frac{1}{V_m} \left( \dot{f}^L \Delta H_m^L + c_P \dot{T} \right) = \text{div}(\kappa \text{grad}(T)) + \dot{Q}$$

## The Equivalent Heat Capacity Method Using Thermo-Calc

If it is further assumed that the fraction liquid  $f^L$  is a unique function of temperature one has:

$$[Eq. 14] \quad \dot{f}^L = \frac{df^L}{dT} \dot{T}$$

and Eq. 13 may be further simplified to:

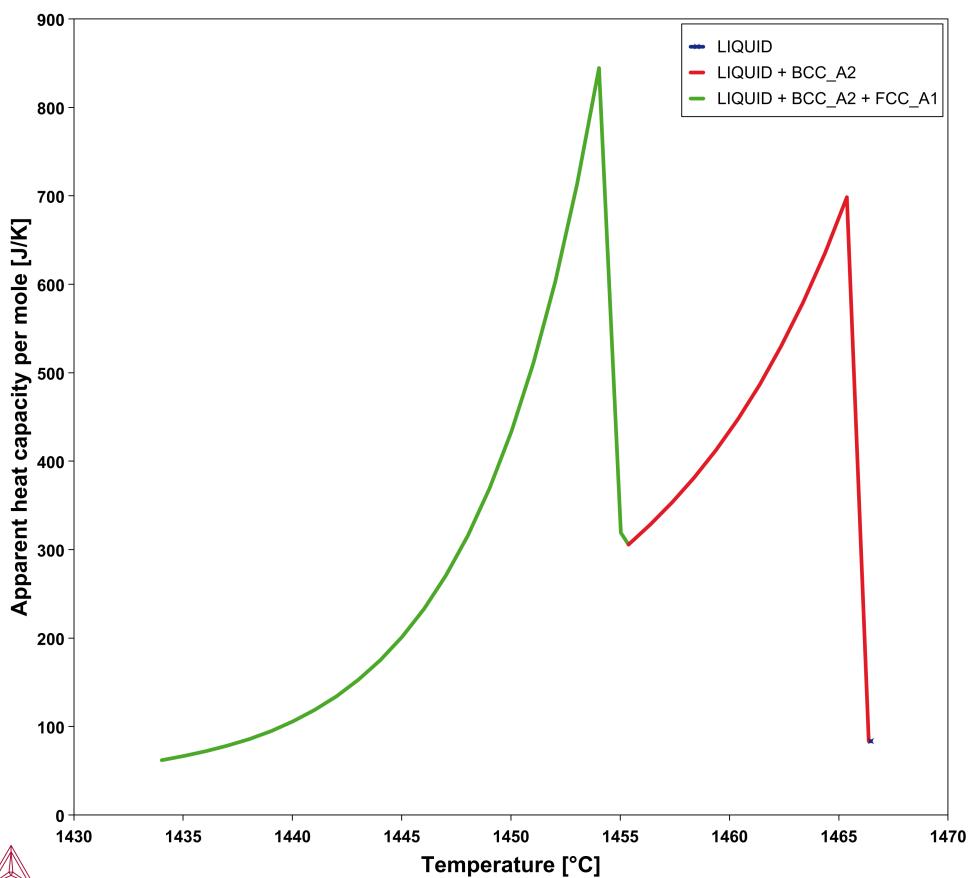
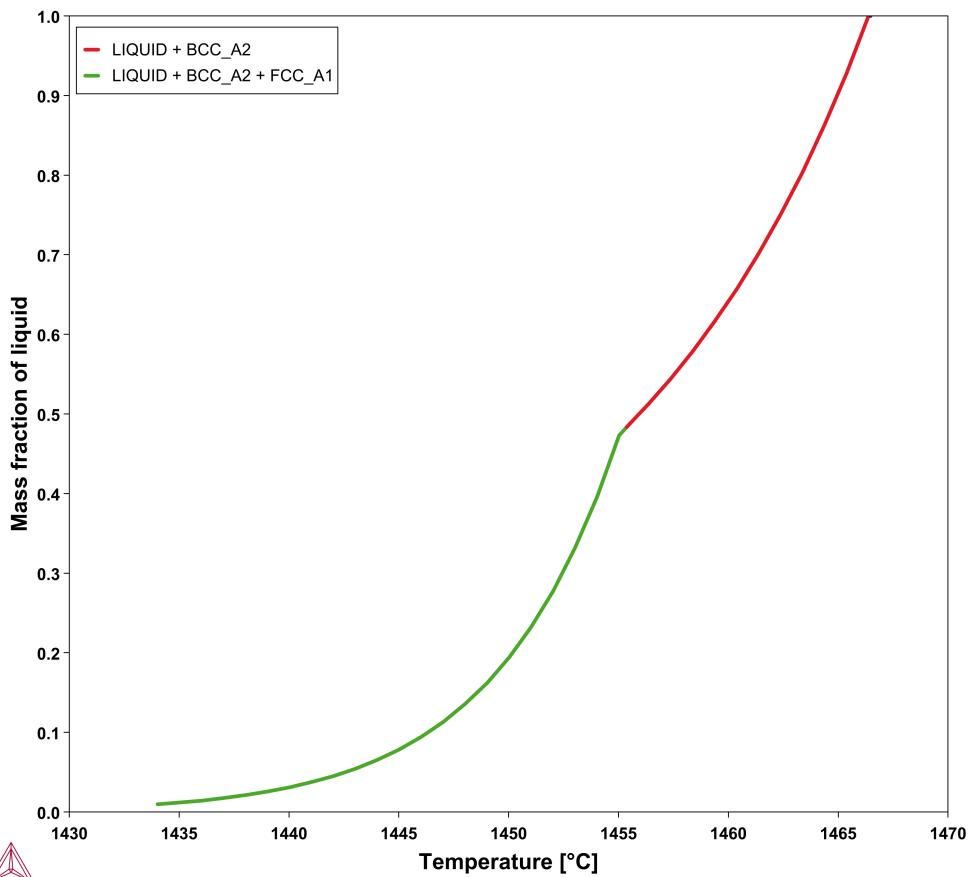
$$[Eq. 15] \quad \frac{c_p^{eff}}{V_m} \dot{T} = \text{div}(\kappa \text{grad}(T)) + \dot{Q}$$

where the effective heat capacity  $c_p^{eff}$  is given by:

$$[Eq. 16] \quad c_p^{eff} = \left( \frac{df^L}{dT} \Delta H_m + c_P \right)$$

Eq. 15 is a normal heat-flow equation and the complication of the liquid/solid phase transformation is taken into account by means of an effective heat capacity. This method is referred to as the equivalent heat-capacity method by Rappaz [1989Rap].

It then remains to be discussed how to determine  $f^L(T)$ . It must be given by some extra information. Traditionally it was taken from experimental information but more recently it has been taken from the Scheil equation. The original equation was based on a number of approximations which are unnecessary today when thermodynamic and properties databases and efficient software such as Thermo-Calc are available. In fact, when using Scheil in Thermo-Calc one can directly calculate  $c_p^{eff}(T)$ , referred to as apparent heat capacity, for a given initial composition of the liquid. A possible approach thus is to calculate  $c_p^{eff}(T)$  for the alloy under consideration and then store the result as a table and use that in the solution of Eq. 15. The molar volume may be extracted from the same calculation. An example for a 316L type of stainless steel is shown in the plots below.



*Figure 3: Results of a Scheil simulation of Fe-18Cr-10Ni alloy showing the mass fraction of the liquid (left) and the apparent heat capacity (right) both as a function of temperature.*

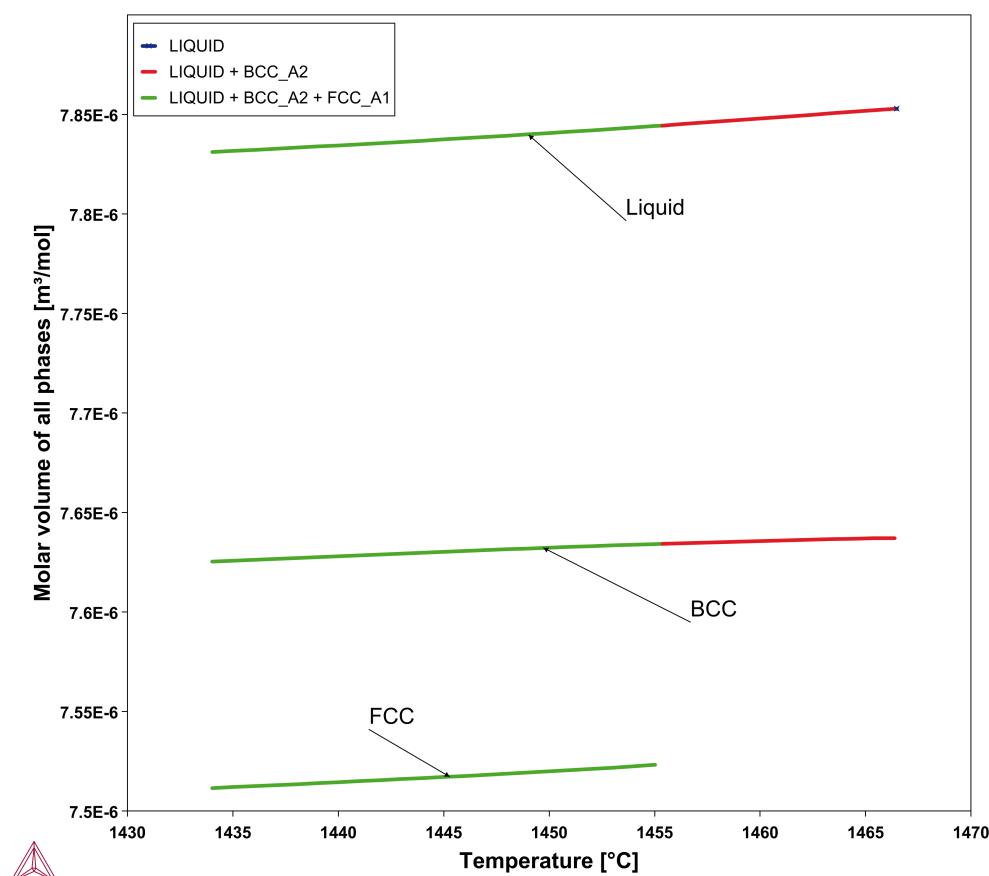
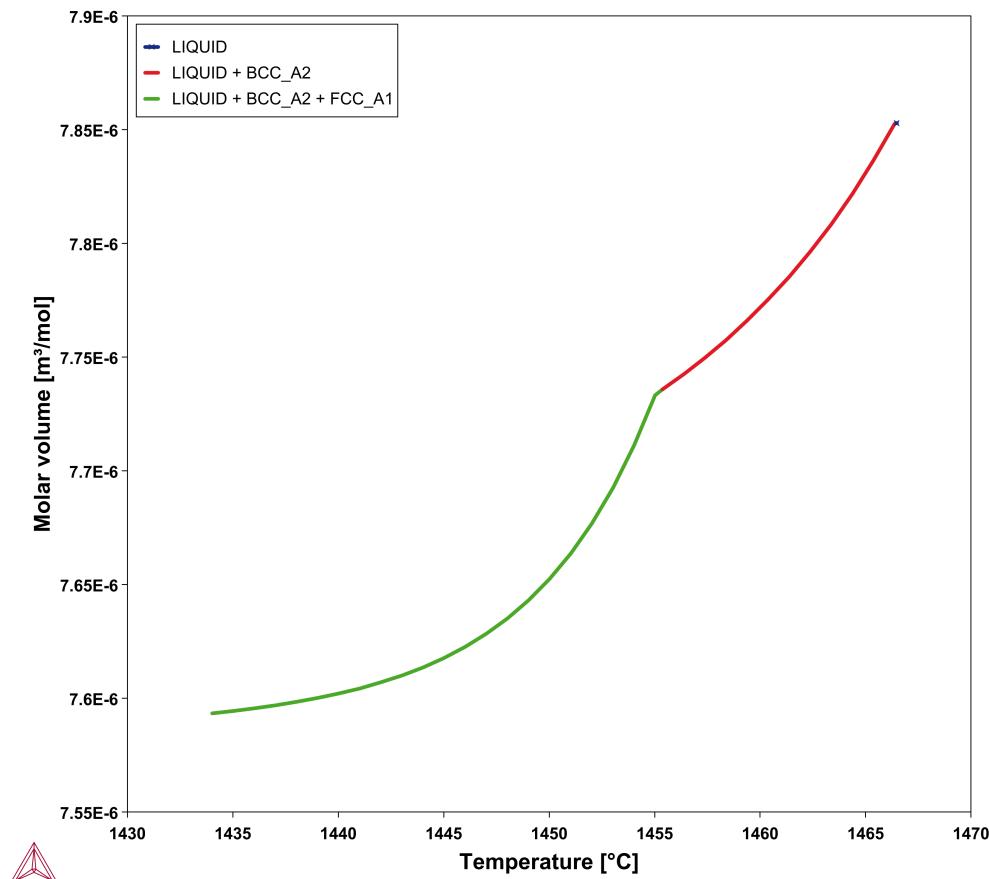


Figure 4: Molar volume from a Scheil simulation of Fe-18Cr-10Ni alloy. The right plot shows all phases as a function of temperature.

## The Enthalpy Method Using Thermo-Calc

In the enthalpy method we keep Eq. 1 and use Eq. 9 to write

$$[Eq. 17] \quad \frac{\dot{H}_m}{V_m} = -\text{div}(J_Q) + \dot{Q}$$

As pointed out by Rappaz [1989Rap] there is no mathematical difference between the enthalpy method and the equivalent heat capacity method because the former is simply the integral of the heat capacity over  $T$ . For numerical reasons the cusps in the heat capacity may be disadvantageous and the enthalpy has a nicer behavior as shown in the plot below, where it gives temperature as a unique function of enthalpy.

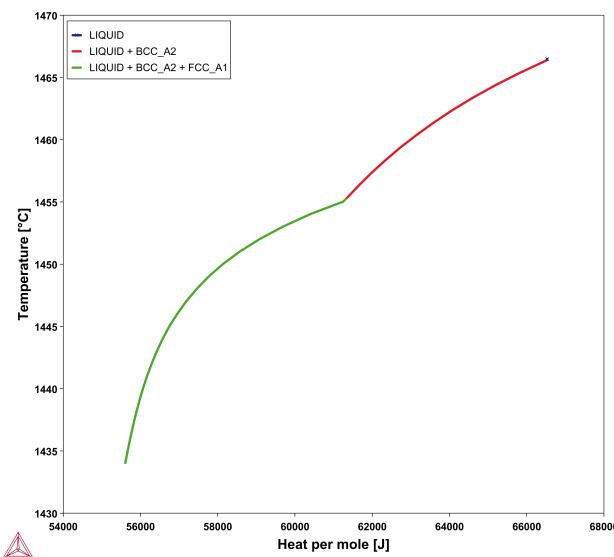


Figure 5: Enthalpy from a Scheil simulation of Fe-18Cr-10Ni alloy.

In the Additive Manufacturing Module, we therefore use Eq. 17 to predict the evolution of temperature during the laser powder bed fusion (LPBF) process for the given material properties and process parameters.

## Steady-state Formulation

An important approximation is when one can solve the stationary heat-flow equation for a volume element moving with the heating source. In that case, we neglect the left-hand side of Eq. 17 and add a translation term as follows:

$$[Eq. 18] \quad \text{div}[\kappa \text{grad}(T)] - \frac{v_b}{V_m} \text{grad}(H_m) + \dot{Q} = 0$$

Where  $v_b$  is the velocity of the heat source. In case of additive manufacturing,  $v_b$  is the scanning speed.

## Fluid Flow

When there is also fluid flow involved, a fluid transport term has to be added to the heat-flow equation and one obtains:

$$[Eq. 19] \quad \frac{\dot{H}_m}{V_m} = \operatorname{div}[\kappa \operatorname{grad}(T)] - \frac{v}{V_m} \operatorname{grad}(H_m) + \dot{Q}$$

where  $v$  is the velocity vector field and may be imposed or obtained from the solution of the Navier-Stokes equation:

$$[Eq. 20] \quad \rho \dot{v} + \rho(v \operatorname{grad})v - \mu(\operatorname{div} \operatorname{grad})v = F_V - \operatorname{grad}P$$

where  $\rho$  is the density related to the molar volume by means of

$$[Eq. 21] \quad \rho = \frac{1}{V_m} \sum_k x_k M_k$$

$M_k$  is the molar weight in kg mol<sup>-1</sup>.  $\mu$  is the viscosity,  $F_V$  is a volume force, e.g., gravitational forces, and  $P$  is the internal pressure. The equation is often combined with approximating the liquid as incompressible.

$$[Eq. 22] \quad \operatorname{div}(v) = 0$$

## Modeling Heat Source

It is crucially important to correctly model the heat source in AM simulations since the heat source not only affects the size of the melt pool but also determines the temperature gradients around the melt pool. In the Additive Manufacturing Module, there are three types of heat source models.

### Gaussian Heat Source

The first model is a surface heat source model which was initially proposed by Pavelic et al. [XX]. By surface heat source model, it is meant that the power input from the heat source is only defined on the top surface of the workpiece, as a Neumann boundary condition on the computational domain, and the heat energy then diffuses into the workpiece depending on the thermal diffusivity of the selected material. As suggested by Pavelic et al., the heat flux (W/m<sup>2</sup>) is defined as Gaussian distribution around the center of the heat source, deposited on the top surface of the domain, as given in the equation below. A schematic representation of the heat flux, as defined by Gaussian heat source is shown in the figure below.

$$Q = \frac{2\epsilon P}{\pi r^2} \exp \left[ -2 \frac{(x-X_p)^2 + (y-Y_p)^2}{r^2} \right]$$

[Eq. 23]

Where  $Q$  is the power density deposited on the top surface ( $\text{W/m}^2$ ),  $\epsilon$  denotes absorptivity of the laser beam,  $P$  is the power of the heat source ( $\text{W}$ ),  $r$  is the laser spot radius, and  $x$  and  $y$  denote coordinates of the computational domain while  $X_p$  and  $Y_p$  represent the location of the heat source.

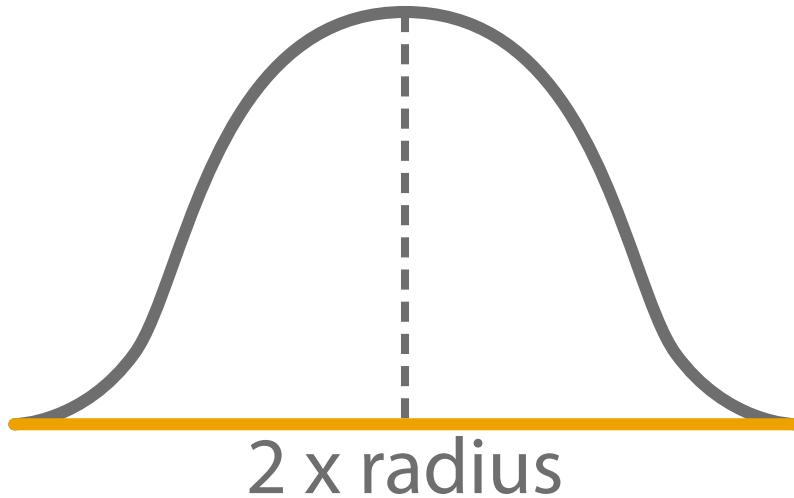


Figure 6: Schematic representation of energy distribution in Gaussian heat source model.

### **Double-ellipsoidal (Goldak) Heat Source**

The second heat source model in the AM Module is a volumetric heat source model which was first proposed by Goldak et al. [1984Gol], and is now commonly used in LBPF simulations. In contrast to the surface heat source model, in the volumetric heat source model, the power input is defined not only on the surface of the workpiece but also inside the powder bed, along the depth of the powder bed. The heat distribution in the double-ellipsoidal heat source model is given by a combination of two ellipsoids; one in the front quadrant of the heat source and the other in the rear quadrant, as shown in the figure below. The power density is thus given by two different expressions, one for each quadrant of the heat source.

$$[Eq. 24] \quad Q_f = f_f \frac{6\sqrt{3}\varepsilon P}{\pi^{\frac{3}{2}} a_f b c} \exp \left[ -2 \frac{(x - X_p)^2}{a_f^2} + \frac{(y - Y_p)^2}{b^2} + \frac{(z - Z_p)^2}{c^2} \right]$$

$$Q_r = f_r \frac{6\sqrt{3}\varepsilon P}{\pi^{\frac{3}{2}} a_r b c} \exp \left[ -2 \frac{(x - X_p)^2}{a_r^2} + \frac{(y - Y_p)^2}{b^2} + \frac{(z - Z_p)^2}{c^2} \right]$$

Where  $Q_f$  and  $Q_r$  are the power densities ( $\text{W/m}^3$ ) in the front and rear quadrant of the heat source, while  $a_f$  and  $a_r$  are the semi-axes of the front and rear ellipsoids, respectively.  $b$  and  $c$  are the semi-axes along the width and depth of the melt pool.  $f_f$  and  $f_r$  are the proportional coefficients for the front and rear ellipsoid of the heat source, with the condition  $f_f + f_r = 2$ .  $f_f$  is then given as follows:

$$[Eq. 25] \quad f_f = \frac{2a_f}{a_f + a_r}$$

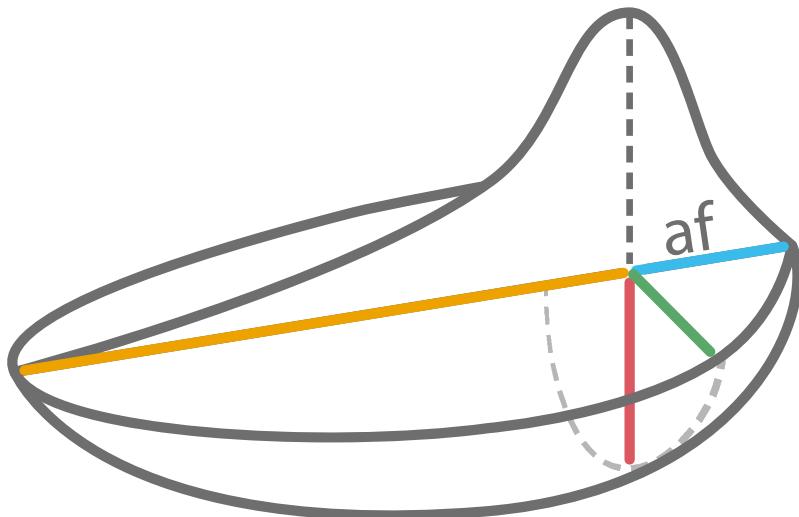


Figure 7: Schematic representation of energy distribution in double-ellipsoidal heat source model.

## Conical Heat Source

The third heat source model in the AM Module is also a volumetric heat source model, which was first employed for welding simulations but due to inherent similarities between welding and LPBF processes, this model is also commonly used for AM simulations. The conical heat source model is defined by a Gaussian heat distribution on the top surface of the workpiece and a conical distribution along the depth of the powder bed. A schematic representation of the energy distribution for conical heat source model is shown below.

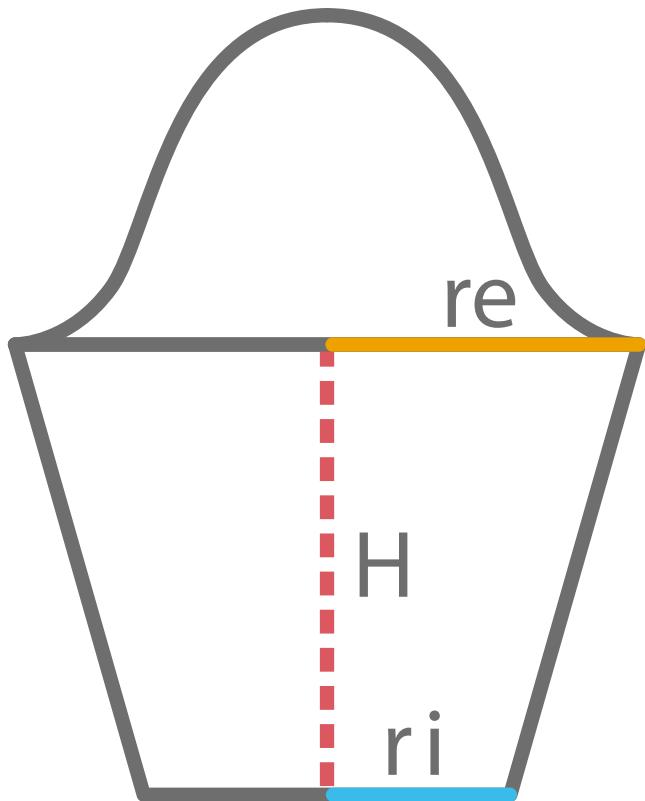


Figure 8: Schematic representation of energy distribution in conical heat source model.

The power density for the conical heat source is given as follows [2019Zha]:

$$Q = \frac{6\epsilon P}{\pi H(r_e^2 + r_e r_i + r_i^2)} \exp \left[ -2 \frac{(x-X_p)^2 + (y-Y_p)^2}{r_o^2} \right] \quad [\text{Eq. 26}]$$

with

$$r_o = r_e + (z - ZP) \frac{(r_e - r_i)}{H}$$

where  $r_e$  and  $r_i$  are the cone radius at the top and bottom, respectively, while  $H$  is the height of the cone.

## Numerical Boundary Conditions

In order to obtain temperature distribution during the LPBF process in the Additive Manufacturing (AM) Module, incorporating fluid flow inside the melt pool, we couple energy equations with the Navier-Stokes equations, as explained earlier. In order to accurately reflect the physical process, both of these equations are subjected to a certain set of boundary conditions, which are given as follows.

### **Boundary Conditions for Energy Equation**

The energy equation is subjected to four different boundary conditions. The first boundary condition is defined on the top surface (either the powder bed surface or the solid substrate) and represents the energy lost due to convection and radiation to the surrounding gas.

$$[Eq. 27] \quad Q_L = h(T - T_{ambient}) + \epsilon\sigma(T^4 - T_{ambient}^4)$$

where  $h$  is the convective heat transfer coefficient,  $\epsilon$  is the surface radiation emissivity and

$$\sigma = 5.669 \times 10^{-8} W/m^2 K^4$$

is the Stefan-Boltzmann constant.  $T_{ambient}$  is the ambient temperature or the temperature of the surrounding gas in the build chamber and can be set in the AM Calculator configuration.

The second boundary condition represents the heat lost through the vertical walls of the domain and for simplicity we have chosen adiabatic boundary conditions for these surfaces. The boundary condition for the vertical walls of the computational domain is thus given as:

$$[Eq. 28] \quad Q_N = 0$$

The third boundary condition reflects the temperature of the base plate and is therefore applied to the bottom of the computational domain. Here we have assumed that the base plate of the build part is kept at a constant temperature and the boundary condition is therefore given as:

$$[Eq. 29] \quad T = T_{baseplate}$$

$T_{baseplate}$  is the base plate temperature and can be set in the AM Calculator configuration.

The fourth and the most important boundary condition is the evaporation boundary condition that represents the heat lost due to evaporation of the material. Evaporation is implemented using a physics-based approach where the heat loss due to evaporation ( $Q_E$ ) is given as:

---

[Eq. 30]  $Q_E = 0.82 J_E \Delta H_v$

where  $J_E$  is the evaporation flux and  $\Delta H_E$  is the evaporation enthalpy. For a multicomponent system, the evaporation flux is given as follows:

[Eq. 31] 
$$J_E = \frac{1}{\sqrt{2\pi MRT}} \left( P_o \exp\left(-\frac{\Delta G_v}{RT}\right) - P \right)$$

where  $\Delta G_v$  is the driving force for evaporation,  $M$  is the molar mass of the gas,  $P$  is the gas pressure inside the chamber,  $P_o$  is the atmospheric pressure, and  $R$  is the universal gas constant. The driving force for evaporation, the evaporation flux, and the molar mass of the gas are all temperature-dependent material properties which are obtained from Thermo-Calc databases and are included in the material library whereas the gas pressure inside the chamber can be set from the AM Calculator configuration.

## **Boundary Conditions for Navier-Stokes Equations**

For the velocity, a no-slip boundary condition is employed on all surfaces of the computational domain. A no-slip boundary assumes that at a solid boundary, the fluid will have zero velocity relative to the boundary. For the pressure, a pinned boundary condition is used.

The most important boundary condition in Navier-Stokes setup is the Marangoni boundary condition that reflects the tangential force on the surface of the melt pool due to temperature variation of surface tension or the so-called Marangoni effect. In AM, large temperature gradients on the surface of the melt pool, leads to the Marangoni effect and is the primary cause of convective flow inside the melt pool. The Marangoni shear stress ( $\tau$ ) is modeled using the following equation:

[Eq. 32] 
$$\tau = \frac{\partial \gamma}{\partial T} \nabla_s T$$

where  $\gamma$  is the surface tension and  $\nabla_s$  represents the tangential component of the spatial derivative.

Surface tension is also a temperature-dependent material property which is obtained from Thermo-Calc databases and is included in the material library.

## **Thermophysical Properties of Powder Material**

When the option “Use separate material properties for powder” is selected, a different thermal conductivity, density and molar volume is used for the powder material as compared to the solid substrate. The above mentioned properties depend on the porosity ( $\phi$ ) of the powder. The density ( $\rho_{\text{powder}}$ ) and molar volume ( $Vm_{\text{powder}}$ ) of the powder are then simply given as follows:

$$\rho_{\text{powder}} = \rho_{\text{solid}}(1 - \phi)$$

$$Vm_{\text{powder}} = Vm_{\text{solid}} \frac{1}{1-\phi}$$

For thermal conductivity of powder  $k_{\text{powder}}$ , an empirical expression is used which was suggested by Xue and Barlow [1991Xue]. The thermal conductivity of powder thus also depends on the conductivity of the surrounding gas. For simplicity, the surrounding gas is assumed to be air. The thermal conductivity of powder is given as follows:

$$k_{\text{powder}} = (6.3 + 22\sqrt{0.09k_{\text{solid}} - 0.016}) \frac{k_{\text{solid}} (1-\phi)}{(k_{\text{solid}} / k_{\text{air}})(10^{0.523-0.594\phi})-1} \quad [\text{Eq. 33}]$$

where  $k_{\text{air}} = 0.05784$

## References

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- [2019Zha] Z. Zhang, Y. Huang, A. Rani Kasinathan, S. Imani Shahabad, U. Ali, Y. Mahmoodkhani, E. Toyserkani, 3-Dimensional heat transfer modeling for laser powder-bed fusion additive manufacturing with volumetric heat sources based on varied thermal conductivity and absorptivity. Opt. Laser Technol. 109, 297–312 (2019).

# Additive Manufacturing Workflow

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# Setting Up the Additive Manufacturing Simulation

Setting up an Additive Manufacturing (AM) Module simulation can be done in one of two workflows.

## General Overview

The general procedure of a simulation using the Additive Manufacturing Module is the following:

1. Define system (Workflow 1 only)
  - a. Choose database
  - b. Select elements and composition
2. Retrieve the materials data (Workflow 1 or 2)
  - a. Either with a Scheil calculation (Workflow 1) or using the materials data library (Workflow 2)
  - b. Apply data smoothing
3. Set up the AM Calculator (Workflow 1 or 2)
  - a. Choose simulation mode
  - b. Set simulation conditions
4. Run the simulation and visualize the results (Workflow 1 or 2)
  - a. 3D plot
  - b. Plot Over Line
  - c. Plot at probe position (only available for transient calculations).

## Workflow 1: When You Need to Obtain the Material Properties Data for the Calculation

Use a System Definer and Scheil Calculator to extract some Scheil data, then feed the data into the AM Calculator. Then add the Plot Renderer to define the specific AM Calculator Plot Renderer features and visualize the results. In this workflow, you can also save the results from the Scheil Calculator into the Material Library and reuse this data in the future.



When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

## Workflow 2: When You Already Have the Material Properties Data Available - Material Library

When you know you have the available material library data available, either by using the provided libraries, importing your own external data, or by saving your own material library after running a Scheil calculation, then you can directly start defining the AM Calculator and add and define one or more plots to visualize the results.



The Scheil Calculator and System Definer function the same as with a regular Thermo-Calc simulation. There are features available on the Scheil Calculator that are particularly useful to these types of calculations. The Plot Renderer is also unique to this calculator but is still based on the standard activity node.

The various activity nodes for each workflow are briefly described below.

### System Definer

The first step of the set-up is to select which database to use and define the material for the simulation. This is done in the System Definer.

In a **System Definer** activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select the species to include as well as change the reference temperature and pressure for your components.

A **System Definer** node can be added either directly to the My Project node or by default when the **Additive Manufacturing** template is added.

### Scheil Calculator (Workflow 1)

Once you have defined your system, you need to retrieve the materials data necessary for the AM calculations. This is done using the Scheil Calculator when you are working in Workflow 1.

A **Scheil Calculator** node can be added either directly to the **System Definer** node or by default when the **Additive Manufacturing** template is added.

### About the Scheil Calculator Settings

The Scheil Calculator in the Additive Manufacturing Module template is configured to generate the data necessary for the AM calculation. It is configured to start the simulation at a temperature of 5000 degrees and capture the evaporation and calculate the material properties down to room temperature. If you add a Scheil Calculator manually from the system definer, you will need to change these settings yourself. If you are working with different materials, different settings might be more suitable to your material.

## Materials Libraries (Workflow 1 or 2)

A Scheil calculation using the Scheil Calculator (Workflow 1) can be saved for reuse in the Materials Libraries. Alternatively, if there is external data available to use, you can skip the Scheil Calculator and just use a library (Workflow 2). There are also some predefined materials libraries included with the installation that can be used, and are used, in the examples AM\_01, AM\_02, and AM\_03 so that users without an AM license and necessary databases can see how this works.

## AM Calculator

Add an **AM Calculator** node to the Scheil Calculator. If you used the **Additive Manufacturing** template (on the **My Projects Configuration** window under **Applications**), click the node to display the **Configuration** settings window.



Cuboid geometries are currently only available for transient simulations. Both Steady-state and Transient models use adaptive mesh refinement to decrease computational cost. You have the option to either choose from the predefined mesh settings that defines the maximum and minimum element size based on the process parameters, or specify the maximum and minimum element size yourself.

You can use this either with or without the Scheil and System Definer if you already have the materials properties calculation you want.

## Choose Materials Data Source

Once the Scheil simulation is complete, click on the AM Calculator 1 node and then the Materials Properties tab to see the material property data obtained from the Scheil calculation. In the Material Properties tab, you can plot the properties required for the AM simulation. This is also where you select the data source that will be used in the simulation. In the Use data from: drop-down list you can choose either Scheil Calculator or Library. The Scheil Calculator option uses the Scheil results that you just calculated, while the Library option uses the data

that was shipped with the software or previously calculated data that you have saved to the Library.

## Visualizations Window

### **Apply Data Smoothing**

Before you run the AM Calculator, it is important that the data you will base the AM calculation on does not have any sharp peaks or curves to be able to solve the numerical problem. To avoid this, you can apply smoothing to your data. The default setting is **Little smoothing** but this can be changed depending on your simulation.

To determine how much smoothing to apply, you can plot the different properties. In the plot drop-down list you can select which property you want to plot to check the data and if there are any sharp peaks or curves in the plot. The plot appears immediately when you select a property. It is recommended to try running the simulations with only applying **Little smoothing**. If the calculation fails, you can increase the smoothing and try again. It is also possible to apply different levels of smoothing on different properties.

## Additive Manufacturing Templates

There are two templates you can use to access the Additive Manufacturing Module settings and features in Thermo-Calc.



You can also add nodes individually to build your own tree.



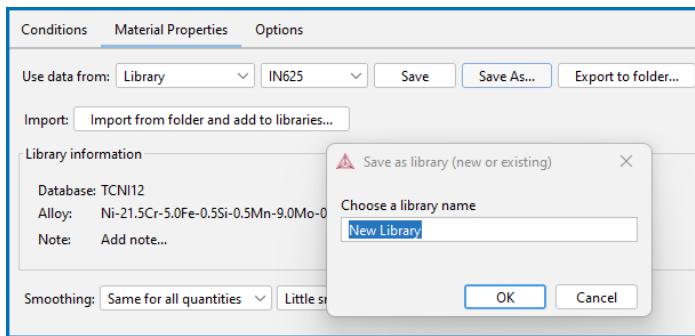
When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

### Additive Manufacturing Template

On the main **Project Configuration** window, under **Applications**, click the **Additive Manufacturing** icon. This adds the following activity nodes as a tree in the Project window – **System Definer**, **Scheil Calculator**, **AM Calculator**, and **Plot Renderer**. When you add this Additive Manufacturing template (and need to generate some materials properties or do not have a material library to use), then some unique default settings for the Scheil Calculator and these particular types of simulations are already set by default. Then you continue defining the AM Calculator by choosing one of the available simulation types: Steady-state, Transient, or Transient with heat source from Steady-state.

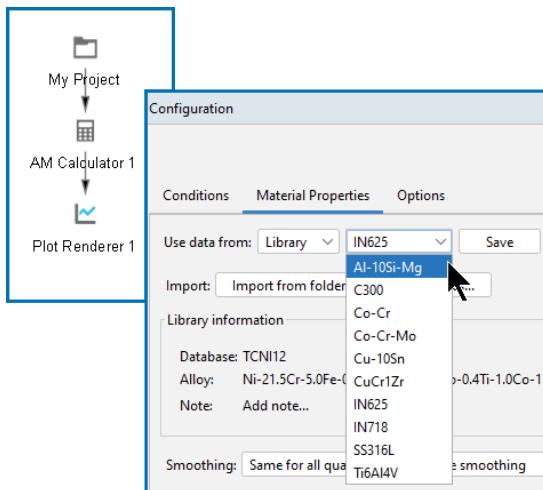


There is also an option on the AM Calculator to save the material properties in a material library, and use these later for a new AM Calculator where you want to make calculations related to the same alloy.



## With Material Library Template

Click **With Material Library** to create an activity tree that only includes the AM Calculator and Plot Renderer nodes. The tree setup does not need the System Definer or Scheil Calculator. Instead you can select (or import) pre-saved Materials Properties data from a library and use these for your AM calculations. For example, if you have already run calculations for the Scheil Calculator for your alloy, and you want to perform a different AM calculation for the same alloy, this data can now be reused where you start the AM Calculator using the second option and use the material property data from the material library.



# Working with the Activity Nodes for an AM Simulation

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## AM Calculator

Depending how you set up your simulation, the **AM Calculator** can either be part of the workflow after a **Scheil Calculator** or directly at the root below the **My Project** node.



There is an **Additive Manufacturing** template available under **Applications** that you can use to quickly set up either one of these workflow options for the AM simulation. See "[Additive Manufacturing Templates](#)" on page 37 and "[Setting Up the Additive Manufacturing Simulation](#)" on page 33.

Once you have added an AM Calculator, the **Configuration** window has these tabs where there are many available features to set on the **Conditions**, **Materials Properties**, and **Options** sections and with the specialized **Plot Renderer** and toolbar on the **Visualizations** window.

There are these simulation type pathways to choose: **Steady-state**, **Transient**, or **Transient with heat source from Steady-state**.

We have understood that in cases where convection is the dominant mode of heat transfer, fluid flow inside the melt pool plays a significant role in determining the correct shape of the melt pool.



For more details about these see "[Additive Manufacturing Simulation Types](#)" on page 15. Also review the "[Additive Manufacturing Module Theory](#)" on page 17 as needed.

**Steady-state:** Compute temperature distribution in a steady-state environment, either on a bare metal substrate or with a powder layer on the top, with the possibility to add fluid flow inside the melt pool.

**Transient:** Compute temperature distribution in a transient case with the given scanning strategy including multiple paths and layers and the possibility to add fluid flow inside the melt pool.

**Transient with heat source from Steady-state:** Compute temperature distribution in a transient case with the given scanning strategy including multiple paths and layers.

- A steady-state simulation runs with the configured heat source and with the possibility to add fluid flow in the melt pool.
- A volume heat source (based on the solution of steady-state calculation) is used in the transient simulation.

There are several settings and these are described separately for each tab.

- "[AM Calculator Conditions Settings](#)" on the next page
- "[AM Calculator Materials Properties Settings](#)" on page 54
- "[AM Calculator Options Settings](#)" on page 52

Also as a successor to the **AM Calculator**, you can right-click the node to add one or more **Plot Renderer** nodes to visualize your results. Although the node works the same as with the other calculators in Thermo-Calc, there are additional features and settings unique to this module. Useful information is included throughout the documentation. See "["AM Calculator Plot Renderer"](#) on page 58 as a starting point.



When setting up an AM simulation, the **Visualizations** window shows both active configuration changes and other design states as set up on the **AM Calculator** as well as the results generated by the **Plot Renderer** calculations.

# AM Calculator Conditions Settings

Once you have added an "AM Calculator" on page 40, the **Configuration** window has these settings tabs where there are many available conditions to set on the **Conditions**, **Materials Properties**, and **Options** tabs and with the specialized **Plot Renderer**.

This topic describes the available main settings on the **Conditions** tab.



"AM Calculator Materials Properties Settings" on page 54 and "AM Calculator Options Settings" on page 52



"Additive Manufacturing Module Theory" on page 17

## Global Settings

### Gas Pressure

Pressure is used to calculate the heat loss due to evaporation from the top surface of the given material.

**Gas pressure:** The pressure of the gas inside the build chamber. The default is 100000 **Pascal**. Select **Atmospheres or Bar**.



When you select a different unit the default value does not change.

Enter a different value in the field.

### Temperature Unit

**Temperature unit:** Select a unit **Kelvin**, **Celsius**, or **Fahrenheit**.

### Base Plate Temperature



If you change the **Temperature unit** then double check that the value in this field is also updated or correct as expected if you are keeping the default. This field does not update automatically when the unit changes.

**Base plate temperature:** The base plate of the build part is assumed to have a constant temperature. This temperature is used as a boundary condition for the base of the computational domain.

The default is 303.15 K.

## Ambient Temperature

The **Ambient temperature** is used to calculate the heat loss from the top surface due to radiation, convection and evaporation.

This setting is the temperature of the air in the immediate surrounding environment.



If you change the **Temperature unit** then double check that the value in this field is also updated or correct as expected if you are keeping the default. This field does not update automatically when the unit changes.

## Fluid Flow including Marangoni Effect

This section becomes available when the **Use separate material properties for powder** checkbox is not selected.



Also see the theory section, "Fluid Flow" on page 25.

Choose to use **Fluid flow including Marangoni effect** if you want to calculate and include for the effect of fluid flow due to gradient of surface tension in the melt pool. The checkbox is selected by default. This solves the Navier-Stokes equation to include fluid flow inside the melt pool due to the Marangoni effect.

If you want to use separate properties for the powder layer, click to clear the checkbox to enable **Use separate material properties for powder** fields and then continue with the settings below.

## Use Separate Material Properties for Powder

---

This option is available when the **Fluid flow including Marangoni effect** checkbox is NOT selected.

**Use separate material properties for powder:** Select to use different density and thermal conductivity for the powder layer; otherwise by default the same properties as for the solid are used.

**Powder density:** The powder density as a percentage (0-100%) of the solid material. The default is 80 % of the solid material.

## Geometry

For a **Steady-state** simulation, it is just the height needed. For **Transient** or **Transient with heat source from Steady-state** these are volumetric and you also define the width and length. For all simulation types also define the coarseness of the mesh.

### ***Height for Steady-state Simulation***

**Height:** Enter the build height (mm). Length and width of the computational domain is automatically chosen as a function of the heat source parameters and the scanning speed.

### ***Height, Width, and Length for Transient Simulations***

- **Height:** Enter the initial build height (mm). Powder layer(s) with the given layer thickness will be added on the top. In mm.
- **Width:** Enter the build width (along y direction). In mm.
- **Length:** Enter the build length (along x direction). In mm.

## ***Mesh***

**Mesh:** The initial mesh size —**Coarse**, **Medium**, **Fine**, or **Custom**. It is adaptive and refined as required.

If **Custom** is selected, enter the maximum and minimum element sizes:

- **Maximum element size:** The initial element size (in  $\mu\text{m}$ ) in the mesh.
- **Minimum element size:** The minimum element size (in  $\mu\text{m}$ ) that the adaptive mesh can refine to.

## Heat Source

The heat source model has either a **Gaussian**, **Double ellipsoidal**, or **Conical distribution**.



"Modeling Heat Source" on page 25 in the theory section.

**Gaussian** is a surface heat source, and it is applied to the top surface of the domain. Then the heat is diffused based on the diffusivity of the material. This is most commonly used heat source in the industry

But in cases where the melt pool tends to form in a keyhole formation then you need to include more multiphysics phenomena to get the correct shape of the meltpool. Then the volumetric heat sources give you better control of the shape of the meltpool and the temperature gradient around the heat source.

**Double ellipsoidal**, also referred to as Goldak, is a volume heat source model where the heat intensity is in the front and the back of the heat source is defined with the help of two different ellipsoids. The axis of each ellipsoid is needed.

The **Conical distribution** is also a volumetric heat source where heat intensity is described as Gaussian distribution at the top surface, defined by a top radius, that varies linearly in the depth of the workpiece until it reaches a bottom radius within the prescribed depth.

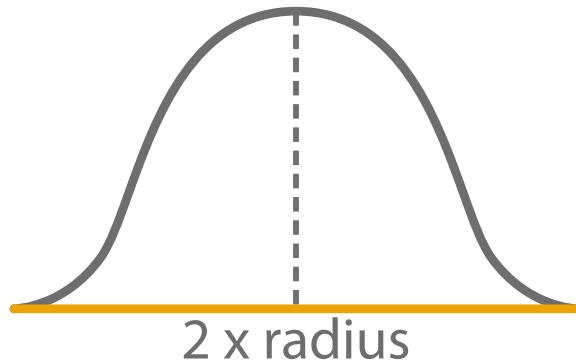
After choosing the type of heat source, then enter parameters as required.

For all models enter:

- **Power:** Power for the selected heat source model. The default is 120 W.
- **Absorptivity:** Absorptivity % for the selected heat source model. The default is 60 %.

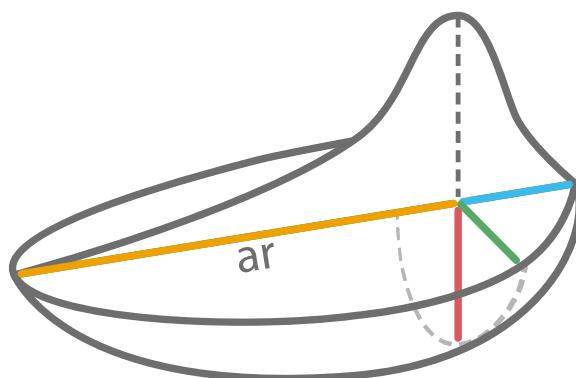
For **Gaussian**, also enter:

- **Beam radius:** Beam radius size for the **Gaussian** heat source model. The default is 110  $\mu\text{m}$ . Hover over the field in the GUI to view this example of it.

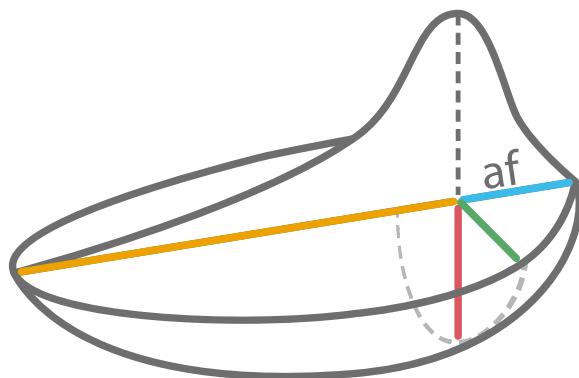


For **Double ellipsoidal**, also enter as required. For each field you can hover over it in the GUI to see these images that show you the location.

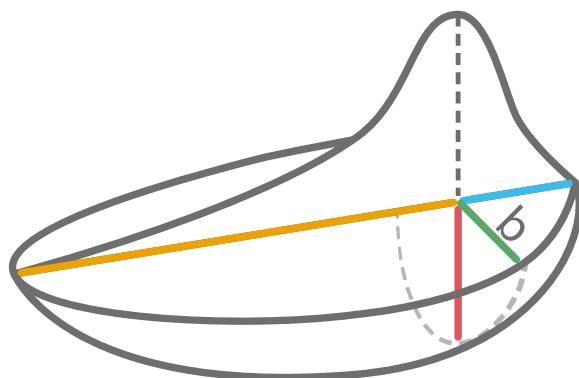
- **ar** (default is 70  $\mu\text{m}$ ).



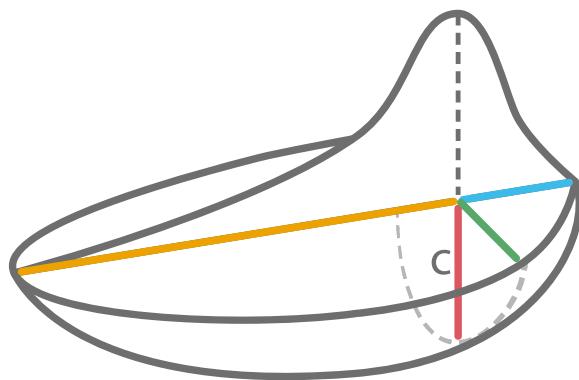
- **af** (default is 70  $\mu\text{m}$ ).



- **b** (default is 85  $\mu\text{m}$ ).

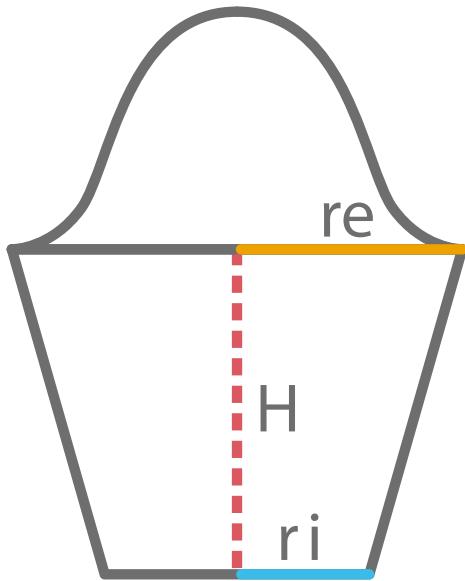


- **c** (default is 200  $\mu\text{m}$ ).



For **Conical distribution**, also enter the following. For each field you can hover over it in the GUI to see these images that show you the location.

- **re** (default is 100  $\mu\text{m}$ ).
- **ri** (default is 60  $\mu\text{m}$ ).
- **H** (default is 100  $\mu\text{m}$ ).



## Scanning Strategy

The scanning strategy determines the build geometry for one or multiple layers. Green layer on the top of the geometry is the powder and the grey part is the solid substrate.

For **Steady-state** simulations, you only need to define the **Scanning speed** and **Layer thickness**.

- **Scanning speed:** The velocity of the moving heat source. The default is 500 mm/s.
- **Layer thickness:** The thickness of the powder layer. The default is 40 mm. When you change the layer thickness, the meshing size changes too.

For both transient simulations, you continue to define the settings below.

## Pattern

**Pattern:** Select the scanning pattern—**Single track**, **Bidirectional**, or **Unidirectional**.

- Select **Unidirectional** to use same scanning direction of the heat source for all tracks.
- Select **Bidirectional** to flip scanning direction of the heat source between alternate tracks.

## Single Track

- **Margin:** Offset of the laser scanning path from the sides of the computational domain. In case of Single track, offset is placed from the sides transverse to the scanning direction, whereas the scanning path is always in the middle of the domain going along the length of the workpiece.
- **Number of layers:** Enter the number of layers or scroll using the arrows.
- **Powder fill time:** Powder recoating time (unit = s) between two consecutive layers. This does not include lift time.

## Bidirectional and Unidirectional

- **Margin:** Offset of the laser scanning path from the sides of the computational domain.
- **Hatch spacing:** Separation (unit = mm) between two consecutive tracks.
- **Lift time:** Time (unit = s) between two tracks where the heat source is inactive.
- **Number of layers:** Enter the number of layers or scroll using the arrows.
- **Powder fill time:** Powder recoating time (unit = s) between two consecutive layers. This does not include lift time.
- **Rotation between layers:** Rotation (unit = degrees) of the scanning direction between two consecutive layers. The scanning pattern of the first layer is always aligned to the X axis then the second layer will be rotated (if you choose this setting) with the specified angle then the next layer will be rotated at the same angle as compared to the previous layer and so on. This way you can change the rotation of the layers.

## Top Boundary Conditions



"Numerical Boundary Conditions" on page 29 in the theory section.

### Radiation Emissivity

**Radiation emissivity:** To include the effect of radiation from the top surface to the surrounding gas, enter a value between 0 and 1. If you want to neglect the heat loss, then enter 0 to disable radiation.

### Convective Heat Transfer Coefficient

**Convective heat transfer coefficient:** The convective heat transfer coefficient for the top surface to the surrounding gas. If you want to ignore this then enter 0 to disable convective heat transfer.

### Evaporation

**Evaporation:** Select the checkbox to include the effect of evaporation heat loss due to heating of the powder layer or the metallic surface close to the evaporation temperature.



The **Evaporation** heat loss is calculated based on the settings on the **Materials Properties** tab, i.e. evaporation enthalpy per mole, the driving force for evaporation per mole quantity and the molar mass of gas. These are also calculated by the databases.

## Probe Positions (Transient Simulations Only)

You can add probes in the domain that record temperature and all other temperature related properties when the simulation is being run. You can either specify the coordinates or click Pick coordinate to choose on the geometry. Important to add the probes before the simulation is run or it is not recorded.

## Using Probe Data in Diffusion and Precipitation Calculations



When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.



"AM Calculator: Working with Probe Data" on page 56

## AM Calculator Options Settings

Once you have added an "AM Calculator" on page 40, the **Configuration** window has these settings tabs where there are many available conditions to set on the **Conditions**, **Materials Properties**, and **Options** tabs and with the specialized **Plot Renderer**.

This section describes the settings for the **Options** tab.



"AM Calculator Conditions Settings" on page 42 and "AM Calculator Materials Properties Settings" on page 54

### ***Streamline Upwind Petrov-Galerkin (SUPG)***

Select the **Streamline upwind Petrov-Galerkin (SUPG)** checkbox to enable SUPG stabilization scheme for the energy and Navier-Stokes equations.

### ***Damping Factor for the Damped Newton Iteration***

Select the **Damping factor for the damped Newton iteration** checkbox to add a damping factor for the damped Newton iteration and enter a value between 0 and 1. The default is 0.7.

It may improve stability but it slows down convergence of the simulation.

### ***Save Interval for Transient Simulation***

Select the interval to save results from transient simulations. If the number of steps are specified, choose if the step size should increase linearly or exponentially.

From the **Save interval for transient simulation** list choose:

- **Automatic (with max number of steps):** The default is 100 **Linear** steps. Or enter another number of steps in the field and/or select **Exponentially increasing** to increase the step size exponentially.
- **Total number of steps:** The default is 100 **Linear** steps. Or enter another number of steps in the field and/or select **Exponentially increasing**
- **Every Nth time step:** The default is 1 or enter or use the up and down arrows to choose

another number.

- **Time in seconds:** The default is 0.01 or enter another number in the field.

### ***Number of Cores***

Select or enter the **Number of cores** available for the simulations. The default value is the total number of physical cores available in the system.

# AM Calculator Materials Properties Settings

Once you have added an "AM Calculator" on page 40, the **Configuration** window has these settings tabs where there are many available conditions to set on the **Conditions**, **Materials Properties**, and **Options** tabs and with the specialized **Plot Renderer**.

This section describes the settings for the **Materials Properties** tab.



"AM Calculator Conditions Settings" on page 42 and "AM Calculator Options Settings" on page 52

## **Use data from**

If there is a Scheil Calculator predecessor to the AM Calculator, you can import the material properties from a **Library** or **Scheil Calculator**. When the AM template is added, the default is to import material properties from Scheil calculations.

When the **with Material Library** template is used, then the AM Calculator > Materials properties are available to import from a **Library** only.

In this case you also can **Save**, **Save as**, **Export to folder**, **Delete**, and **Rename** the material data both from Scheil and from material library. With Save or Save as, original data is saved i.e. without any smoothing. With Export to folder, the data is saved with Smoothing. the material data both from Scheil and from material library.

## **Import**

You can import material properties contained in a folder.

Click the **Import from folder and add to libraries** button and navigate to the folder location where the material properties are located.

## **Smoothing**

From the **Smoothing** list, select **Same for all quantities** (where **Little smoothing** is the default) or **Per quantity**. Then either define the smoothing once (**Same for all quantities**) or individually for each quantity. Options are **No smoothing**, **Little smoothing**, **Medium smoothing**, **Large smoothing**, or **Linear**.

Available quantities to define smoothing:

- Heat and heat capacity
- Density
- Thermal conductivity
- Dynamic viscosity
- Surface tension
- Molar volume
- Molar mass of gas
- Driving force for evaporation per mole
- Evaporation enthalpy per mole

## ***Plot***

From the **Plot** list, choose what quantity to plot

- Heat
- Apparent heat capacity per kg
- Density
- Thermal conductivity
- Dynamic viscosity
- Surface tension
- Molar volume
- Molar mass of gas
- Driving force for evaporation per mole
- Evaporation enthalpy per mole

## AM Calculator: Working with Probe Data



When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

### Workflow to Include Probe Data from Diffusion or Precipitation Simulations



You can use an installed example to visualize how the probes are set up for a Diffusion Calculator. See "["AM\\_05: Using AM Calculator Probe Data with the Diffusion Module \(DICTRA\)" on page 100](#)". The process is similar for a Precipitation Calculator.

1. Set up the probes on the **AM Calculator**. Probes are available for transient calculations only. See "["AM Calculator Conditions Settings" on page 42](#)". This must be done before you can use the probe data in the calculations connected to a Diffusion Calculator or Precipitation Calculator.
2. If not already done, add a **Diffusion Calculator** or **Precipitation Calculator** as a successor to the **AM Calculator**.
3. Set up your Diffusion or Precipitation Calculator as needed. Follow the basic settings details for the **Thermal Profile** section.
4. Once the standard settings are completed, and as long as probes are set up, on the **Configuration** window, the section **Probes** is available. Until the AM Calculator is run, the list is empty. After the AM simulation is completed, the data is imported into the table you can choose how to **Condense time-temperature data**. These settings are described below.

## Probes

The list of **Probes** is available as long as *Probe Positions* are set up on the AM Calculator and the AM Calculator is performed to generate the data, which is fed into the applicable Calculator (Diffusion or Precipitation). Select the probe you want to plot, for example as a Segregation Profile as shown in example AM\_05.

## Condense Time-Temperature Data

Use the **Condense time-temperature data** setting to adjust how many time-temperature points are included in the **Thermal Profile** displayed in the **Visualizations** window. For example, for a complex calculation you can choose a **Medium** or **Large** setting to save fewer time steps at this stage of design, which in turn can ensure that a complex diffusion or precipitation calculation is able to finish.

Choose **None**, **Small**, **Medium**, **Large**, or **Custom**.

- **None** (the default) includes all points, i.e. no points are condensed together and all point data are included in the **Thermal Profile** preview. When using the **Custom** setting, this is equivalent to entering a value greater than  $1$  in the field.
- **Small** condenses a minimum number of points, which means that a *large* number of time steps are used in the calculation and thus lots of time steps are shown.
- **Medium** is when that a medium number of points are condensed together, which means that a *medium* number of time steps are used in the calculation.
- **Large** is when a large number of points are condensed together, which means that there are few, or a *small* number of time steps used in the calculation.
- When **Custom** is selected you can fine-tune the number of points to include. Enter a value between  $0$  and  $1$ , where  $0$  maximizes condensing the points (the same as choosing **Large**),  $1$  minimizes condensing the points (the same as choosing **Small**), and  $0.5$  is a medium number of points being condensed (the same as choosing **Medium**). If you enter a value greater than  $1$ , it is the same as choosing **None**, i.e. all data points are included. The larger the value, the more points are condensed, until only two points are shown.

## AM Calculator Plot Renderer

Once you have added an "AM Calculator" on page 40, you can add the specialized **Plot Renderer**. The following is information about the settings available for a **Plot Renderer** when it is a successor to an **AM Calculator**.

**Rescale plotting data range over all time steps:** Select this to scale min and max values of legends and plots over all time steps.

**Filter by material types:** Select to visualize a specific material type(s) from the list. This option is only available when "Use separate material properties for powder" is selected in the AM Calculator configuration.

Options to choose **3D Plot** or **Plot Over Line** tabs available on the Configuration window.



"Rotate, Zoom, and Pan 3D Plots: AM Calculations" on page 64



"AM Visualizations Window Plot Toolbar" on page 62

### Plot Settings

You can plot the material properties (2D) so you can specify the quantities and add as many lines as you want directly to the plot in the visualizatoins window. What you see is Distance vs Temperature, first is first layer, 2nd 2nd layer, etc etc. on the 2D plots. You can select the different times from the list at the top at different points and see it on the plot. at 26 minutes you can see where it is as the peak of the melt pool max temperature

### Add a Quantity and Remove a Quantity Buttons

Use the **Add quantity** and **Remove quantity** buttons to add additional setting groups that include all of the available settings described below. Click the checkbox next to these buttons to enable or disable any particular settings group.

### Axis Variable

Set the state variable you want plotted along the X-axis and the Y-axis. The available variables in the list are based on how your system is set up.

Below are additional details related to the *Axis variable* chosen.

Variable options are

- **Temperature, Surface tension, Thermal conductivity, Dynamic viscosity, Flow velocity field.** Then also choose a unit for your selection from the applicable drop-down list.

## Display

Based on the **Axis variable** selected, choose the way to **Display** it.

- For Temperature, Surface tension, Thermal conductivity, or Dynamic viscosity, choose **Contour, Surface colormap, or Iso-surface**.
- For Flow velocity field, choose the object shape to display velocity vectors: **Arrow, 2D glyph, Cone, or Line**.

The settings are further described in separate sections below.

## Tubes

Available for a **Contour** Display.

The **Tubes** checkbox is selected by default and this displays contour plots as 3D tubes. Click to clear the checkbox and instead display the contours as 2D lines.

## Values

Available for display types **Contour** and **Iso-surface**. For Iso-surface you can also specify the opacity of surface plot in %.

Choose the **Values**: **Automatic** (the default), **Custom values**, **Custom range**, **Solidus**, **Liquidus**, or **Solidus and Liquidus**.

- For **Automatic**, enter the **Number of steps**.
- For **Custom values** enter a number in the field.
- For **Custom range** enter the **Min** and **Max** number of lines, then **Number of steps**.

- Select **Solidus** to plot contour/iso-surface at solidus temperature.
- Select **Liquidus** and **Solidus and Liquidus** to plot contour/iso-surface at both solidus and liquidus temperatures.

Some settings are further described in separate sections below.

## **Number of Steps**

Available for **Contour** and **Iso-surface** Display types, and when **Automatic** or **Custom range** Values are selected.

Enter or choose the **Number of steps**.



In some cases for a **Custom range** selection, you need to expand the Configuration window to the right to access this setting.

## **Opacity**

Available for **Surface colormap** and **Iso-surface** (available for all **Values** options).

Enter a value between 0-100 as the percent (%) of **Opacity**.

## **Slice**

Select the **Slice** checkbox to visualize the **Axis variable** on a cross-sectional plane. You can choose the normal of the cross-sectional plane and the distance of the plane from the center of the heat source.

Then choose **X-direction**, **Y-direction**, or **Z-direction**, for the **Distance from center of heat source** and for the **beam radius**

## **Coloring and Range**

Choose **Rainbow**, **Cool to warm**, **Purple Orange**, **Green Purple**, **Blue Brown**, **Green Red**, **Solid color**.

For all but **Solid color**, choose a **Range—Automatic** or **Custom**. Then for **Custom** enter a **Min** and **Max** number.

## **Legend**

Click the **Legend** checkbox to include or click to clear to exclude a legend.

## **Scale Glyph by Velocity Magnitude**

This setting is for a **Flow velocity field Axis variable**. It is available for all **Display** types.

Select the **Scale glyph by velocity magnitude** checkbox to scale the velocity display object (glyph) according to the velocity magnitude. Otherwise the glyphs are scaled uniformly.

## **Glyph Scale Factor**

This setting is for a **Flow velocity field Axis variable**.

Enter a numerical value for the **Glyph scale factor**.

## **Show Glyph in Every**

This setting is for a **Flow velocity field Axis variable**.

For the **Show glyph in every setting**, enter or select the number of grid **points** where velocity glyphs are displayed.

## AM Visualizations Window Plot Toolbar

The **Visualizations** window by default has tabs included to help you visualize both the set up using the **AM Calculator** and the results that are calculated via the **Plot Renderer**.



"Rotate, Zoom, and Pan 3D Plots: AM Calculations" on page 64

<b>Button</b>	<b>Name</b>	<b>Action</b>
	Zoom to heat source position	Click to zoom to the heat source.
	Set view to 3D	Click to reset the view where you zoom out to see the whole geometry.
	Set view direction to YZ	Click to orient to a side view in the YZ-axes direction.
	Set view direction to XZ	Click to orient to a side view in the XZ-axes direction.
	Set view direction to XY	Click to orient to a top view in the XY-axes direction.
	Azimuth rotation, Ctrl+ for invert rotation	Click to rotate around the free axis. Press and hold CTRL + click the mouse to control the direction turned.
	Elevation rotation, Ctrl+ for invert rotation	Click to rotate around the free axis. Press and hold CTRL + click the mouse to control the direction turned.
	Roll rotation, Ctrl+ for invert rotation	Rotate around the free axis Click Ctl+button to control the direction turned
	Save camera view angle	There are two attributes that are saved when the <b>Save camera view angle and zoom level</b> button is clicked. The view angle of the camera and the zoom level.

<b>Button</b>	<b>Name</b>	<b>Action</b>
	and zoom level	<p>Then when you click the <b>Apply saved camera view and zoom level</b>, it mirrors the view angle of the camera and the zoom level. This is available for any 3D plot tab on the Visualizations window.</p> <p>Only one camera position can be saved/retained at any time for use.</p>
	Apply saved camera view angle and zoom level	<p>First use the <b>Save camera view angle and zoom level</b> to save the desired view. Then click the <b>Apply saved camera view and zoom level</b> button to mirror the view angle of the camera and the zoom level. This is available for any 3D plot tab on the Visualizations window.</p> <p>Only one camera position can be saved/retained at any time for use.</p>
	Show grid	Click to turn on and off the mesh grid.
	Show heat source	Click to show and hide the heat source.
	Mirror geometry	When in steady state you only see half the geometry. Click to show the whole geometry, click again to show half the geometry.
—	Hide layers	Enter a number of layers to hide
	Show Outer Box	Click to turn on and off the outer box geometry.
	Show Size of the Melt Pool	Click to show or hide the melt pool. This is the same thing as showing the size of the liquidus iso-surface plot. When clicked you also see the measurements in the <b>Event Log</b> window and shows on the <b>Visualizations</b> window.
	Show Size of Melt Pool plus Mushy Zone	Click to show or hide the melt pool and mushy zone. This is the same thing as showing the size of the solidus iso-surface plot. When clicked you also see the measurements in the <b>Event Log</b> window and shows on the <b>Visualizations</b> window.
	Show Manual Ruler	<p>Click to use the manual ruler to measure the melt flow.</p> <ul style="list-style-type: none"> <li>• Double click each time to add the start and end points.</li> <li>• To align a ruler on the x-, y-, or z- axis: Hold CTRL when adding or moving the end point. The ruler snaps to the closest point on the same axis.</li> <li>• To move a ruler: Click and hold a point, then drag to reposition.</li> <li>• Right-click a point to delete it.</li> </ul>

## Rotate, Zoom, and Pan 3D Plots: AM Calculations

When working with the Additive Manufacturing (AM) Module and the results from an "AM Calculator" on page 40 simulation, two general plot types are added to the **Visualizations** window: a *3D plot* and a *Plot over line 2D plot*. The 2D plot has the same functionality as for other calculations but the 3D plot is specific to this Module.

In addition to the **Visualizations** window for an AM 3D plot having its own set of buttons (see "AM Visualizations Window Plot Toolbar" on page 62) there are also different ways to work with the 3D plots with respect to rotating, zooming, and panning the geometry around the window.



In combination with the following actions use these buttons on the toolbar: **Set View to 3D** and **Set View Direction** .

- **Rotate the geometry** : Left-click and hold the mouse, then move it around the window to rotate in any direction. Hold CTRL + left mouse button to rotate on a specific axis.
- **Zoom in and out**: Scroll the mouse wheel or right-click and move the mouse up and down in the window.
- **Pan the geometry**: Hold Shift + left mouse button then move the mouse up or down, left or right, to move the geometry around the window without zooming.



Go to the Help (press F1 in Thermo-Calc) to view a short video showing the use of these actions.

## Additive Manufacturing (AM) Module Examples Collection



A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run three examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.



Read more about the [Additive Manufacturing \(AM\) Module](#) on our website. You can also use the [Getting Started Guide](#) to learn about the key features available.

In this section:

## AM\_01: Transient Simulation of a Single Track

The following example is part of a series showing some of the features of the Additive Manufacturing (AM) Module and the **AM Calculator**. In this example, a single track simulation is performed using the **Transient** model of the AM Calculator.



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The first three examples (AM\_01, AM\_02, and AM\_03) use predefined Material Properties libraries that are embedded with the examples for use for all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO mode. See "Available Options" on page 7 for details.

### Project File Information

- Folder: Additive Manufacturing
- File name: *AM\_01\_Transient\_DE\_No\_Marangoni.tcu*

Open the example project file and click **Perform Tree** to generate the plots associated with it.



When you run (Perform) this example, it can take over two hours to complete the calculations.

### Material Properties

These properties are the same for both AM\_01 and AM\_02.

- Inconel 738LC: Ni-15.8 Cr-8.6 Co-2.7 W-3.3 Ti-3.6 Al-1.8 Ta-1.8 Mo-0.04 Fe-0.8 Nb-0.002 Mn-0.1 C Mass percent.
- Database: TCNI12

- The material property was pre-calculated, and stored as a built-in material library of the Additive Manufacturing (AM) Module.

## Reference

[2021Gra] D. Grange, A. Queva, G. Guillemot, M. Bellet, J.-D. Bartout, C. Colin, Effect of processing parameters during the laser beam melting of Inconel 738: Comparison between simulated and experimental melt pool shape. *J. Mater. Process. Technol.* 289, 116897 (2021).

## Model Configuration

The transient model solves for the heat equation in the entire 3D domain, including the melt pool, and is therefore, computationally expensive to solve. The fluid flow inside the melt pool due to the Marangoni effect is not included in this example. The double ellipsoidal, or the so-called Goldak heat source model, is used to predict melt pool size and temperature distribution during single track scanning. The parameters for the double ellipsoidal heat source are computed using optimization in a steady-state case for the given process parameters (power and scanning speed) and the melt pool size reported in the paper by Grange et al. [2021Gra]. The resulting parameters are shown in Figure 9.

A screenshot of the Thermo-Calc AM Calculator interface. The 'Heat Source' tab is selected. Under 'Double ellipsoidal', the following parameters are entered:

Power: 230.0	W Absorptivity: 88.06	% ar: 97.3	μm af: 99.04	μm b: 41.67	μm c: 181.11	μm
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Figure 9: Optimized heat source parameters entered on the AM Calculator for the experiment given in Grange et al. [2021Gra] with power = 230 W and scanning speed = 960 mm/s.

The geometry for a transient simulation, as given in the paper by Grange et al. [2021Gra], is shown in Figure 10. The base plate is 2 mm in length, 0.5 mm in width, and with a thickness of 0.95 mm. A layer of powder with a thickness of 55 μm is deposited on the solid substrate. The powder layer, however, has the same material properties as the solid substrate. The laser beam with a power of 230 W develops linear scanning with constant velocity 960 mm/s. The trajectory evolves from initial position (x, y) = (0.25, 0.25) mm to final position (1.75, 0.25) mm on the top surface.

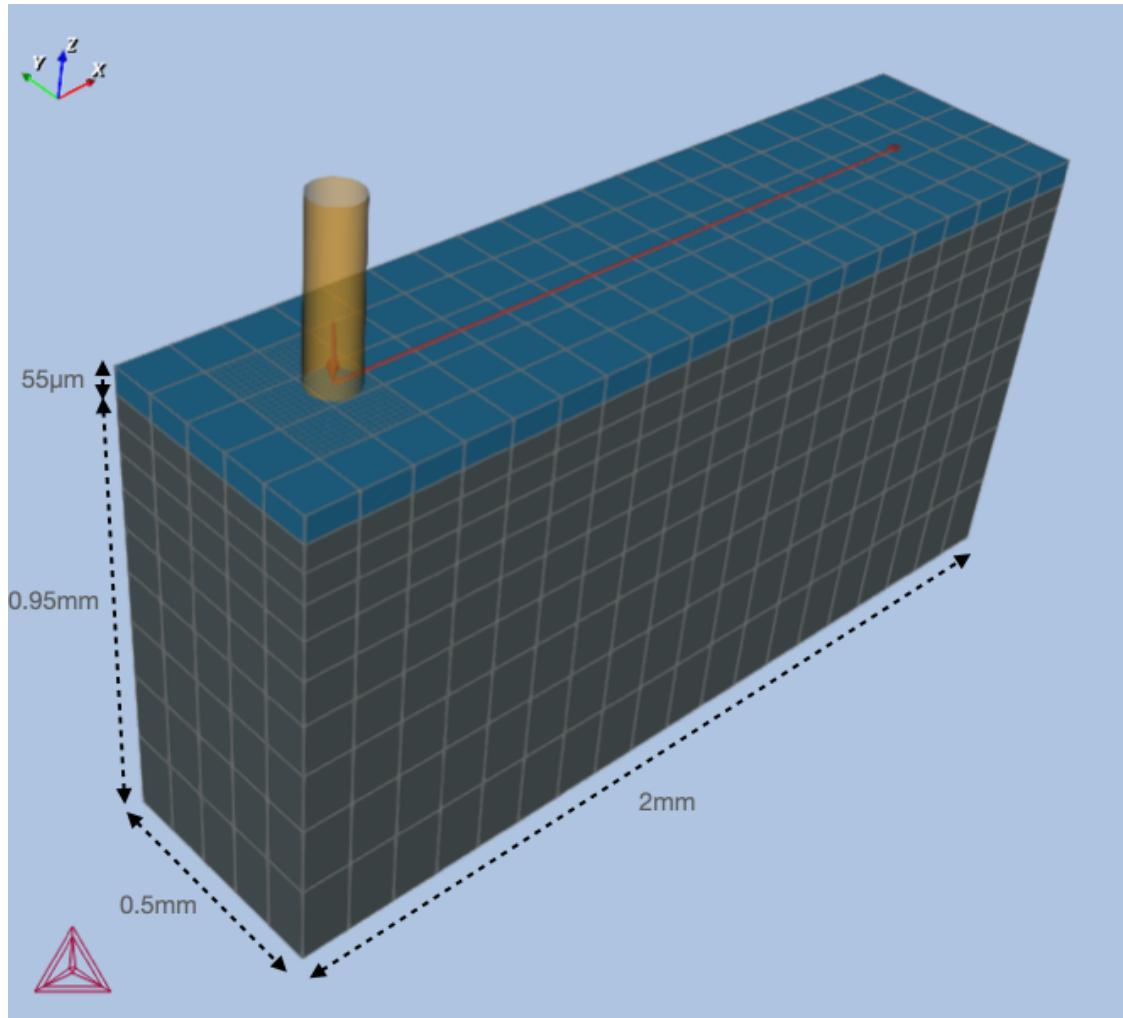


Figure 10: The geometry used for the Additive Manufacturing (AM) Module examples AM\_01 and AM\_02.

Two probes monitor the temporal evolution of temperature at positions shown in Figure 11. The results can be presented by tabulated data or as 2D graph plots.

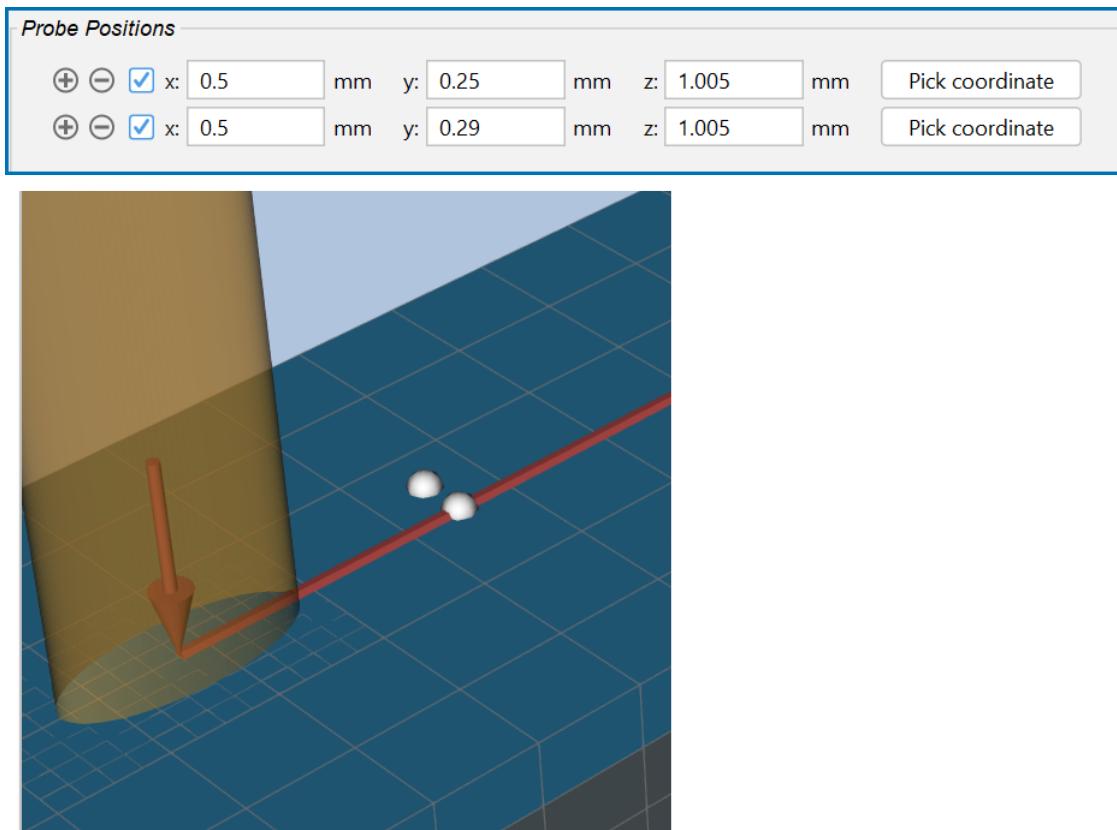


Figure 11: Probe positions for Probes P1 and P2, where P1 is placed exactly on the scanning track while P2 is placed at a distance of 0.04 mm from the track, as shown in a close up of the probes on the Visualizations window.

## Visualizations

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

- **Geometry:** View the geometry and adjust parameters visually by changing inputs on the Configuration window. Add probes as shown in [Figure 12](#).
- Melt pool and other dynamically changing features can also be visualized and changed.
- **Plot 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, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

Figure 12 shows the surface plot of temperature distribution after the scanning process is completed. It is noted that the melt pool shape reaches a steady-state when the laser beam approaches the end of the scanning track. The melt pool dimensions at the end of scanning track is given in the table.

Melt Pool Dimension	Size (mm)
Width	0.125
Depth	0.144
Length	1.12



If you are in the project file, click the **Probe plot** node in the Project window and the **3D Plot** tab in the Visualizations window.

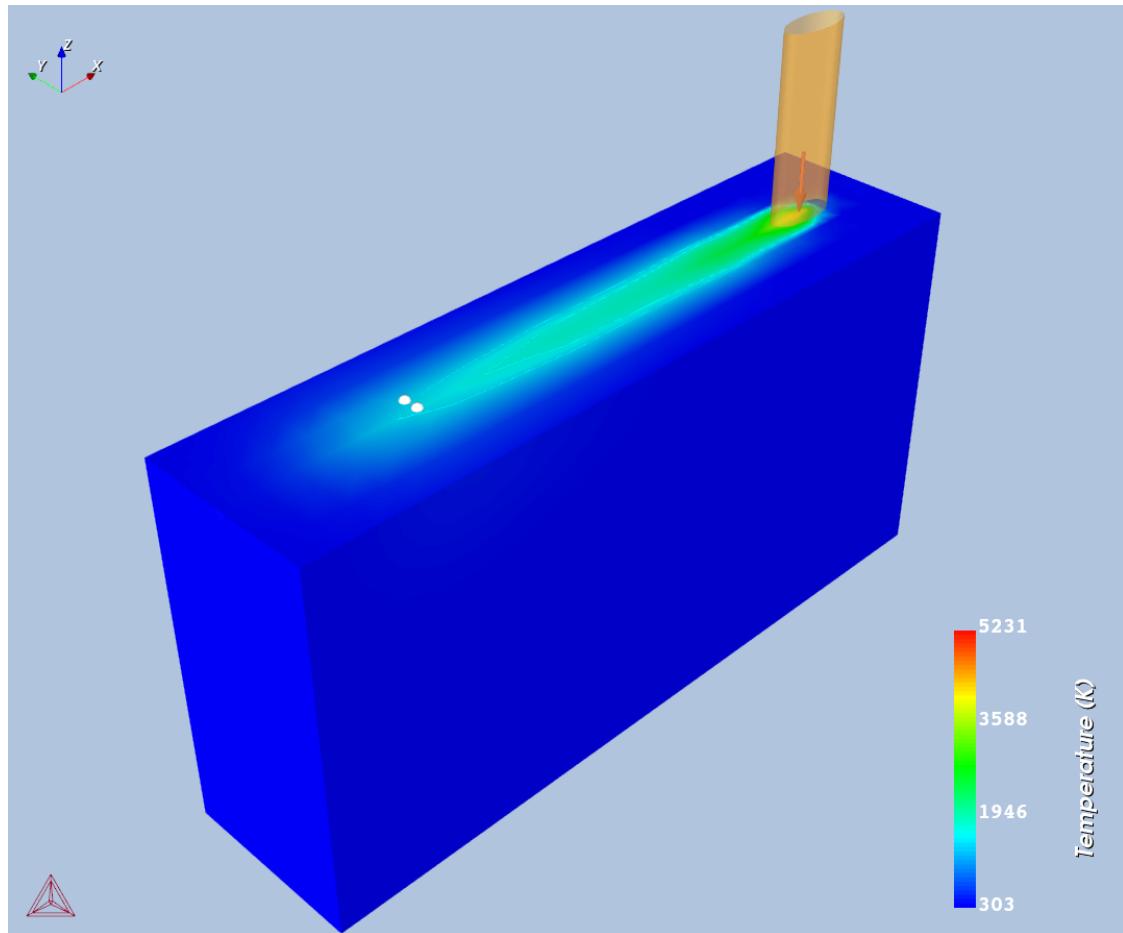
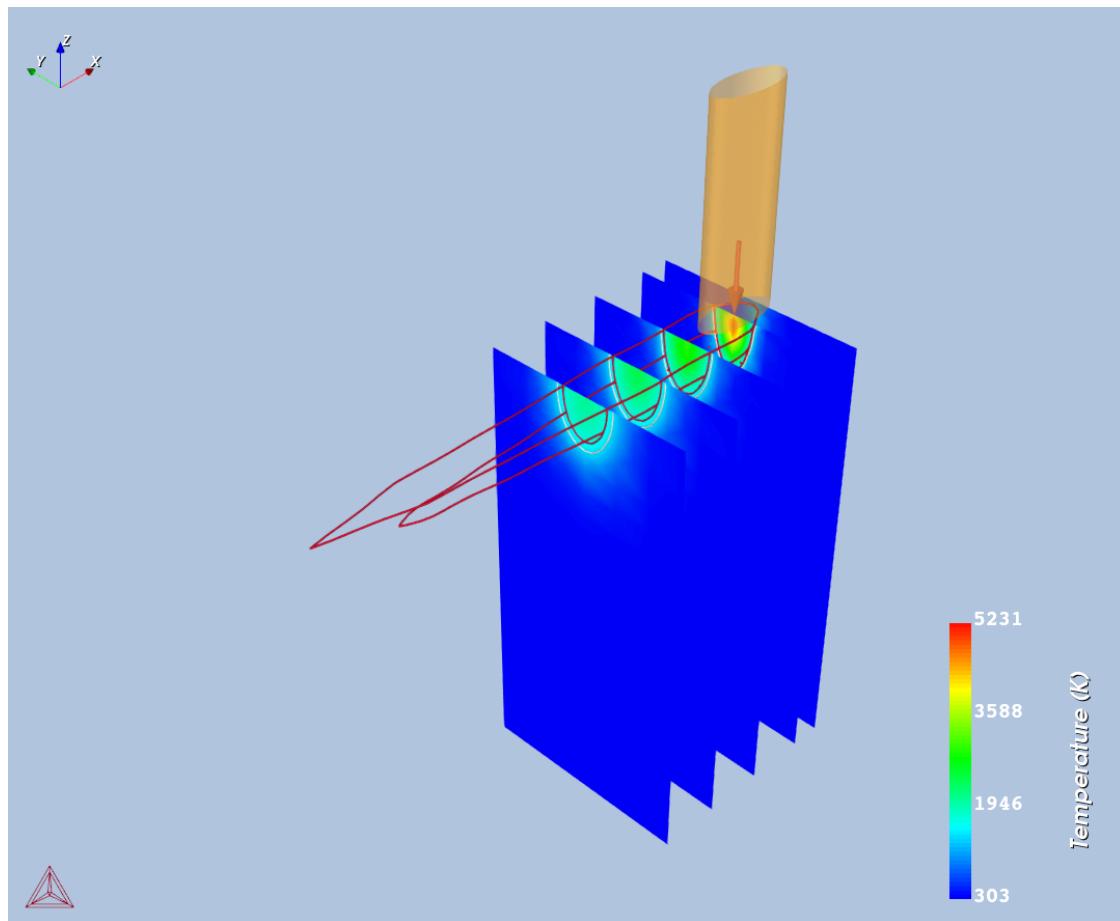


Figure 12: Surface plot of temperature distribution after the single track scan is completed. Probes P1 and P2 can also be seen on the top surface.

It is also possible to plot quantities at different cross-sections inside the domain by selecting the **Slice** checkbox on the Plot Renderer Configuration window under the 3D Plot tab. [Figure 13](#) shows the temperature slices plotted at cross-sections orthogonal to the scanning direction.



*Figure 13: Slices of the computational domain, orthogonal to the scanning direction, showing temperature distribution at different cross-sections. Red tubes show the contour of the melt pool (at liquidus temperature).*

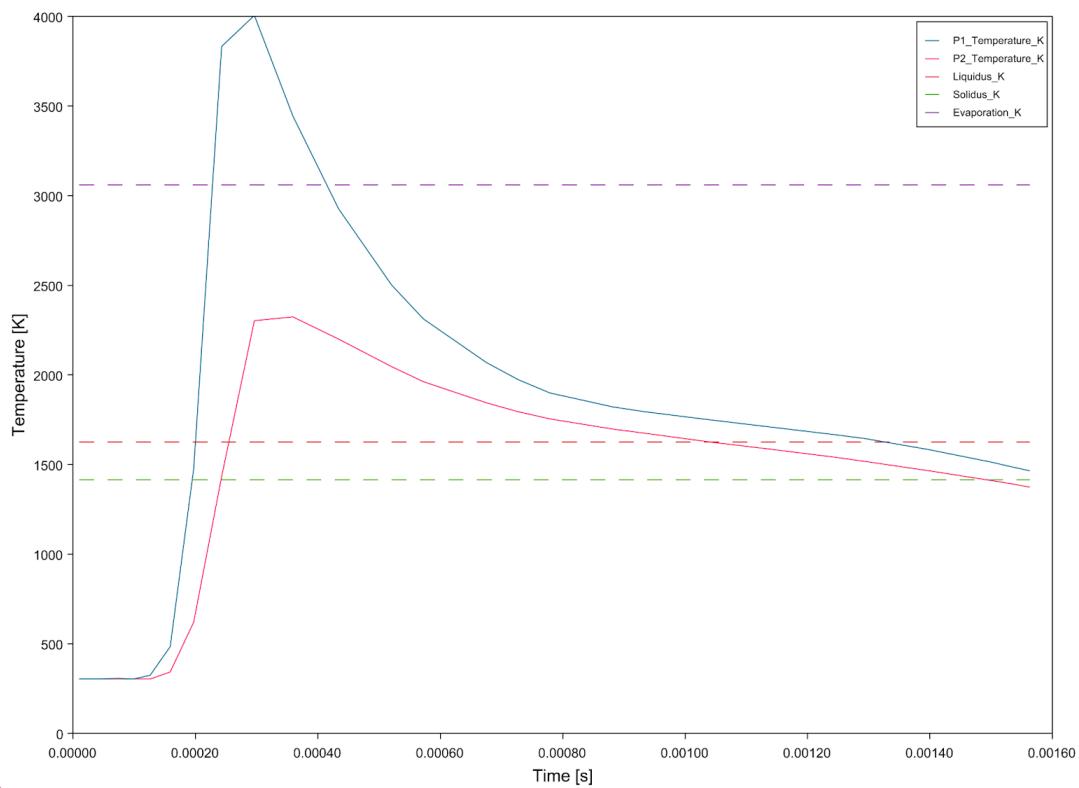


Figure 14: 2D probe plot showing temperature evolution as a function of time at probes P1 and P2.

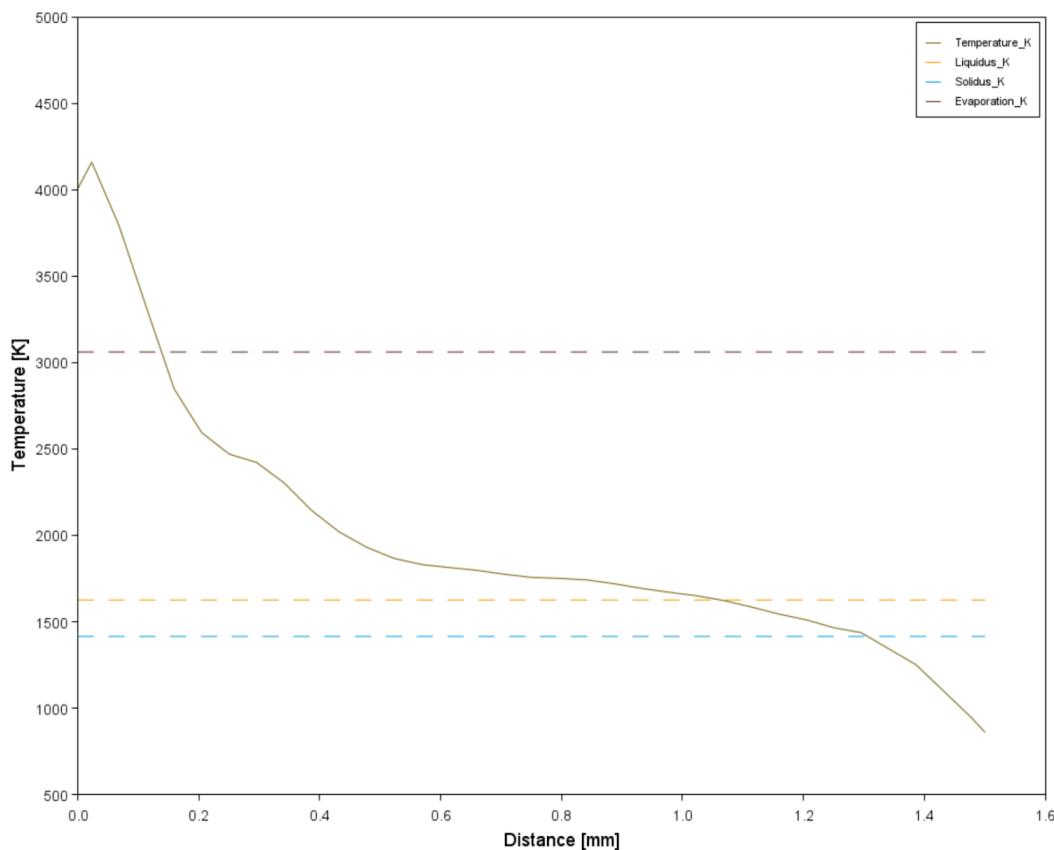


Figure 15: 2D plot over line showing temperature in the tail of the melt pool as a function of distance plotted along the scanning track.

## Other Resources



Read more about the [Additive Manufacturing \(AM\) Module](#) on our website. You can also use the [Getting Started Guide](#) to learn about the key features available.



Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the [website](#) or our [YouTube channel](#).

## AM\_02: Transient and Steady-state Simulations of a Single Track

The following example is part of a series showing some of the features of the Additive Manufacturing (AM) Module and the **AM Calculator**. This example builds on the work done by Grange et al. [2021Gra] and is similar to example AM\_01. The difference however is that in this example a single track simulation is performed using **Transient with heat source from Steady-state** model instead of the **Transient** model.

The **Transient with heat source from Steady-state** model exploits the assumption that the melt pool size and temperature distribution reaches a steady-state almost instantly and thus first solves for a **Steady-state** case with the given process parameters. The result from the **Steady-state** in the form of temperature distribution in the melt pool is then mapped as a heat source in the transient simulation. This novel approach is much faster and efficient than the approach used in example AM\_01 where the heat equation is solved in the entire 3D domain.



A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run three examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.



The first three examples (AM\_01, AM\_02, and AM\_03) use predefined Material Properties libraries that are embedded with the examples for use for all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO mode. See "Available Options" on page 7 for details.

### Project File Information

- Folder: Additive Manufacturing
- File name: *AM\_02\_TransientSS\_DE.tcu*

Open the example project file and click **Perform Tree** to generate the plots associated with it.



When you run (Perform) this example, it can take over two hours to complete the calculations.

## Material Properties

These properties are the same for both AM\_01 and AM\_02.

- Inconel 738LC: Ni-15.8 Cr-8.6 Co-2.7 W-3.3 Ti-3.6 Al-1.8 Ta-1.8 Mo-0.04 Fe-0.8 Nb-0.002 Mn-0.1 C Mass percent.
- Database: TCNI12
- The material property was pre-calculated, and stored as a built-in material library of the Additive Manufacturing (AM) Module.

## Reference

[2021Gra] D. Grange, A. Queva, G. Guillemot, M. Bellet, J.-D. Bartout, C. Colin, Effect of processing parameters during the laser beam melting of Inconel 738: Comparison between simulated and experimental melt pool shape. *J. Mater. Process. Technol.* 289, 116897 (2021).

## Model Configuration

The transient model solves for the heat equation in the entire 3D domain, including the melt pool, and is therefore, computationally expensive to solve. The fluid flow inside the melt pool due to the Marangoni effect is not included in this example. The double ellipsoidal, or the so-called Goldak heat source model, is used to predict melt pool size and temperature distribution during single track scanning. The parameters for the double ellipsoidal heat source are computed using optimization in a steady-state case for the given process parameters (power and scanning speed) and the melt pool size reported in the paper by Grange et al. [2021Gra]. The resulting parameters are shown in Figure 16.

A screenshot of the AM Calculator software interface. The 'Heat Source' section is highlighted. It shows the following parameters: 'Double ellipsoidal' selected from a dropdown menu, 'Power: 230.0 W', 'W Absorptivity: 88.06', '% ar: 97.3', 'μm af: 99.04', 'μm b: 41.67', 'μm c: 181.11 μm'. The input fields for power, absorptivity, and axis lengths have a light blue background, while the dropdown and other labels are white.

Figure 16: Optimized heat source parameters entered on the AM Calculator for the experiment given in Grange et al. [2021Gra] with power = 230 W and scanning speed = 960 mm/s.

The geometry for a transient simulation, as given in the paper by Grange et al. [2021Gra], is shown in Figure 17. The base plate is 2 mm in length, 0.5 mm in width, and with a thickness of 0.95 mm. A layer of powder with a thickness of 55  $\mu\text{m}$  is deposited on the solid substrate. The powder layer, however, has the same material properties as the solid substrate. The laser beam with a power of 230 W develops linear scanning with constant velocity 960 mm/s. The trajectory evolves from initial position  $(x, y) = (0.25, 0.25)$  mm to final position  $(1.75, 0.25)$  mm on the top surface.

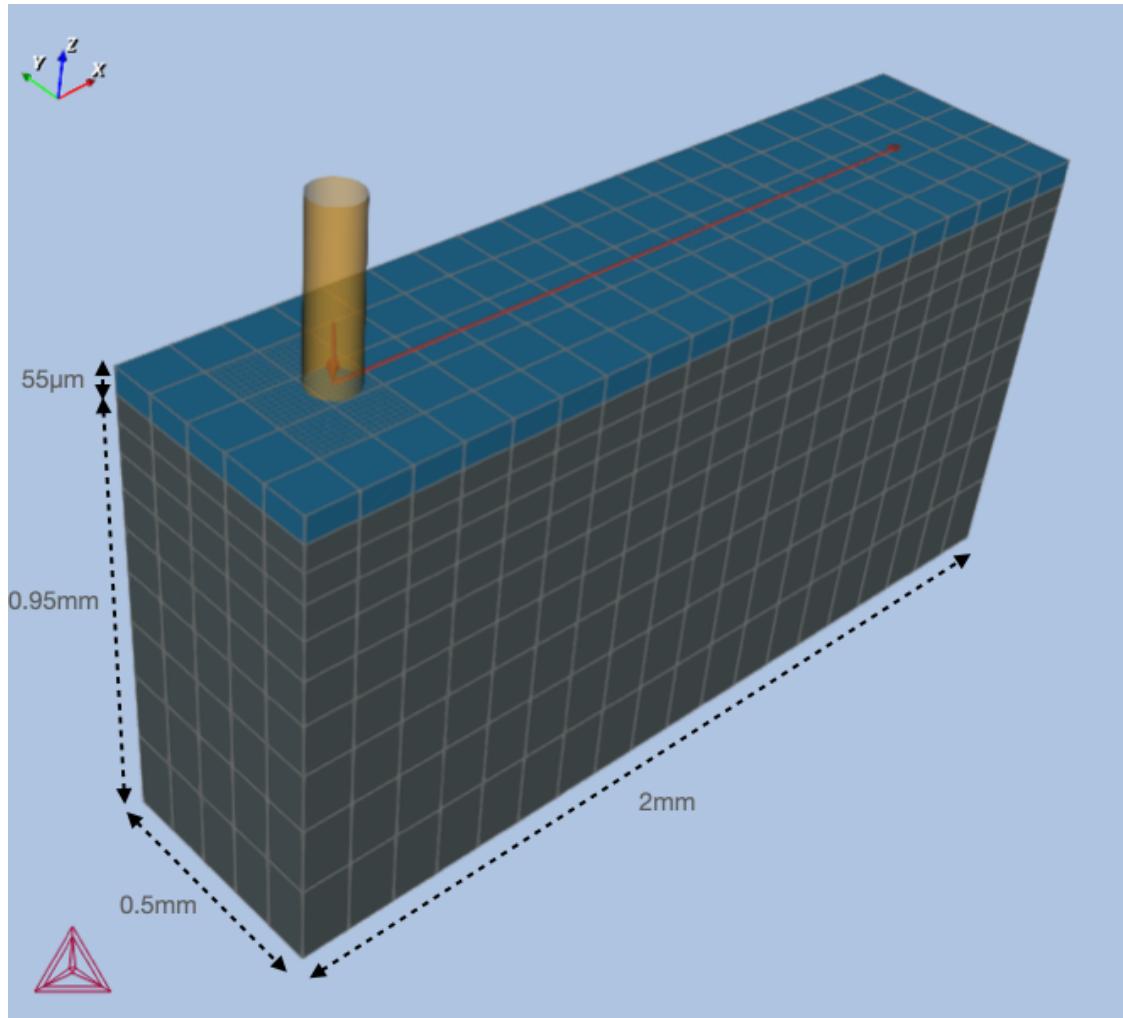


Figure 17: The geometry used for the Additive Manufacturing (AM) Module examples AM\_01 and AM\_02.

Two probes monitor the temporal evolution of temperature at positions shown in Figure 18. The results can be presented by tabulated data or as 2D graph plots.

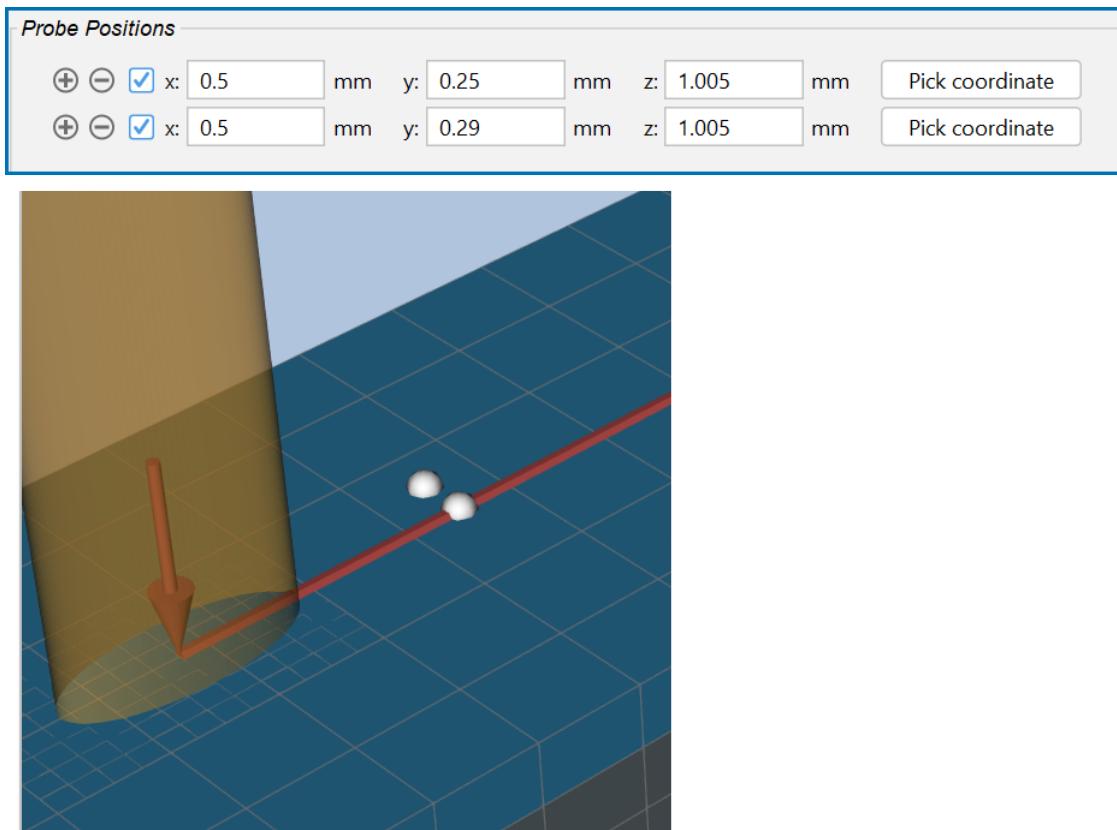


Figure 18: Probe positions for Probes P1 and P2, where P1 is placed exactly on the scanning track while P2 is placed at a distance of 0.04 mm from the track, as shown in a close up of the probes on the Visualizations window.

## Visualizations

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

- **Geometry:** View the geometry and adjust parameters visually by changing inputs on the Configuration window.
- Melt pool and other dynamically changing features can also be visualized and changed.
- **Plot 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, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

With the example open and after it is run, the following is a summary of what is visible on the **Visualizations** window.

Figure 19 shows the surface plot of temperature distribution after the single track scanning is completed. The temperature profile is qualitatively similar to the one in example AM\_01, however the maximum temperature is slightly lower in example AM\_02. This could be due to selection of a coarse mesh in both examples which sometimes could affect the maximum temperature.

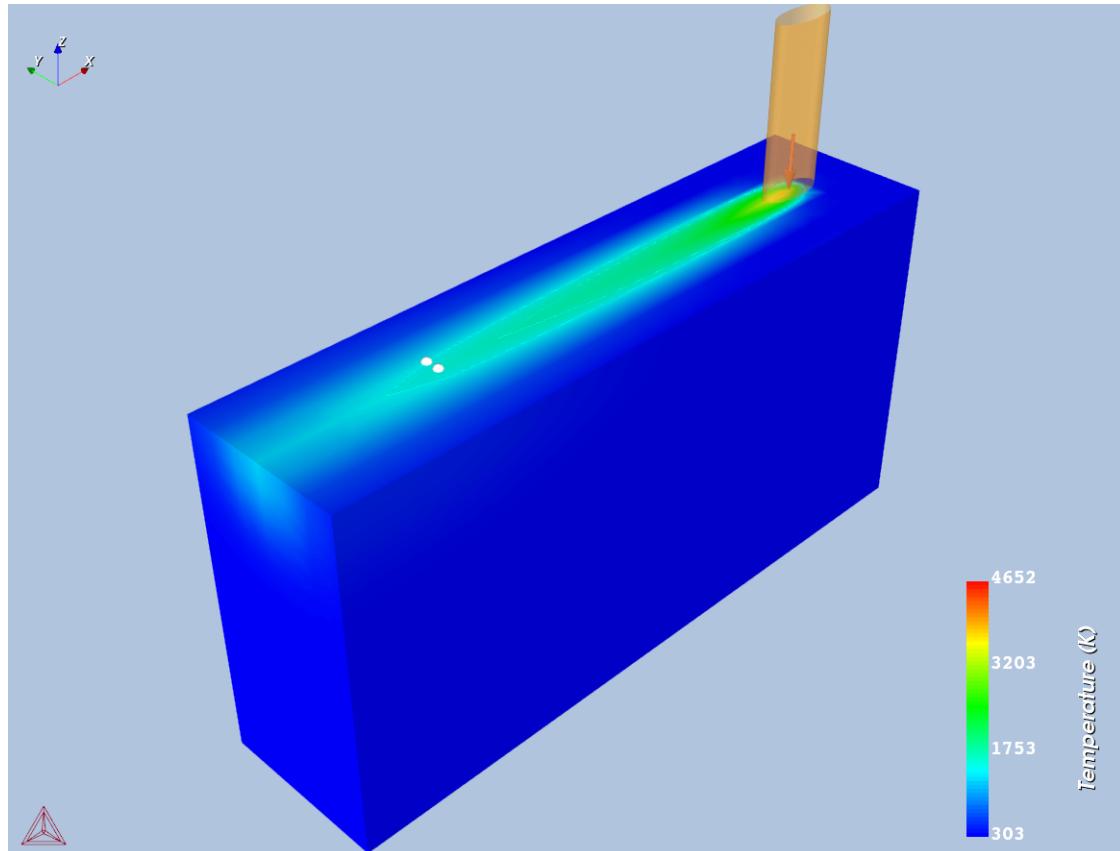
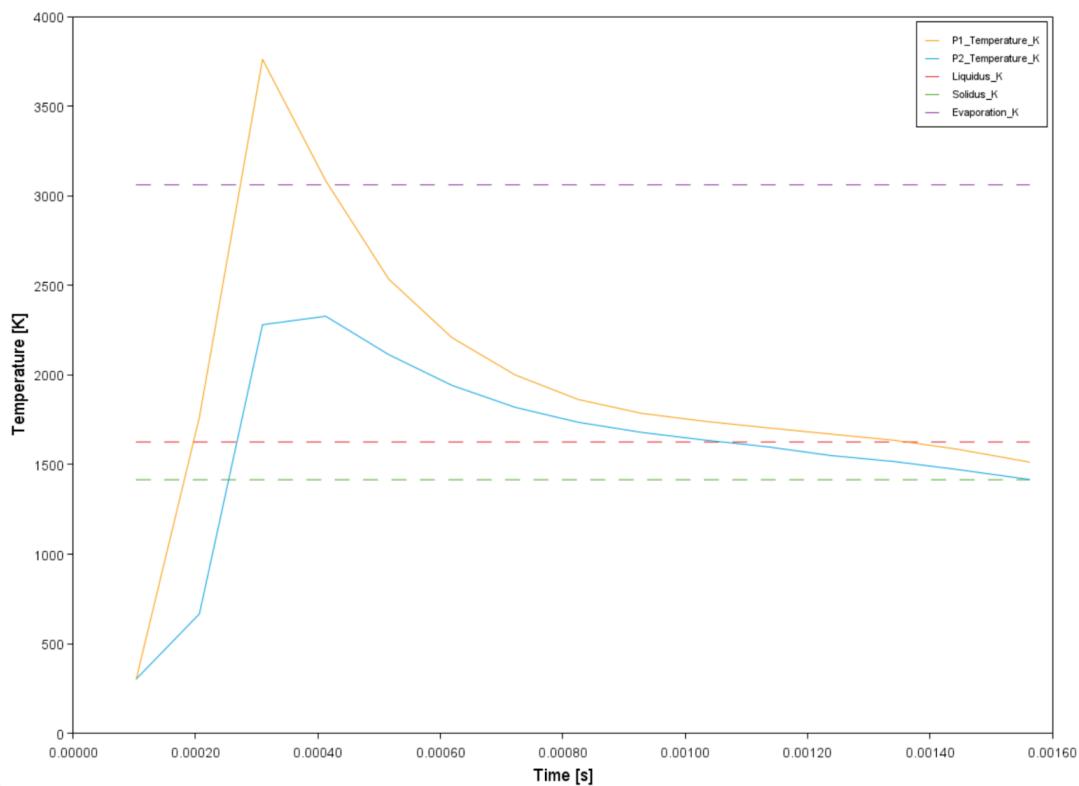


Figure 19: Surface plot of temperature distribution after the single track scan is completed. Probes P1 and P2 can also be seen on the top surface.

The melt pool dimensions for AM\_02 are given in the following table, which are very similar to the melt pool dimensions obtained in example AM\_01.

Melt Pool Dimension	Size (mm)
Width	0.127
Depth	0.129
Length	1.12

A qualitative comparison between AM\_01 and AM\_02 can also be made by looking at probe plots. The probe plot for AM\_02 is given in [Figure 20](#).



*Figure 20: 2D probe plot showing temperature evolution as a function of time at probes P1 and P2.*

Despite the fact that maximum temperature is higher in AM\_01, the temperature profile in the tail of the melt pool and close to the melt pool is very similar. This can also be concluded by comparing plot over lines for the two examples, where the plot over line for AM\_02 is given in [Figure 21](#).

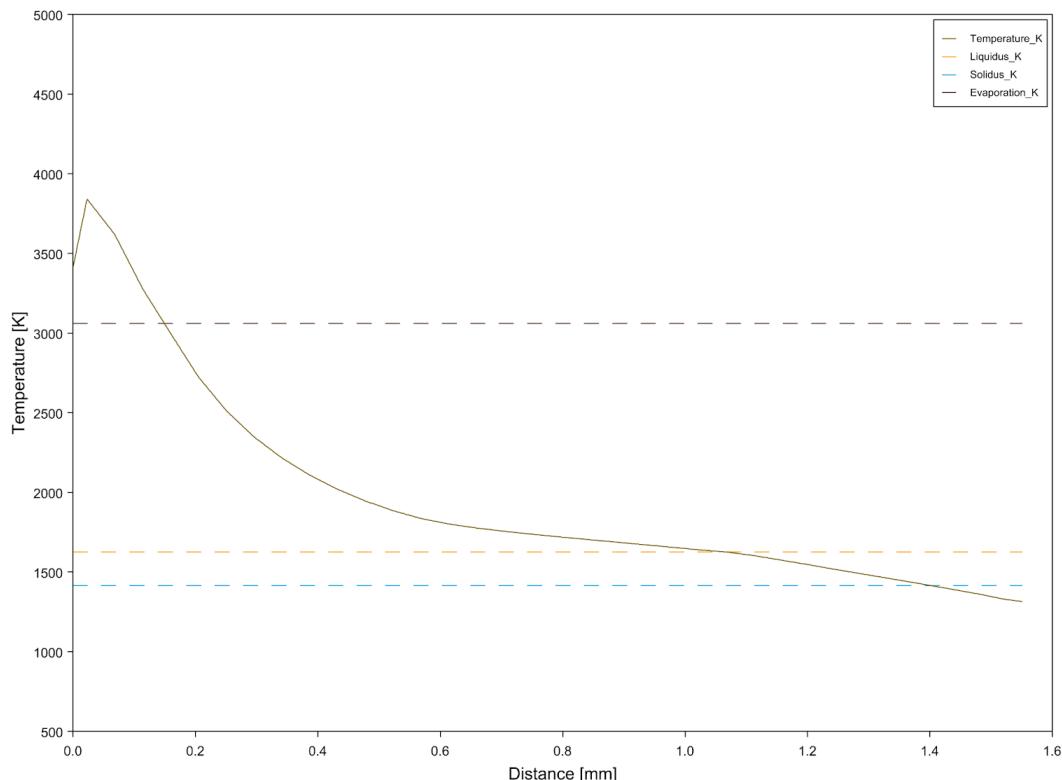


Figure 21: 2D plot over line showing temperature in the tail of the melt pool as a function of distance plotted along the scanning track.

## Other Resources



Read more about the [Additive Manufacturing \(AM\) Module](#) on our website. You can also use the [Getting Started Guide](#) to learn about the key features available.



Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the [website](#) or our [YouTube channel](#).

## AM\_03: Steady-state Simulations

The following example is part of a series showing some of the features of the Additive Manufacturing (AM) Module and the **AM Calculator**.



A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run three examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.



The first three examples (AM\_01, AM\_02, and AM\_03) use predefined Material Properties libraries that are embedded with the examples for use for all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO mode. See "["Available Options" on page 7](#) for details.

In this example steady-state simulations are performed for IN625 with different conditions i.e.

- i. without fluid flow in the melt pool,
- ii. with fluid flow in the melt pool due to Marangoni effect, and
- iii. using separate material properties for the powder.

and then the results are compared to demonstrate the effects of fluid flow and separate material properties for the powder on the temperature distribution as well as on the shape of the melt pool.



For the first two simulations, the same material properties are used for both powder and solid substrate while for the third simulation no fluid flow is included in the melt pool.



In steady-state simulations it is assumed that the heat source (laser beam) moves with a uniform speed relative to the base plate. In this case, the model is solved by modifying governing equations to a reference frame attached to a moving heat source. Furthermore, in steady-state mode you can make use of symmetry along the width of the geometry and solve for only half of the domain.

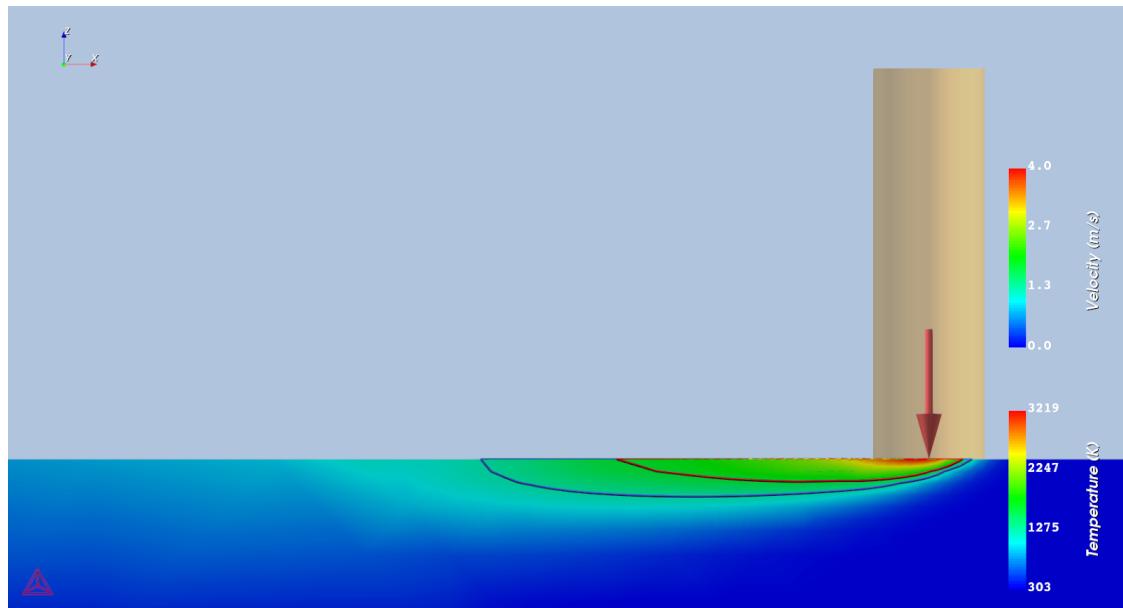
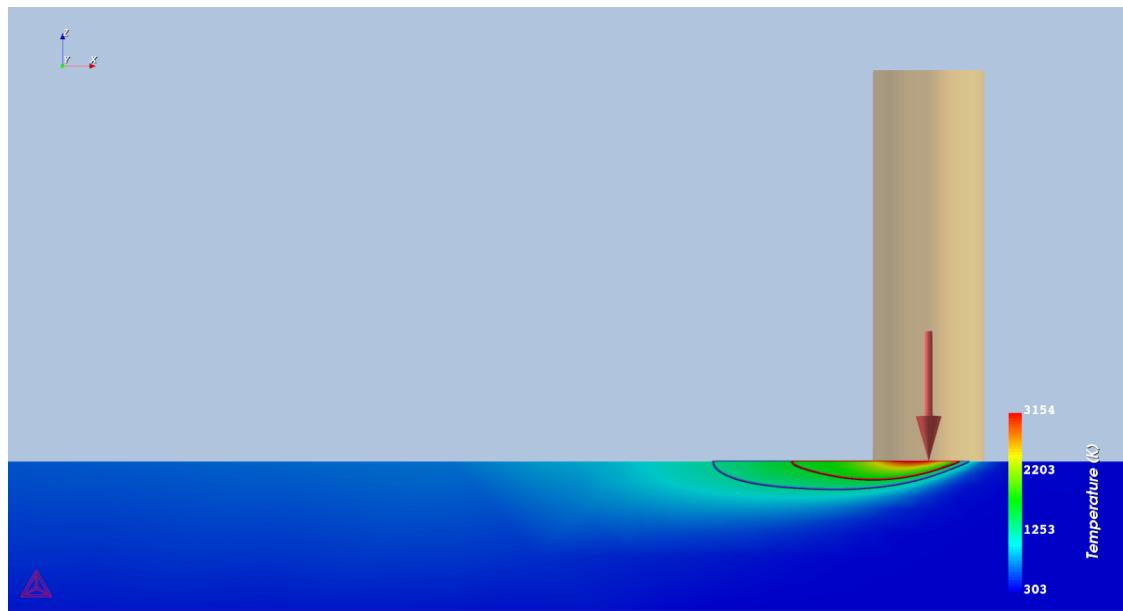
## Project File Information

- Folder: Additive Manufacturing
- File name: *AM\_03\_Steady.tcu*



When you run (Perform) this example, it takes a few minutes for the calculations to complete.

## ***Results Discussion***



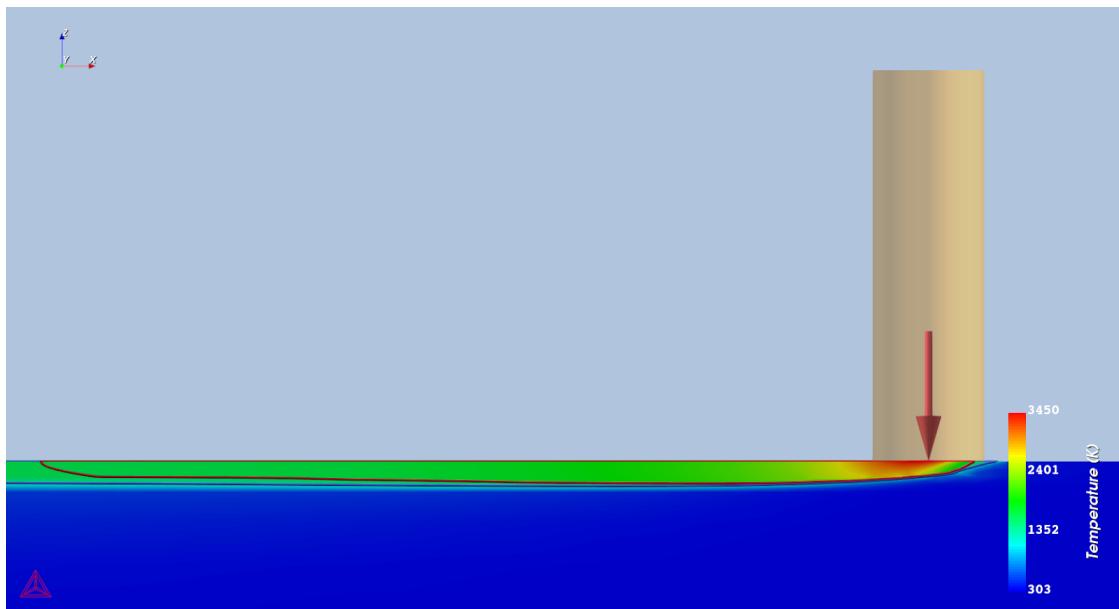


Figure 22: A comparison of the melt pool depth for different simulation conditions; (top) without fluid flow, (middle) with fluid flow in the melt pool and (bottom) with different material properties for the powder layer. Isocontours show the boundaries of (inner) melt pool and (outer) mushy zone.

The table shows a comparison of the melt pool dimensions for different simulation conditions.

Simulation set up	Melt Pool Dimensions (mm)		
	Width	Depth	Length
Without fluid flow	0.156	0.032	0.300
With fluid flow	0.188	0.040	0.619
Separate powder material properties	0.250	0.039	1.670

Figure 22 shows the effect of fluid flow on temperature distribution and size of the melt pool for the given process parameters. A quantitative comparison is also given in the table. It can be seen that with the addition of fluid flow due to gradient in surface tension (Marangoni effect), the melt pool tends to increase its dimensions in all three directions. This is because the negative gradient in surface tension with respect to the temperature creates an outward flow on the surface of the melt pool which consequently increases the width and length of the melt pool, as shown in Figure 23.

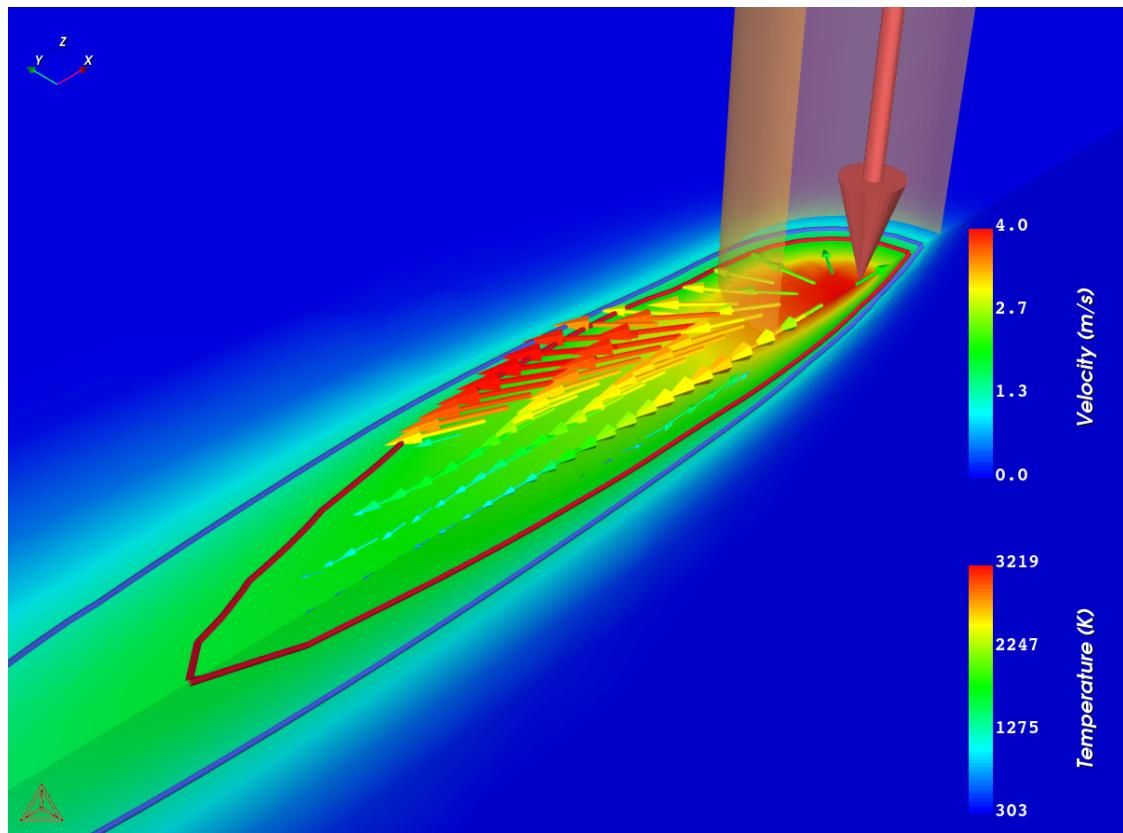


Figure 23: Vectors showing flow field in the melt pool due to gradient in surface tension. The colours of the vectors represent the magnitude of the velocity. Surface colormap shows the temperature distribution.

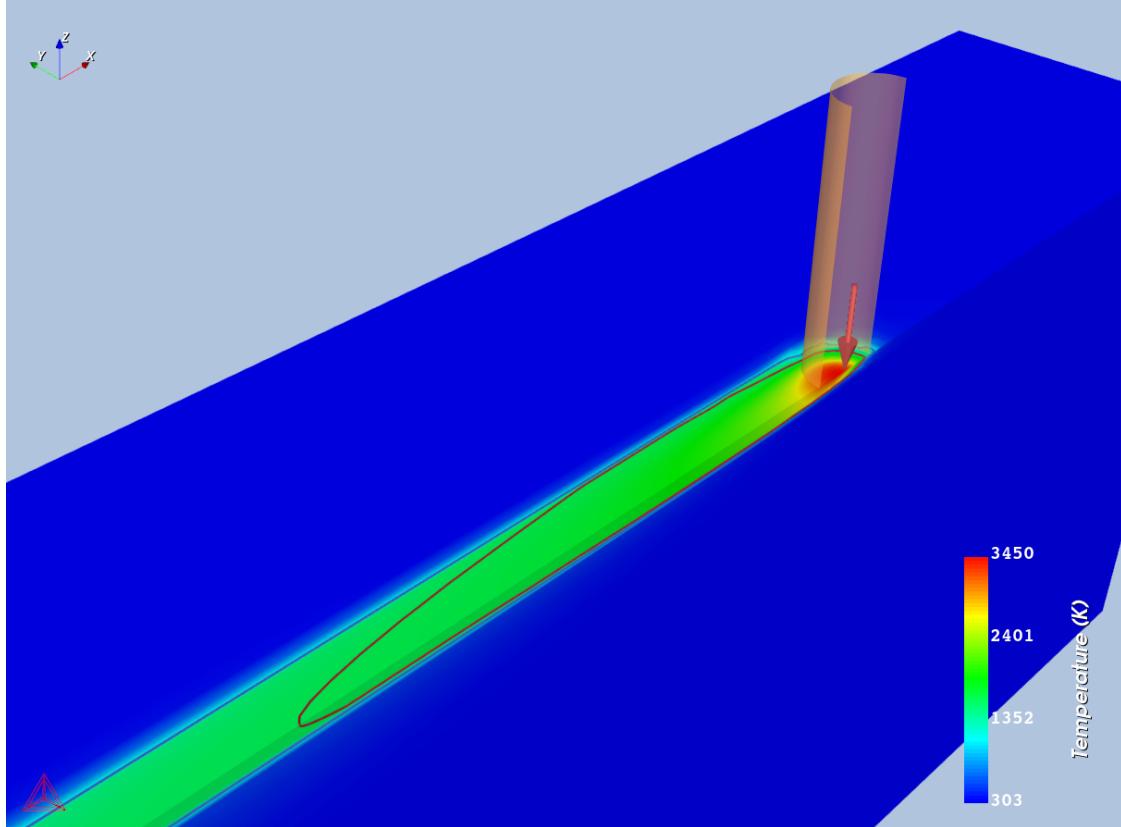
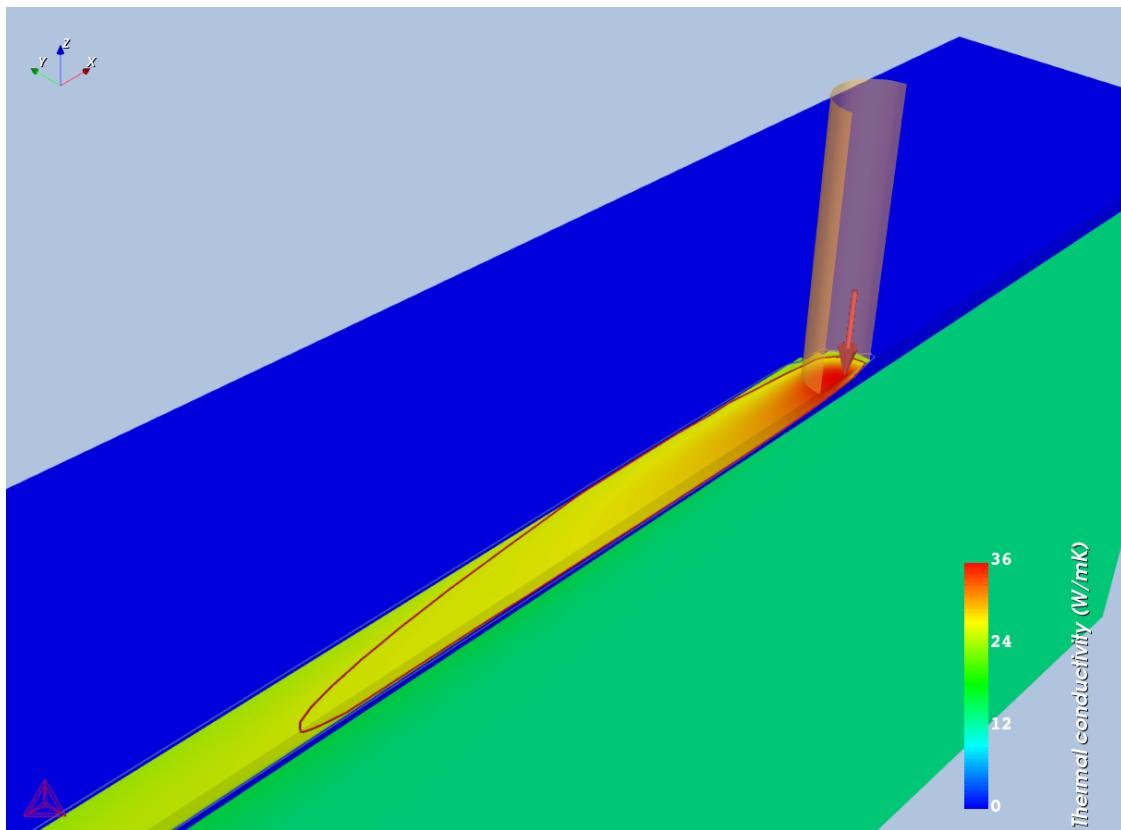


Figure 24: (top) Surface colormap of temperature dependent thermal conductivity showing different values in powder and liquid/solid and (bottom) the corresponding temperature distribution.

Using separate material properties for powder has a significant effect on both the temperature distribution and the size of the melt pool. This is because a lower thermal diffusivity in the powder makes the temperature to diffuse more towards the length of the melt pool hence causing a significant increase in the length of the melt pool (shown in Figure 24) as compared to the first two cases. There is also an obvious increase in the width of the melt pool while the depth of the melt pool is almost the same as with the fluid flow. Furthermore, the maximum temperature is also highest in the case with separate material properties.

## Visualizations

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

- **Geometry:** View the geometry and adjust parameters visually by changing inputs on the Configuration window.
- Melt pool and other dynamically changing features can also be visualized and changed.
- **Plot** 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, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

## Other Resources



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## AM\_04: Scheil Transient Steady-state

In this example, three different simulations are performed: Steady-state, Transient Single track, and Transient Multilayer. Both Transient\_Single track and Transient\_Multilayer use **Transient with heat source from Steady-state** model to compute time-dependent temperature distribution in the given geometry. The primary difference between this example and the previous examples (AM\_01 to AM\_03) is that, in this case, the material properties data is retrieved from the Scheil Calculator whereas in the previous examples the material properties are taken from the preinstalled material library. Furthermore, this example simulates scanning of two layers of powder where the second layer is spread on the top of the first layer when scanning of the first layer is completed.



Material chosen for this example is Ti-6Al-4V. To run this example requires both version TCTI5.0 and newer of the TCS Ti/TiAl-based Alloys Database (TCTI) in addition to a license for the Additive Manufacturing (AM) Module. Some portions of this example are also covered in the [Getting Started Guide](#) on our website.

### Project File Information

- Folder: Additive Manufacturing
- File name: *AM\_04\_Scheil\_TransientSS.tcu*

Open the example project file and click **Perform Tree** to generate the plots associated with it.



When you run (Perform) this example, it takes several hours to complete the calculations.

### Visualizations

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

- **Geometry:** View the geometry and adjust parameters visually by changing inputs on the Configuration window.
- Melt pool and other dynamically changing features can also be visualized and changed.

- **Plot 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, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

## ***Steady-state***

The Steady-state calculator of this example computes temperature distribution in a steady state for the power of 100W and scanning speed of 600mm/s. The beam radius in this example is taken as 100 $\mu\text{m}$ . For the geometry, the steady-state model only needs the height of the solid substrate as the input, which is taken as 2.0mm. The solid substrate is covered with a powder layer of thickness 55 $\mu\text{m}$ . This example also takes into account the effect of fluid flow due to Marangoni forces inside the melt pool.

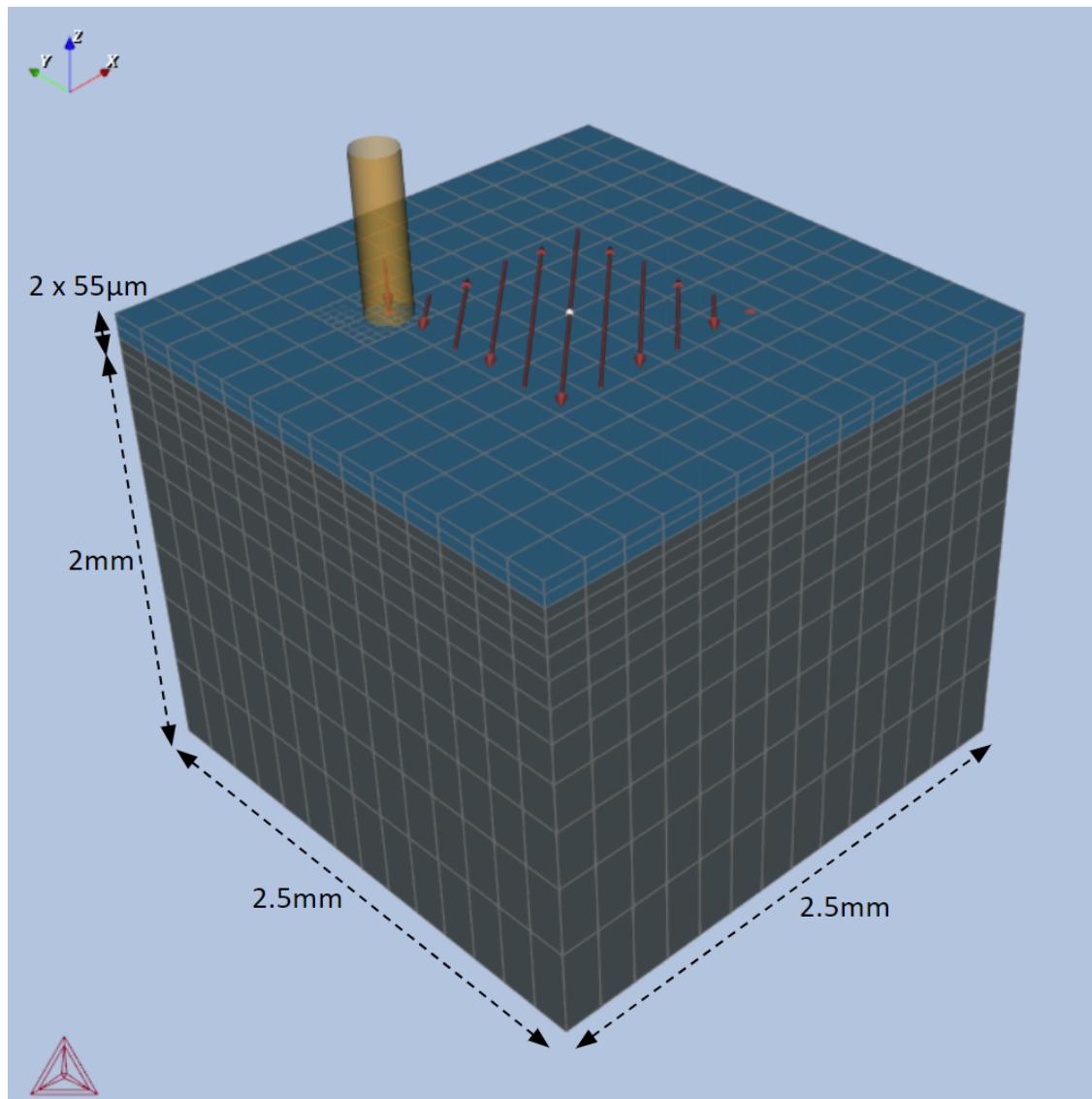


Figure 25: Geometry definition for Transient Multilayer. The scanning strategy shows the scanning pattern on the top most layer.

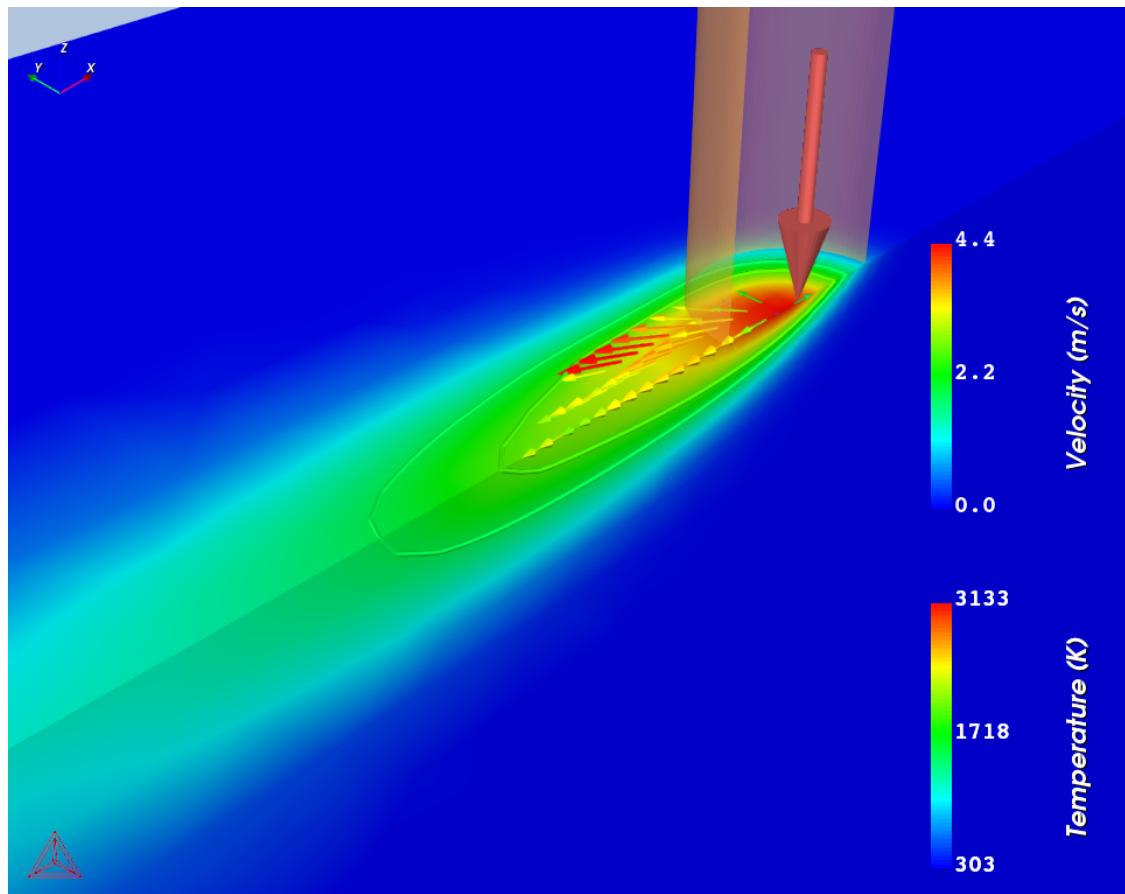


Figure 26: Temperature distribution around the melt pool and mushy zone for the Steady-state case. Velocity vectors representing the fluid flow inside the melt pool can also be seen.

## Transient Single Track

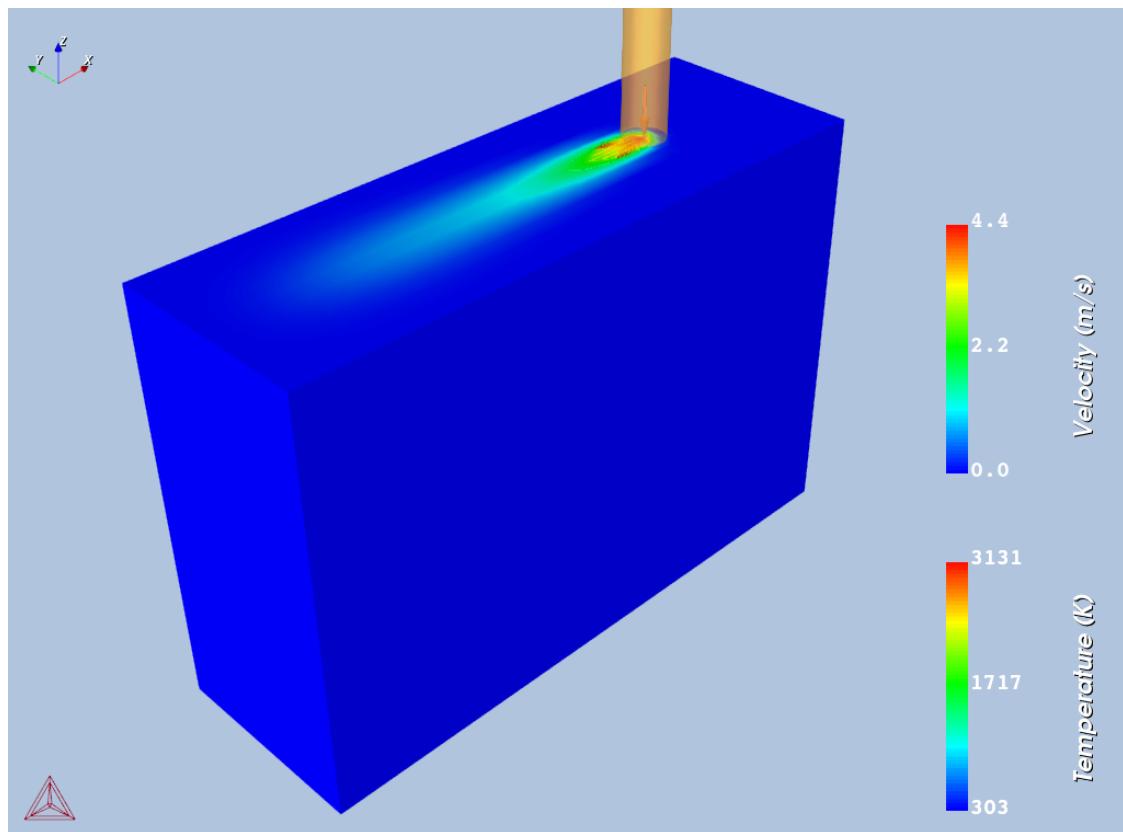


Figure 27: Surface colormap showing temperature distribution at the end of single track transient simulation. The velocity vectors around the heat source show the direction of fluid flow in the melt pool.

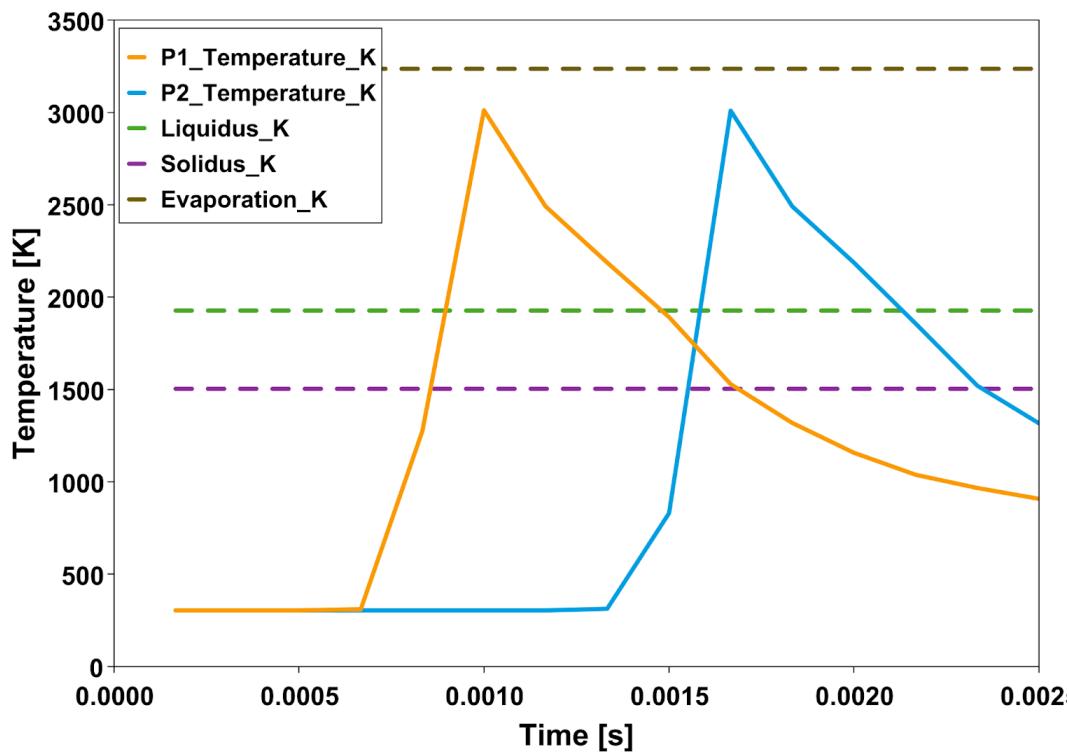


Figure 28: 2D Plots showing temperature as a function of time from Probe 1 (orange) and Probe 2 (blue) after the single track scan is completed.

## Transient Multilayer

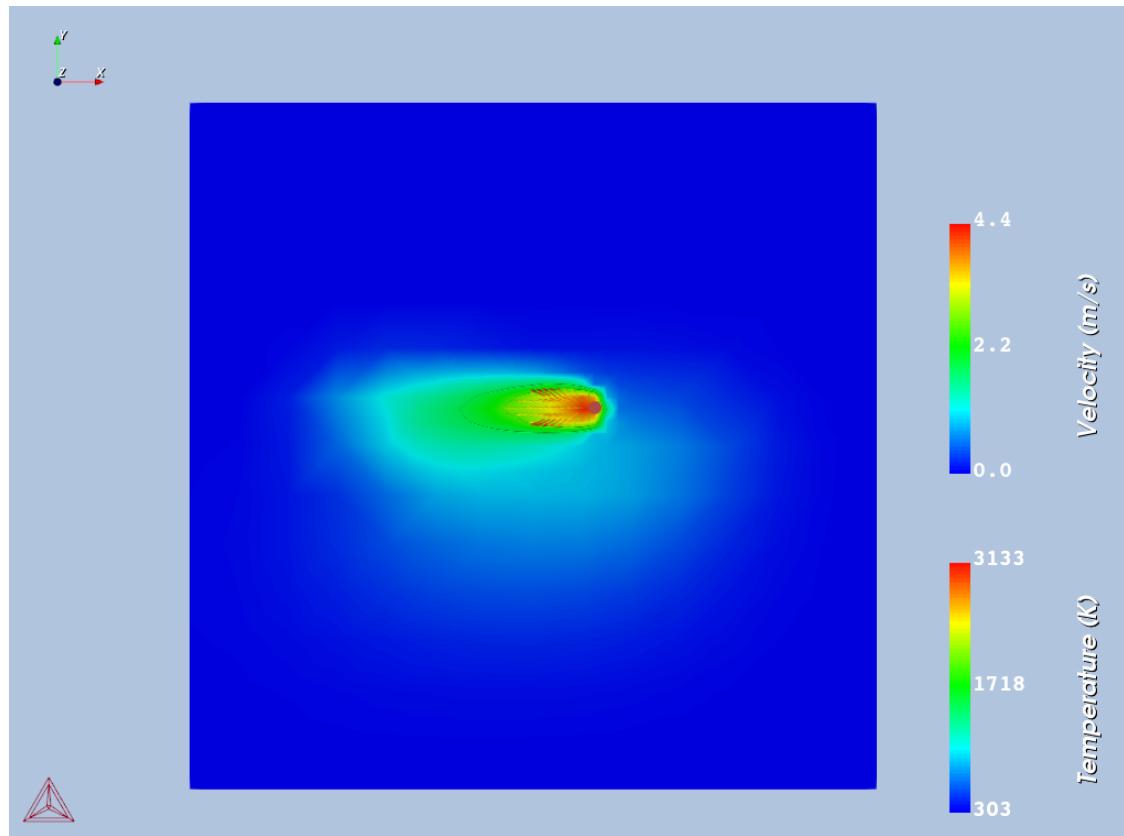


Figure 29: Temperature distribution on the top surface of the workpiece during scanning of the first layer.

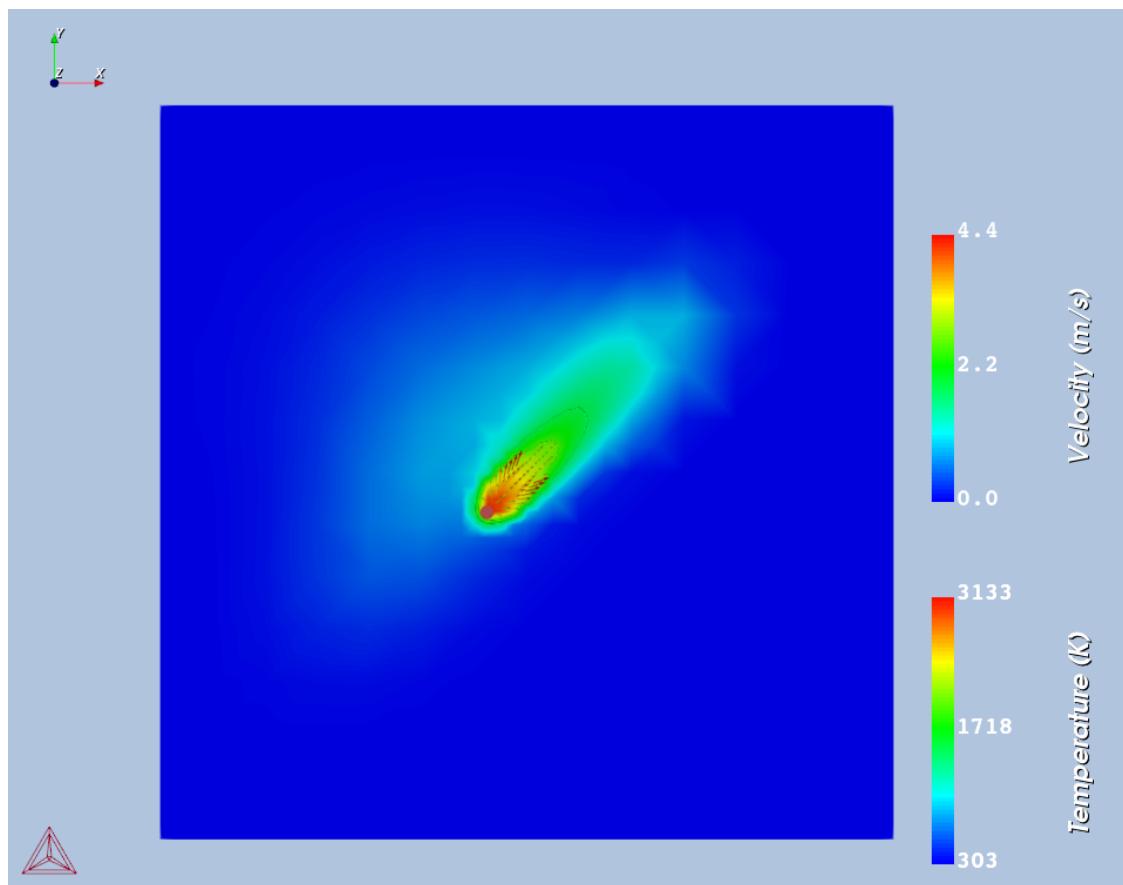


Figure 30: Temperature distribution on the top surface of the workpiece during scanning of the second layer.

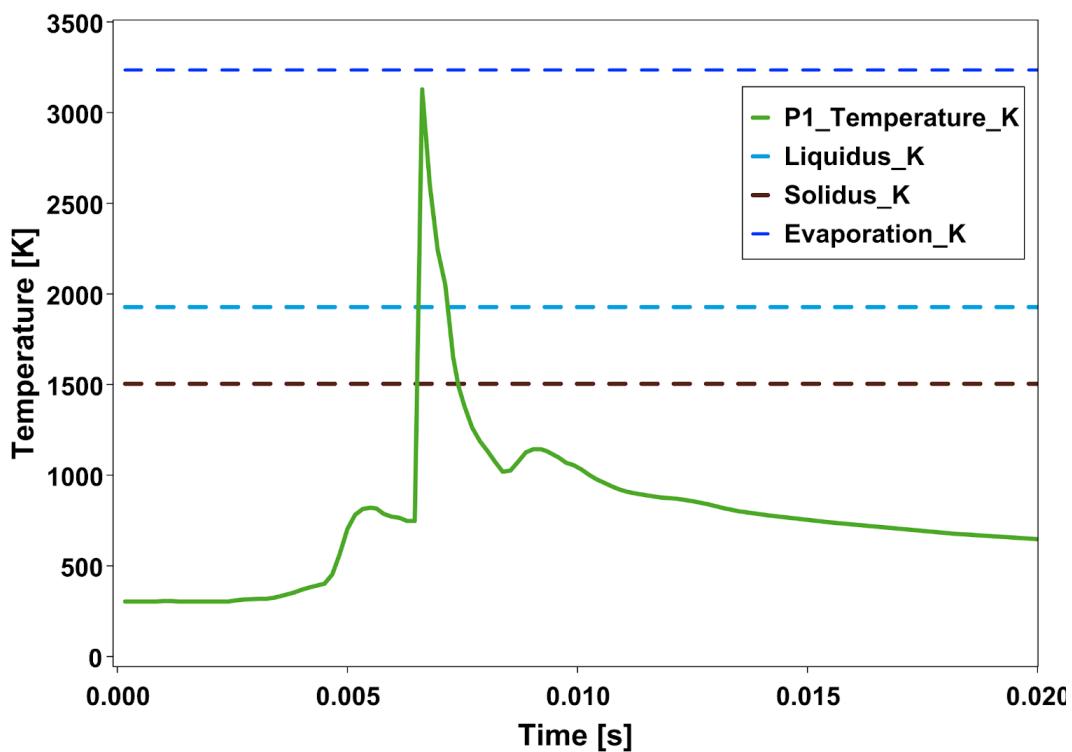


Figure 31: 2D Plots showing temperature as a function of time from Probe 1 after scanning the first layer.

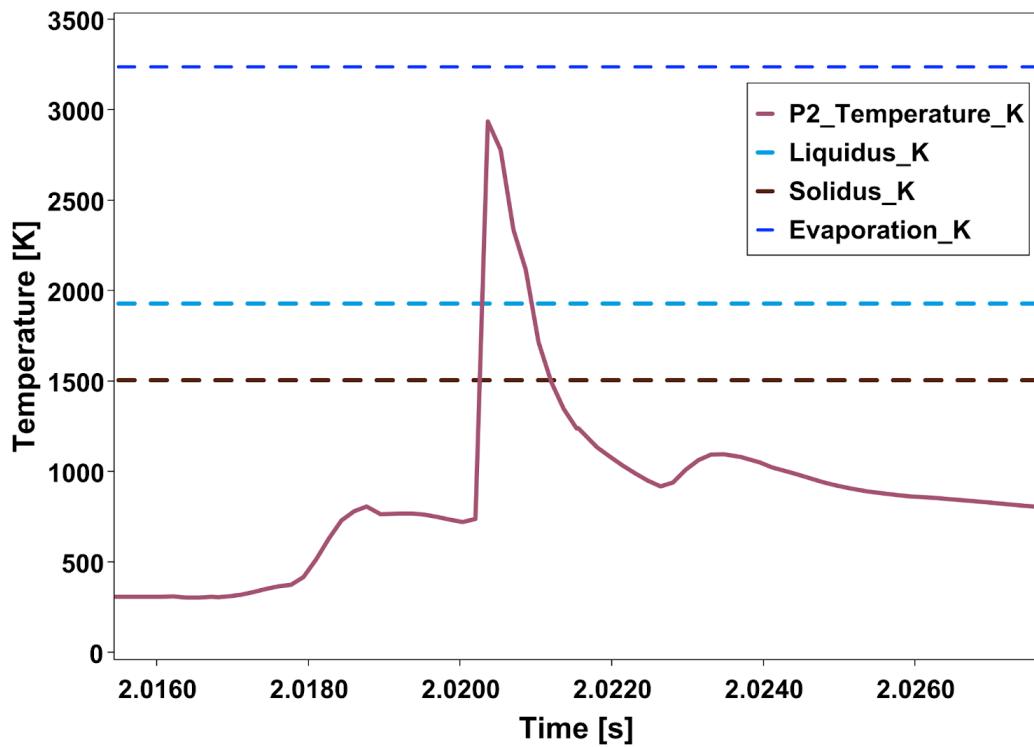


Figure 32: 2D Plots showing temperature as a function of time from Probe 2 after scanning the second layer.

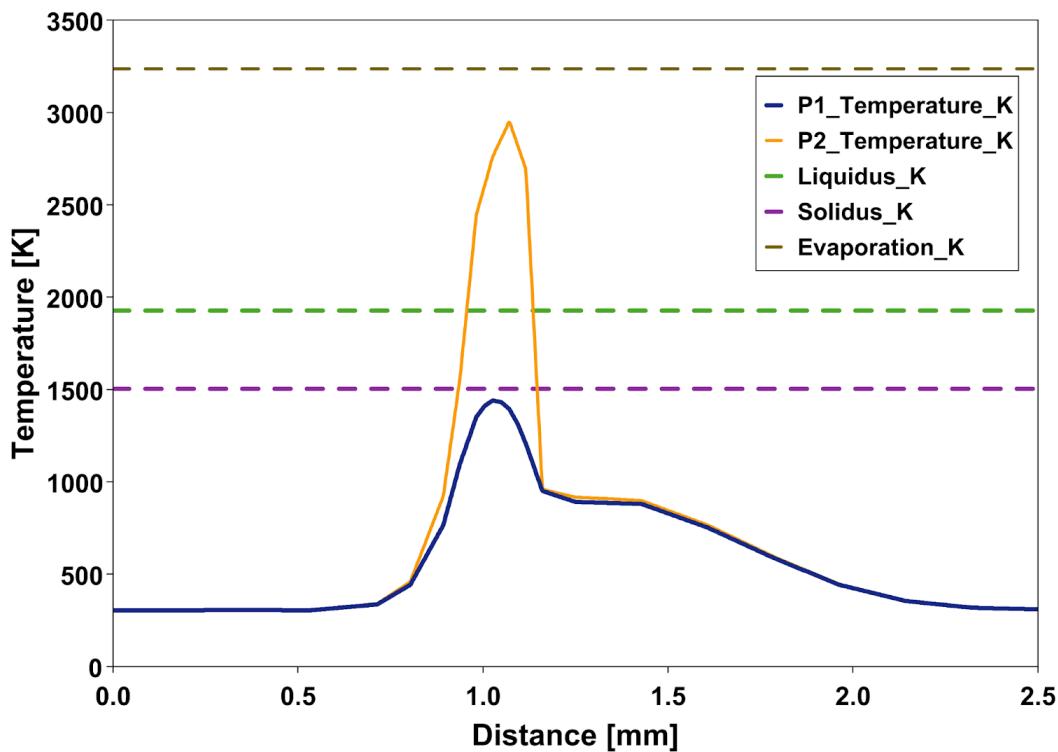


Figure 33: 2D Plot over line showing temperature profiles plotted along the lines, parallel to the width of the geometry placed on the top of the first layer (P1) and the second layer (P2).

## AM\_05: Using AM Calculator Probe Data with the Diffusion Module (DICTRA)

The microstructure of a hot-work tool steel additively manufactured using laser powder-bed fusion (L-PBF) is studied in detail by microstructure characterization and computational thermodynamics and kinetics by C.-Y. Chou et al. [2021Cho].

This example demonstrates the application of adding probes to an AM Calculator and then using this data via the Thermal Profile that is set up on a connected Diffusion Calculator. The example also uses a Scheil Calculator to collect some materials data that is then further used with the AM Calculator prior to using the probe data generated by the AM Calculator.



A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. This example also requires a license for the Diffusion Module (DICTRA), plus additional database licenses for the TCS Steel and Fe-alloys Database (TCFE) (TCFE13 and newer), and the TCS Steels/Fe-Alloys Mobility Database (MOBFE) (MOBFE8 and newer).

### Project File Information

- Folder: Additive Manufacturing
- File name: *AM\_05\_AM\_Probe\_to\_Diffusion.tcu*

Open the example project file and click **Perform Tree** to generate the plots associated with it.



When you run (Perform) this example, it takes several hours to complete the calculations.

### Background

According to the thermodynamics of this steel,  $\delta$ -ferrite is the solid phase stable at the highest temperature and would be the first solid phase to form during solidification from a thermodynamic point of view, see [Figure 34](#).

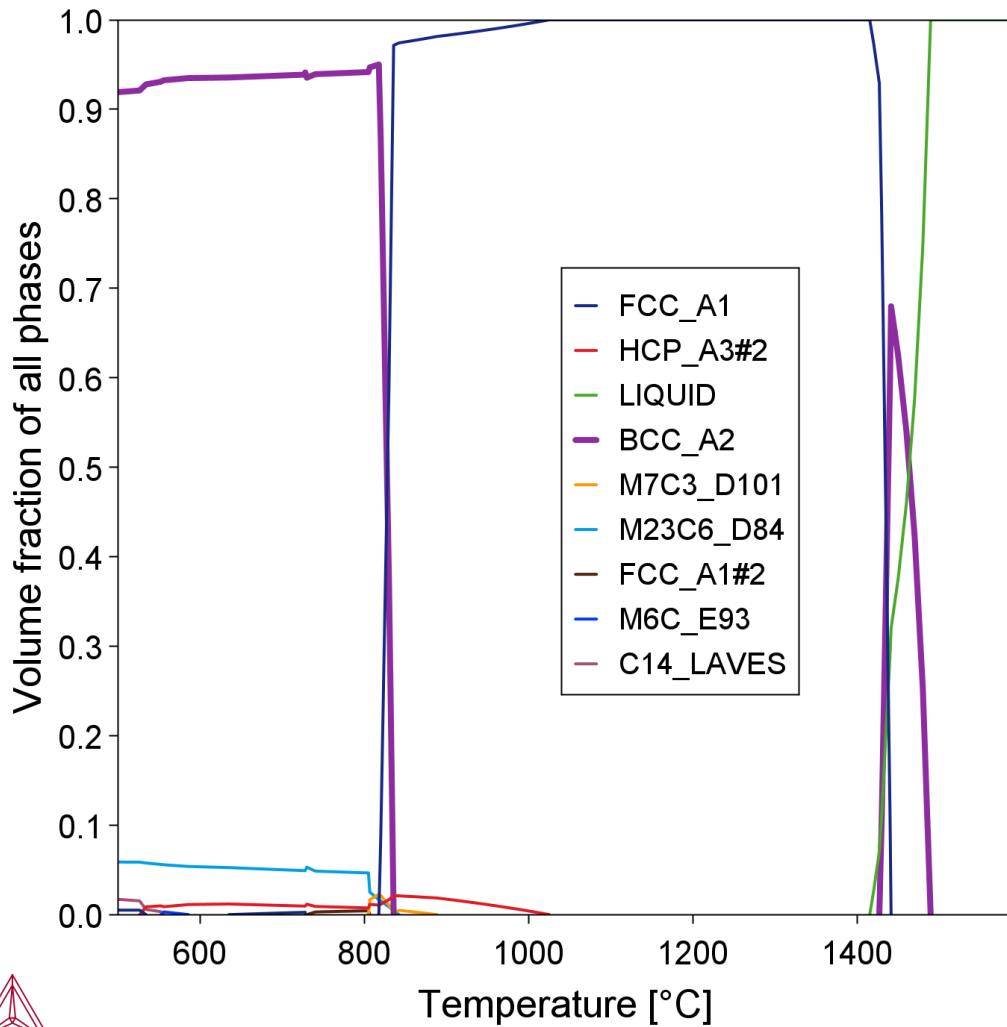


Figure 34: Equilibrium property diagram calculated in Thermo-Calc of the tool steel showing  $\delta$ -ferrite would be the first solid phase to form during solidification according to equilibrium.

However, the high solidification and cooling rates during the L-PBF process lead to suppression of  $\delta$ -ferrite and instead solidification of an austenite phase directly containing a cellular substructure where the alloying elements have segregated to the inter-cellular regions.

The microsegregation can be predicted by reducing the complex solidification behavior to a diffusion problem in one dimension enabling comparisons with the measured segregation profiles quantified at a nanometer scale.

## Configuration and Calculation Set Up

For all calculations, the simplified composition Fe-0.35C-4.93Cr-0.45Mn-2.24Mo-0.25Si-0.54V (mass%) was used with  $\delta$ -ferrite suspended on the System Definer.

The **Additive Manufacturing** template was used to first add the System Definer, Scheil Calculator, AM Calculator and Plot Renderer to the Project window tree. Additionally, a Diffusion Calculator was added as a successor to the AM Calculator in order to automatically import the time-temperature profile from the AM simulation into the diffusion simulation. See [Figure 35](#) (or refer to the example if you have it open) to see the layout.

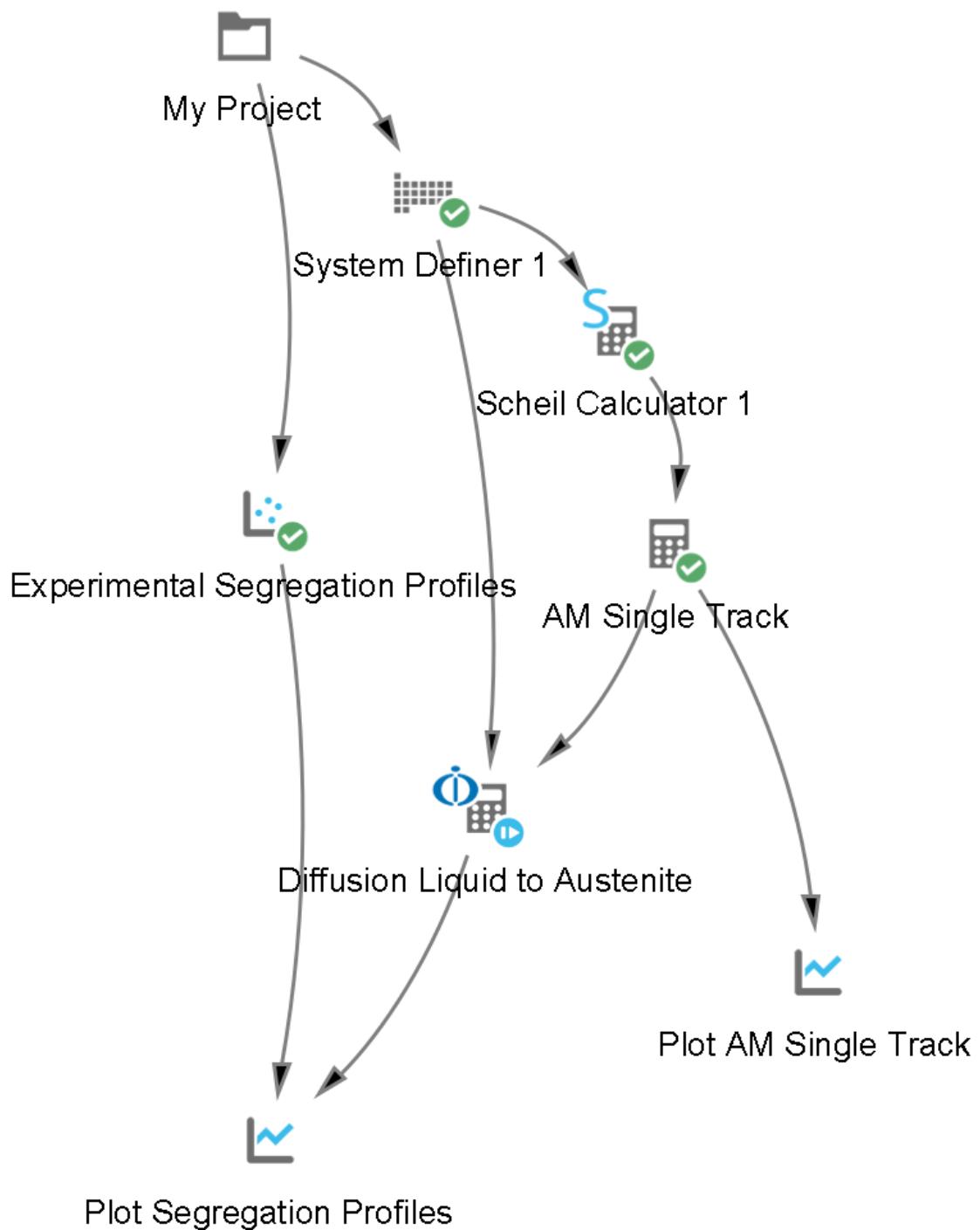
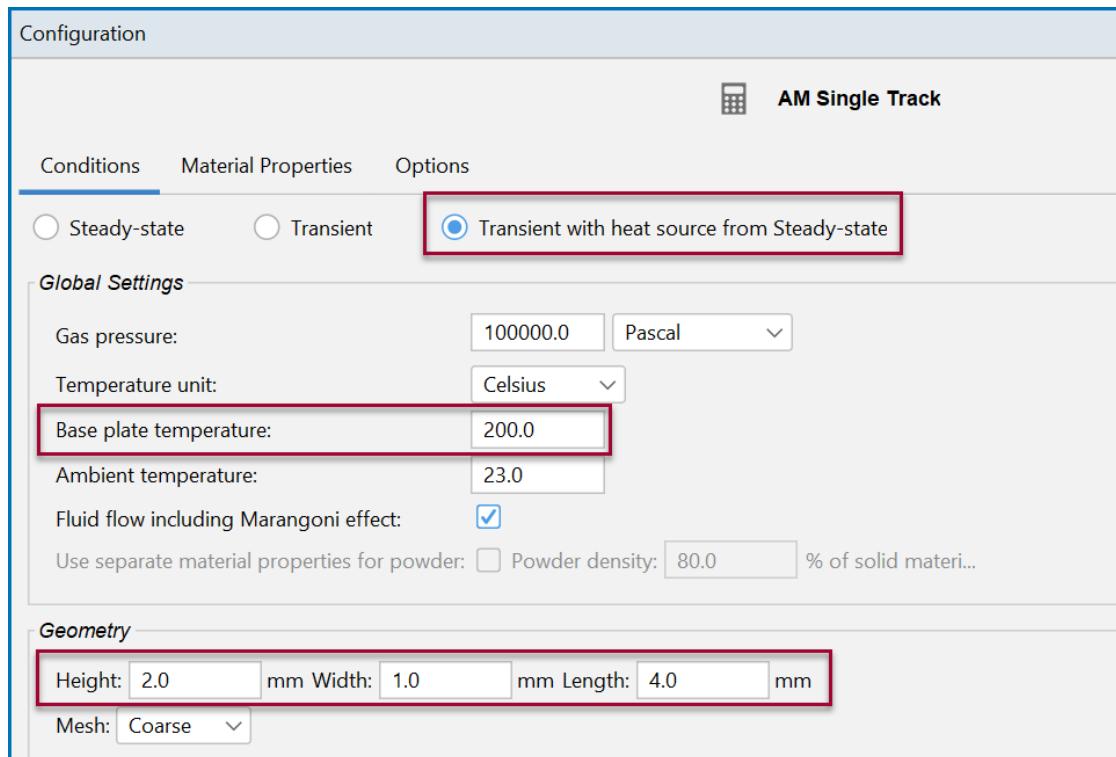


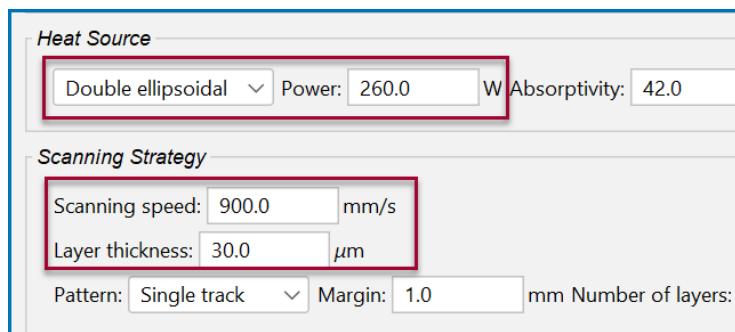
Figure 35: Project tree of the example containing activities from the default Additive Manufacturing template with additional Diffusion Calculator and Experimental File Reader nodes added, where the segregation profiles datasets are pulled from the Experimental File Reader.

On the **AM Calculator Configuration** window, the calculation type **Transient with heat source from Steady-state** is selected with a single track scan pattern and a **Geometry** of 2 mm x 1 mm x 4 mm (height x width x length). The **Base plate temperature** is set to 200 °C.



Additional settings are then made on the **Configuration** window as follows.

The **Double ellipsoidal** volume heat source was previously assessed as a function of linear energy density for a similar material and directly applied to the experimental conditions of a volumetric energy density of 80 J/mm<sup>3</sup>. The laser **Power** is entered at 260 W, **Scanning speed** at 900 mm/s, and powder **Layer thickness** 30 µm. Below is a snapshot of the settings.



A probe was then added in the center of the scan track at a distance of 1.3 mm from the edge. The **Probe Positions** can either be entered directly on the Configuration window or click the **Pick coordinate** button and then click on the geometry in the **Visualizations** window to directly choose the probe point (or points if there is more than one probe added).

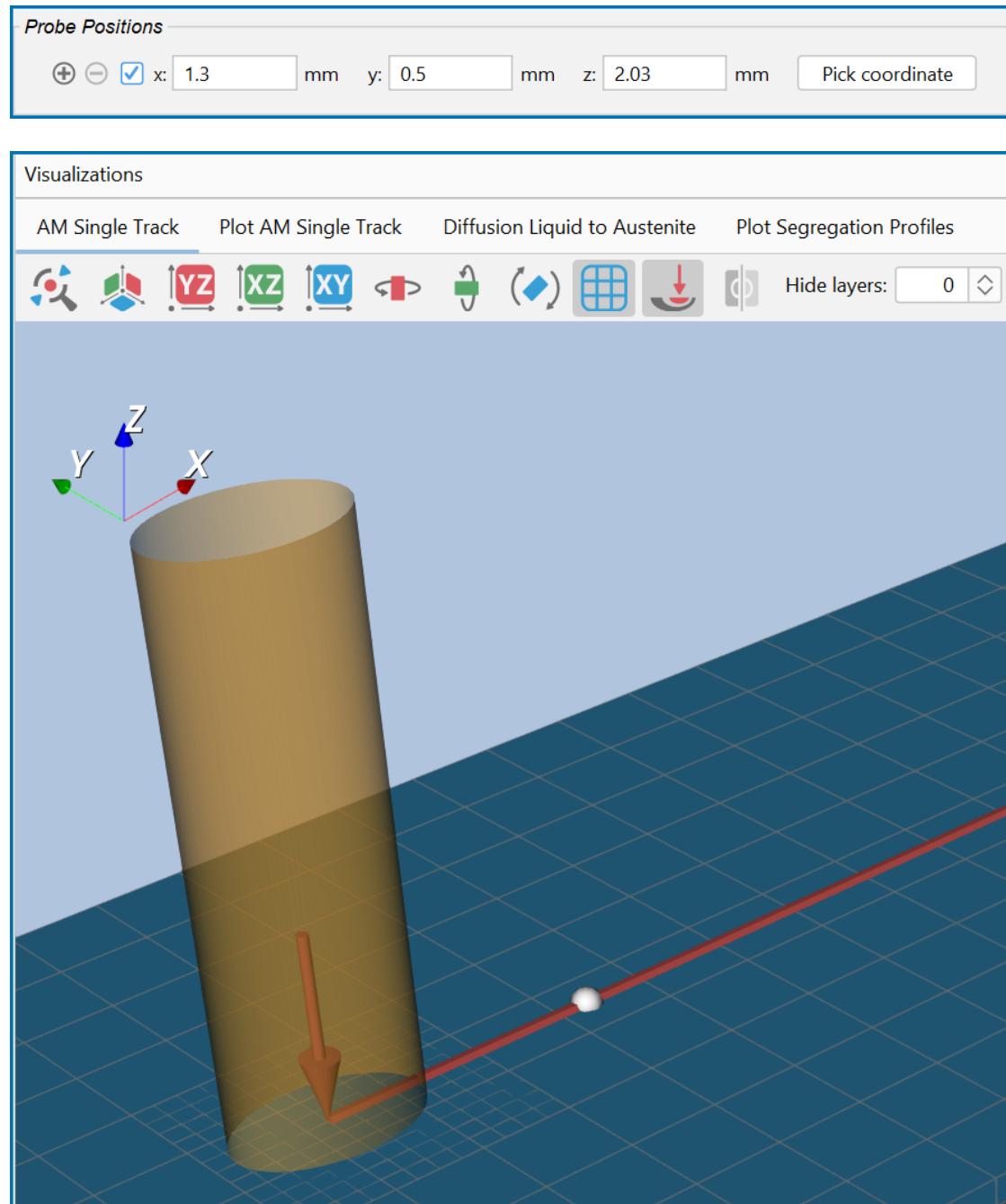


Figure 36: Close up of the probe point added to the geometry for the single track AM simulation.

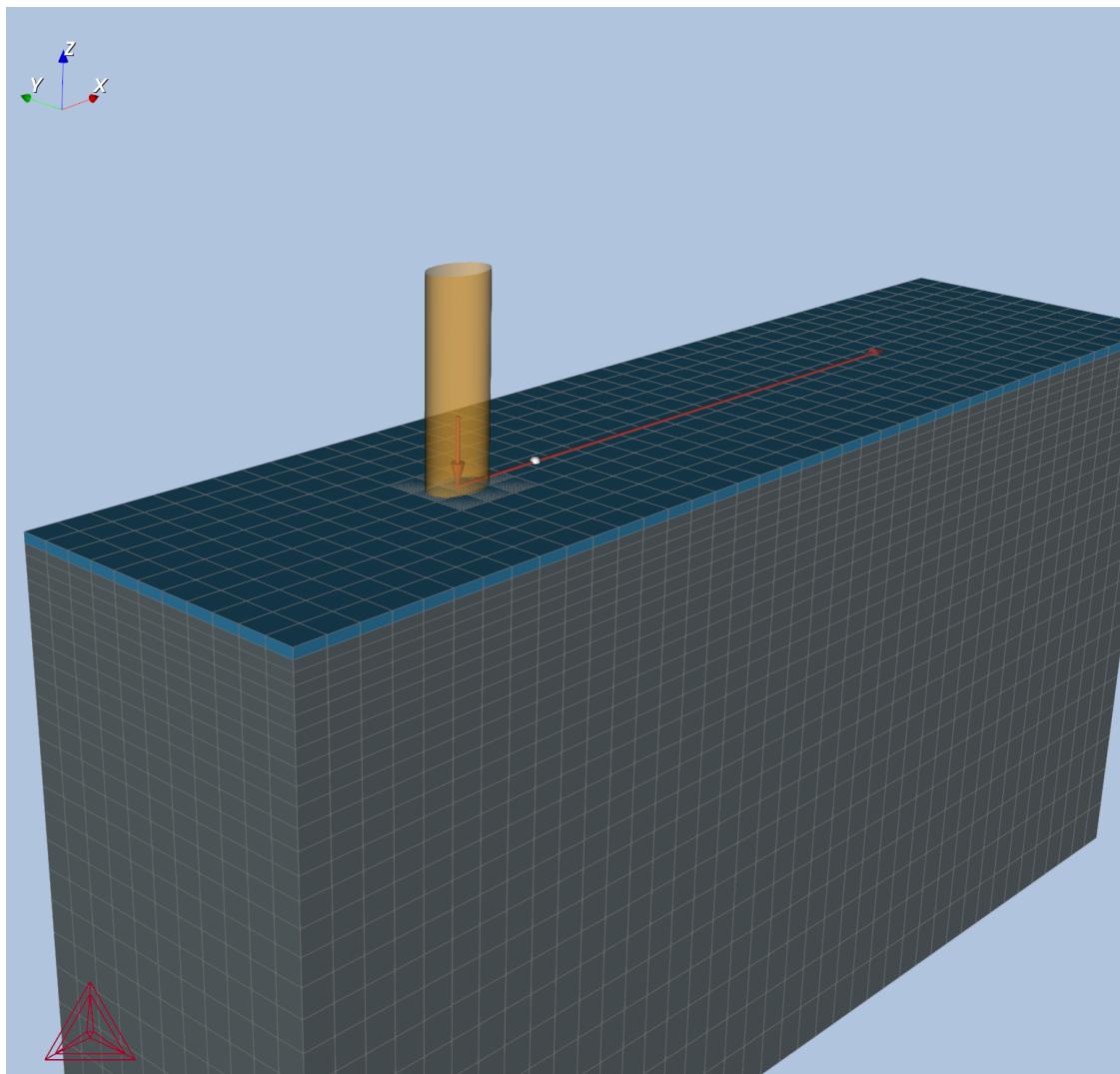
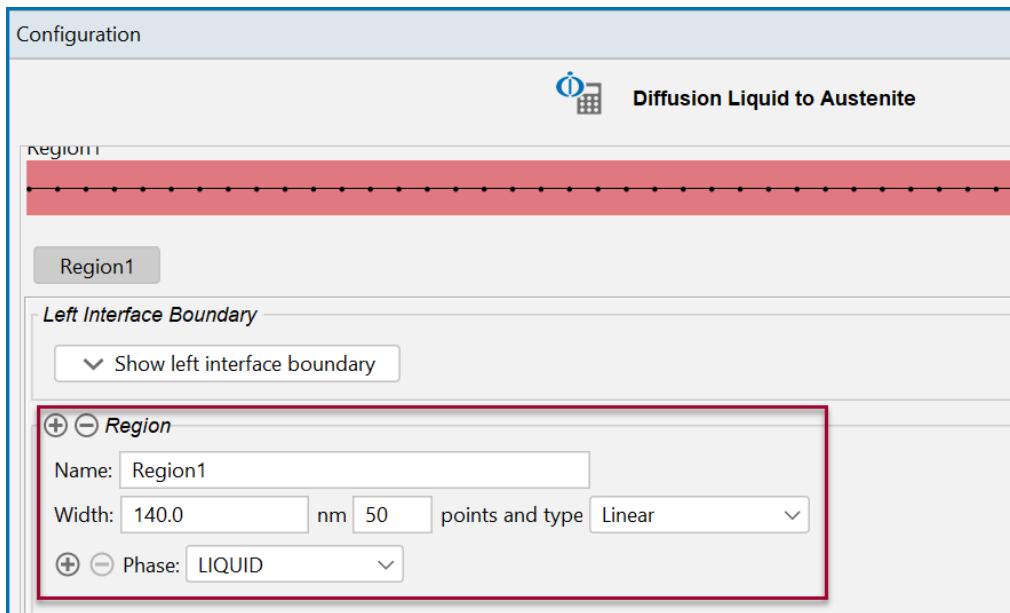


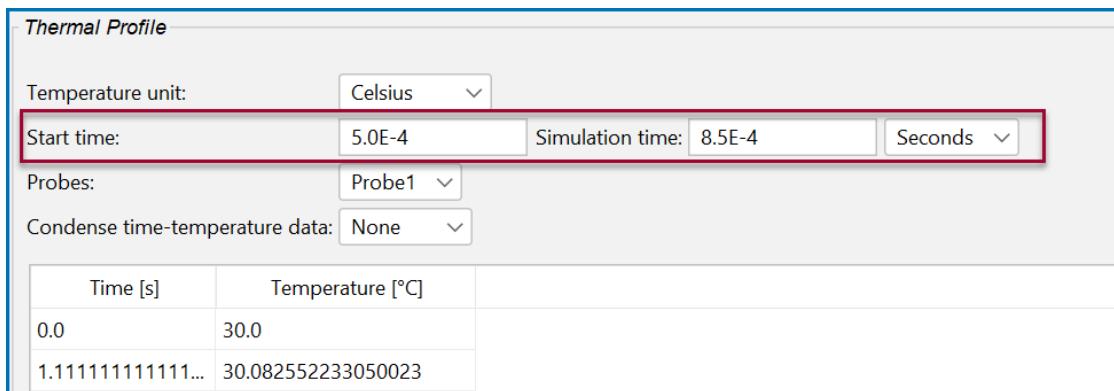
Figure 37: The full geometry set up for the single track AM simulation with a probe point added to the middle of the scan. Open the example to better see the set up and to try working within the window.

## Diffusion Calculations

For the Diffusion Module (DICTRA) solidification calculations using the **Diffusion Calculator**, only the liquid to austenite (FCC) transformation was simulated. On the **Diffusion Calculator Configuration** window, a **Region** of 140 nm with liquid and FCC allowed to form at the right boundary is set.



In the *Thermal Profile* section, the time temperature from the probe was selected between a **Start time** of 5.0E-4 and **Simulation time** of 8.5.0E-4 s in order to only simulate the solidification, which can be viewed on the **Visualizations** window as in [Figure 38](#). Note that the probes need to be added and then run in the AM Calculator to make this data available in for this part of the calculation.



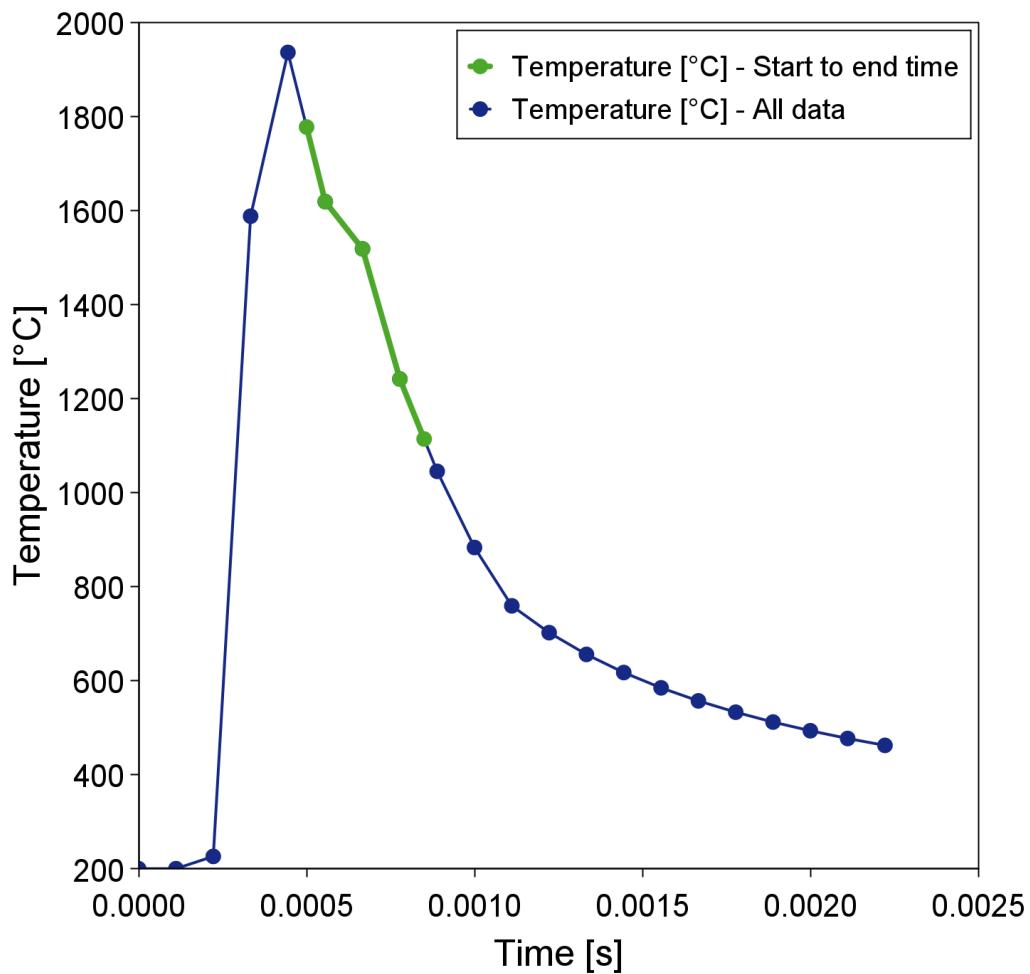


Figure 38: Time temperature profile of the probe in the AM simulation. The green curve show the part of the profile used during the diffusion simulation with the Diffusion Calculator.

The calculated segregation profiles are finally compared with the STEM-EDS line scans as shown in Figure 39.

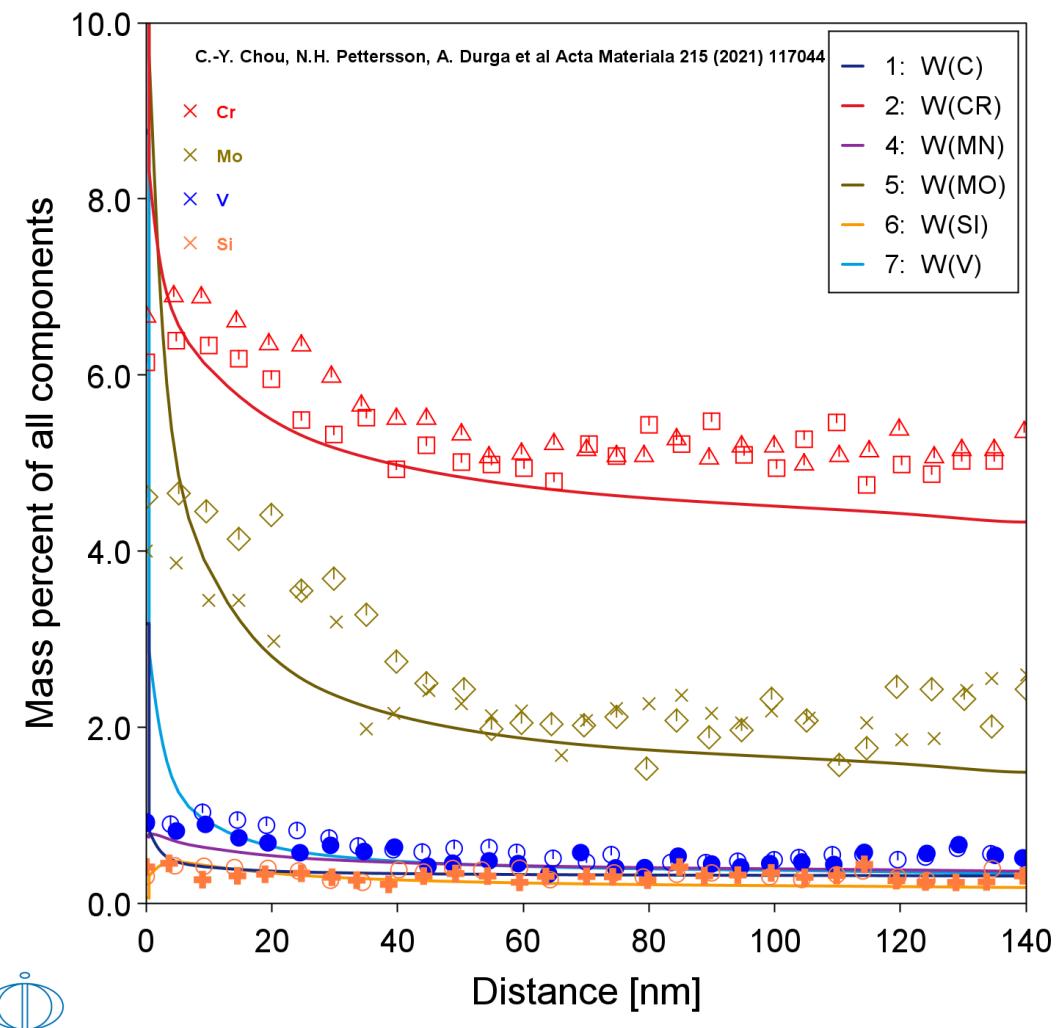


Figure 39: The simulated segregation profile with overlaid experimental STEM-EDS line scans from C.-Y. Chou et al. [2021Cho].

## Visualizations

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s). This example highlights some of these capabilities:

- **Probes:** Probes are added to the AM Calculator during the set up either by entering coordinates or directly adding these to the geometry. See [Figure 36](#) and [Figure 37](#) for example.
- **Thermal Profile:** The Diffusion Calculator Thermal Profile settings automatically include the probe data and you can visualize to help you continue the simulation. See [Figure 38](#).

- **Plot 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, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window. See [Figure 39](#).

## Reference

[2021Cho] C.-Y. Chou, N. H. Petterson, A. Durga, F. Zhang, C. Oikonomou, A. Borgenstam, J. Odqvist, G. Lindwall, Influence of solidification structure on austenite to martensite transformation in additively manufactured hot-work tool steels. *Acta Mater.* 215, 117044 (2021).

## Other Resources



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