Tutorial 22. Modeling Solidification

Introduction

This tutorial illustrates how to set up and solve a problem involving solidification. This tutorial will demonstrate how to do the following:

- Define a solidification problem.
- Define pull velocities for simulation of continuous casting.
- Define a surface tension gradient for Marangoni convection.
- Solve a solidification problem.

Prerequisites

This tutorial is written with the assumption that you have completed Tutorial 1, and that you are familiar with the ANSYS FLUENT navigation pane and menu structure. Some steps in the setup and solution procedure will not be shown explicitly.

Problem Description

This tutorial demonstrates the setup and solution procedure for a fluid flow and heat transfer problem involving solidification, namely the Czochralski growth process. The geometry considered is a 2D axisymmetric bowl (shown in Figure 22.1), containing liquid metal. The bottom and sides of the bowl are heated above the liquidus temperature, as is the free surface of the liquid. The liquid is solidified by heat loss from the crystal and the solid is pulled out of the domain at a rate of 0.001 m/s and a temperature of 500 K. There is a steady injection of liquid at the bottom of the bowl with a velocity of \(1.01 \times 10^{-3}\) m/s and a temperature of 1300 K. Material properties are listed in Figure 22.1.

Starting with an existing 2D mesh, the details regarding the setup and solution procedure for the solidification problem are presented. The steady conduction solution for this problem is computed as an initial condition. Then, the fluid flow is enabled to investigate the effect of natural and Marangoni convection in a transient fashion.
\[ \rho = 8000 - 0.1 \times T \ \text{kg/m}^3 \]
\[ \mu = 5.53 \times 10^{-3} \ \text{kg/m} - \text{s} \]
\[ k = 30 \ W/\text{m} - \text{K} \]
\[ C_p = 680 \ \text{J/kg} - \text{K} \]
\[ \frac{\partial \sigma}{\partial T} = -3.6 \times 10^{-4} \ \frac{\text{N}}{\text{m} - \text{K}} \]
\[ T_{\text{solidus}} = 1100 \ \text{K} \]
\[ T_{\text{liquidus}} = 1200 \ \text{K} \]
\[ L = 1 \times 10^5 \ \text{J/kg} \]
\[ A_{\text{mush}} = 1 \times 10^5 \ \text{kg/m}^3 - \text{s} \]

**Setup and Solution**

**Preparation**

1. Download `solidification.zip` from the **User Services Center** to your working folder (as described in Tutorial 1).

2. Unzip `solidification.zip`.

   *The file `solid.msh` can be found in the `solidification` folder created after unzipping the file.*

3. Use FLUENT Launcher to start the 2D version of ANSYS FLUENT.
For more information about FLUENT Launcher, see Section 1.1.2 in the separate User’s Guide.

Note: The Display Options are enabled by default. Therefore, after you read in the mesh, it will be displayed in the embedded graphics window.

Step 1: Mesh

1. Read the mesh file solid.msh.

As the mesh is read by ANSYS FLUENT, messages will appear in the console reporting the progress of the reading.

A warning about the use of axis boundary conditions will be displayed in the console, informing you to consider making changes to the zone type, or to change the problem definition to axisymmetric. You will change the problem to axisymmetric swirl in step 2.

Step 2: General Settings

1. Check the mesh.

ANSYS FLUENT will perform various checks on the mesh and will report the progress in the console. Make sure that the minimum volume is a positive number.

2. Examine the mesh (Figure 22.2).
3. Select Axisymmetric Swirl from the 2D Space list.

The geometry comprises an axisymmetric bowl. Furthermore, swirling flows are considered in this problem, so the selection of Axisymmetric Swirl best defines this geometry.

Also, note that the rotation axis is the x-axis. Hence, the x-direction is the axial direction and the y-direction is the radial direction. When modeling axisymmetric swirl, the swirl direction is the tangential direction.
4. Add the effect of gravity on the model.
   ☑ General → ✔ Gravity

   (a) Enable Gravity.
   (b) Enter \(-9.81 \text{ m/s}^2\) for X in the Gravitational Acceleration group box.

**Step 3: Models**

   ☑ Models

   1. Define the solidification model.
      ☑ Models → ✉ Solidification & Melting → Edit…
(a) Enable the Solidification/Melting option in the Model group box.

The Solidification and Melting dialog box will expand to show the related parameters.

(b) Retain the default value of 100000 for the Mushy Zone Constant.

This default value is acceptable for most cases.

(c) Enable the Include Pull Velocities option.

By including the pull velocities, you will account for the movement of the solidified material as it is continuously withdrawn from the domain in the continuous casting process.

When you enable this option, the Solidification and Melting dialog box will expand to show the Compute Pull Velocities option. If you were to enable this additional option, ANSYS FLUENT would compute the pull velocities during the calculation. This approach is computationally expensive and is recommended only if the pull velocities are strongly dependent on the location of the liquid-solid interface. In this tutorial, you will patch values for the pull velocities instead of having ANSYS FLUENT compute them.

For more information about computing the pull velocities, see Section 25.1 in the separate User's Guide.

(d) Click OK to close the Solidification and Melting dialog box.

An Information dialog box will open, telling you that available material properties have changed for the solidification model. You will set the material properties later, so you can simply click OK in the dialog box to acknowledge this information.

Note: ANSYS FLUENT will automatically enable the energy calculation when you enable the solidification model, so you need not visit the Energy dialog box.
Step 4: Materials

In this step, you will create a new material and specify its properties, including the melting heat, solidus temperature, and liquidus temperature.

1. Define a new material.

   ![Create/Edit Materials dialog box]

   (a) Enter liquid-metal for Name.

   (b) Select polynomial from the Density drop-down list to open the Polynomial Profile dialog box.

   *Scroll down the list to find polynomial.*

   ![Polynomial Profile dialog box]
i. Set Coefficients to 2.
ii. Enter 8000 for 1 and -0.1 for 2 in the Coefficients group box.

As shown in Figure 22.1, the density of the material is defined by a polynomial function: \( \rho = 8000 - 0.1T \).

iii. Click OK to close the Polynomial Profile dialog box.

A Question dialog box will open, asking you if air should be overwritten. Click No to retain air and add the new material (liquid-metal) to the FLUENT Fluid Materials drop-down list.

(c) Select liquid-metal from the FLUENT Fluid Materials drop-down list to set the other material properties.

(d) Enter 680 J/kg – k for \( C_p \).
(e) Enter 30 W/m – k for Thermal Conductivity.
(f) Enter 0.00553 kg/m – s for Viscosity.
(g) Enter 100000 j/kg for Pure Solvent Melting Heat. 
   Scroll down the group box to find Pure Solvent Melting Heat and the properties that follow.

(h) Enter 1100 K for Solidus Temperature.

(i) Enter 1200 K for Liquidus Temperature.

(j) Click Change/Create and close the Create/Edit Materials dialog box.

Step 5: Cell Zone Conditions

Cell Zone Conditions
1. Set the boundary conditions for the fluid (fluid).
   (a) Select liquid-metal from the Material Name drop-down list.
   (b) Click OK to close the Fluid dialog box.

Step 6: Boundary Conditions
   (a) Set the boundary conditions for the fluid (fluid).
   (b) Click OK to close the Fluid dialog box.
1. Set the boundary conditions for the inlet (inlet).

   - ![Boundary Conditions](image)

   - **(a)** Enter 0.00101 m/s for **Velocity Magnitude**.
   - **(b)** Click the **Thermal** tab and enter 1300 K for **Temperature**.

   - ![Velocity Inlet](image)

   - **(c)** Click **OK** to close the **Velocity Inlet** dialog box.
2. Set the boundary conditions for the outlet (outlet).
   
   ![Boundary Conditions](image)

   Here, the solid is pulled out with a specified velocity, so a velocity inlet boundary condition is used with a positive axial velocity component.

   ![Velocity Inlet](image)

   (a) Select Components from the Velocity Specification Method drop-down list. The Velocity inlet dialog box will change to show related inputs.

   (b) Enter 0.001 m/s for Axial-Velocity.

   (c) Enter 1 rad/s for Swirl Angular Velocity.

   (d) Click the Thermal tab and enter 500 K for Temperature.
(e) Click OK to close the Velocity Inlet dialog box.

3. Set the boundary conditions for the bottom wall (bottom-wall).

   ![Boundary Conditions Dialog Box]

(a) Click the Thermal tab.

   i. Select Temperature from the Thermal Conditions group box.
   ii. Enter 1300 K for Temperature.

(b) Click OK to close the Wall dialog box.
4. Set the boundary conditions for the free surface (free-surface).

The specified shear and Marangoni stress boundary conditions are useful in modeling situations in which the shear stress (rather than the motion of the fluid) is known. A free surface condition is an example of such a situation. In this case, the convection is driven by the Marangoni stress and the shear stress is dependent on the surface tension, which is a function of temperature.

(a) Select Marangoni Stress from the Shear Condition group box.

The Marangoni Stress condition allows you to specify the gradient of the surface tension with respect to temperature at a wall boundary.

(b) Enter -0.00036 n/m – k for Surface Tension Gradient.

(c) Click the Thermal tab to specify the thermal conditions.
i. Select Convection from the Thermal Conditions group box.
ii. Enter 100 w/m²·K for Heat Transfer Coefficient.
iii. Enter 1500 K for Free Stream Temperature.

(d) Click OK to close the Wall dialog box.

5. Set the boundary conditions for the side wall (side-wall).

(a) Click the Thermal tab.

![Wall dialog box](image)

i. Select Temperature from the Thermal Conditions group box.
ii. Enter 1400 K for the Temperature.

(b) Click OK to close the Wall dialog box.
6. Set the boundary conditions for the solid wall (solid-wall).

(a) Select **Moving Wall** from the Wall Motion group box. 
*The Wall dialog box will expand to show additional parameters.*

(b) Select **Rotational** in the lower box of the Motion group box. 
*The Wall dialog box will change to show the rotational speed.*

(c) Enter 1.0 rad/s for **Speed**.
(d) Click the **Thermal** tab to specify the thermal conditions.

![Wall dialog box](image)

i. Select **Temperature** from the **Thermal Conditions** selection list.

ii. Enter 500 K for **Temperature**.

(e) Click **OK** to close the **Wall** dialog box.
Step 7: Solution: Steady Conduction

In this step, you will specify the discretization schemes to be used and temporarily disable the calculation of the flow and swirl velocity equations, so that only conduction is calculated. This steady-state solution will be used as the initial condition for the time-dependent fluid flow and heat transfer calculation.

1. Set the solution parameters.

   • **Solution Methods**

![Solution Methods](image)

(a) Retain the default selection of SIMPLE from the Pressure-Velocity Coupling drop-down list.

(b) Select PRESTO! from the Pressure drop-down list in the Spatial Discretization group box.

   *The PRESTO! scheme is well suited for rotating flows with steep pressure gradients.*

(c) Retain the default selection of First Order Upwind from the Momentum, Swirl Velocity, and Energy drop-down lists.
2. Enable the calculation for energy.
   ![Solution Controls](image)
   ![Equations](image)
   (a) Deselect Flow and Swirl Velocity from the Equations selection list to disable the calculation of flow and swirl velocity equations.
   (b) Click OK to close the Equations dialog box.

3. Set the Under-Relaxation Factors.
   ![Solution Controls](image)
   (a) Retain the default values.
4. Enable the plotting of residuals during the calculation.
   - Monitors ➔ Residuals ➔ Edit...

   (a) Make sure Plot is enabled in the Options group box.
   (b) Click OK to close the Residual Monitors dialog box.

5. Initialize the solution.
   - Solution Initialization
(a) Retain the default value of 0 for Gauge Pressure, Axial Velocity, Radial Velocity, and Swirl Velocity.

Since you are solving only the steady conduction problem, the initial values for the pressure and velocities will not be used.

(b) Retain the default value of 300 K for Temperature.

(c) Click Initialize.

6. Define a custom field function for the swirl pull velocity.

Define → Custom Field Functions...

In this step, you will define a field function to be used to patch a variable value for the swirl pull velocity in the next step. The swirl pull velocity is equal to \( \Omega r \), where \( \Omega \) is the angular velocity and \( r \) is the radial coordinate. Since \( \Omega = 1 \) rad/s, you can simplify the equation to simply \( r \). In this example, the value of \( \Omega \) is included for demonstration purposes.

![Custom Field Function Calculator](image)

(a) Select Mesh... and Radial Coordinate from the Field Functions drop-down lists.

(b) Click the Select button to add radial-coordinate in the Definition field.

If you make a mistake, click the DEL button on the calculator pad to delete the last item you added to the function definition.

(c) Click the \( \times \) button on the calculator pad.

(d) Click the 1 button.

(e) Enter omegar for New Function Name.

(f) Click Define.

Note: To check the function definition, you can click Manage... to open the Field Function Definitions dialog box. Then select omegar from the Field Functions selection list to view the function definition.

(g) Close the Custom Field Function Calculator dialog box.
7. Patch the pull velocities.

As noted earlier, you will patch values for the pull velocities, rather than having ANSYS FLUENT compute them. Since the radial pull velocity is zero, you will patch just the axial and swirl pull velocities.

(a) Select Axial Pull Velocity from the Variable selection list.
(b) Enter 0.001 m/s for Value.
(c) Select fluid from the Zones to Patch selection list.
(d) Click Patch.

You have just patched the axial pull velocity. Next you will patch the swirl pull velocity.

(e) Select Swirl Pull Velocity from the Variable selection list.

Scroll down the list to find Swirl Pull Velocity.
(f) Enable the Use Field Function option.

(g) Select \texttt{omegar} from the Field Function selection list.

(h) Make sure that fluid is selected from the Zones to Patch selection list.

(i) Click Patch and close the Patch dialog box.

8. Save the initial case and data files (\texttt{solid0.cas.gz} and \texttt{solid0.dat.gz}).

   \textbf{File} \rightarrow \textbf{Write} \rightarrow \textbf{Case} & \textbf{Data}...

9. Start the calculation by requesting 20 iterations.

   \textbf{Run Calculation}

   \begin{center}
   \includegraphics[width=0.4\textwidth]{Run_Calculation.png}
   \end{center}

   (a) Enter 20 for \textbf{Number of Iterations}.

   (b) Click \textbf{Calculate}.

   \textit{The solution will converge in approximately 11 iterations.}
10. Display filled contours of temperature (Figure 22.3).

(a) Enable the Filled option.

(b) Select Temperature... and Static Temperature from the Contours of drop-down lists.

(c) Click Display (Figure 22.3).

Figure 22.3: Contours of Temperature for the Steady Conduction Solution
11. Display filled contours of temperature to determine the thickness of mushy zone.
   ![Graphics and Animations](image1)
   ![Contours](image2)
   ![Set Up...](image3)

(a) Disable **Auto Range** in the **Options** group box.

*The Clip to Range option will automatically be enabled.*

(b) Enter 1100 for Min and 1200 for Max.

(c) Click **Display** (See Figure 22.4) and close the **Contours** dialog box.

![Figure 22.4: Contours of Temperature (Mushy Zone) for the Steady Conduction Solution](image4)
12. Save the case and data files for the steady conduction solution (solid.cas.gz and solid.dat.gz).

   File → Write → Case & Data...

**Step 8: Solution: Transient Flow and Heat Transfer**

*In this step, you will turn on time dependence and include the flow and swirl velocity equations in the calculation. You will then solve the transient problem using the steady conduction solution as the initial condition.*

1. Enable a time-dependent solution.
   - General

   ![General Settings]

   (a) Select Transient from the Time list.
2. Set the solution parameters.

(a) Retain the default selection of First Order Implicit from the Transient Formulation drop-down list.

(b) Ensure that PRESTO! is selected from the Pressure drop-down list in the Spatial Discretization group box.

3. Enable calculations for flow and swirl velocity.
(a) Select Flow and Swirl Velocity and ensure that Energy is selected from the Equations selection list.

Now all three items in the Equations selection list will be selected.

(b) Click OK to close the Equations dialog box.

4. Set the Under-Relaxation Factors.

Solution Controls

(a) Enter 0.1 for Liquid Fraction Update.

(b) Retain the default values for other Under-Relaxation Factors.

5. Save the initial case and data files (solid01.cas.gz and solid01.dat.gz).

File → Write → Case & Data…
6. Run the calculation for 2 time steps.
   - Run Calculation

   - Enter 0.1 s for Time Step Size.
   - Set the Number of Time Steps to 2.
   - Retain the default value of 20 for Max Iterations/Time Step.
   - Click Calculate.

7. Display filled contours of the temperature after 0.2 seconds.
   - Graphics and Animations → Contours → Set Up...

   - Make sure that Temperature... and Static Temperature are selected from the Contours of drop-down lists.
   - Click Display (See Figure 22.5).
Figure 22.5: Contours of Temperature at $t = 0.2$ s

8. Display contours of stream function (Figure 22.6).

   ![Stream Function Contours](image)

   (a) Disable Filled in the Options group box.
   (b) Select Velocity... and Stream Function from the Contours of drop-down lists.
   (c) Click Display.

Figure 22.6: Contours of Stream Function at $t = 0.2$ s
As shown in Figure 22.6, the liquid is beginning to circulate in a large eddy, driven by natural convection and Marangoni convection on the free surface.

9. Display contours of liquid fraction (Figure 22.7).

(a) Enable Filled in the Options group box.
(b) Select Solidification/Melting... and Liquid Fraction from the Contours of drop-down lists.
(c) Click Display and close the Contours dialog box.

![Contours of Liquid Fraction](image)

Figure 22.7: Contours of Liquid Fraction at \( t = 0.2 \) s

The liquid fraction contours show the current position of the melt front. Note that in Figure 22.7, the mushy zone divides the liquid and solid regions roughly in half.

10. Continue the calculation for 48 additional time steps.

(a) Enter 48 for Number of Time Steps.
(b) Click Calculate.

After a total of 50 time steps have been completed, the elapsed time will be 5 seconds.
11. Display filled contours of the temperature after 5 seconds (Figure 22.8).

(a) Ensure that Filled is enabled in the Options group box.
(b) Select Temperature... and Static Temperature from the Contours of drop-down lists.
(c) Click Display.

As shown in Figure 22.8, the temperature contours are fairly uniform through the melt front and solid material. The distortion of the temperature field due to the recirculating liquid is also clearly evident.

In a continuous casting process, it is important to pull out the solidified material at the proper time. If the material is pulled out too soon, it will not have solidified (i.e., it will still be in a mushy state). If it is pulled out too late, it solidifies in the casting pool and cannot be pulled out in the required shape. The optimal rate of pull can be determined from the contours of liquidus temperature and solidus temperature.

12. Display contours of stream function (Figure 22.9).

(a) Disable Filled in the Options group box.
(b) Select Velocity... and Stream Function from the Contours of drop-down lists.
(c) Click Display.
As shown in Figure 22.9, the flow has developed more fully by 5 seconds, as compared with Figure 22.6 after 0.2 seconds. The main eddy, driven by natural convection and Marangoni stress, dominates the flow.

To examine the position of the melt front and the extent of the mushy zone, you will plot the contours of liquid fraction.

![Contours of Stream Function](image)

Figure 22.9: Contours of Stream Function at t = 5 s

13. Display filled contours of liquid fraction (Figure 22.10).

   ![Graphics and Animations](image) ![Contours](image) ![Set Up…](image)

   (a) Enable Filled in the Options group box.

   (b) Select Solidification/Melting... and Liquid Fraction from the Contours of dropdown lists.

   (c) Click Display and close the Contours dialog box.

The introduction of liquid material at the left of the domain is balanced by the pulling of the solidified material from the right. After 5 seconds, the equilibrium position of the melt front is beginning to be established (Figure 22.10).
Figure 22.10: Contours of Liquid Fraction at $t = 5$ s

14. Save the case and data files for the solution at 5 seconds (solid5.cas.gz and solid5.dat.gz).

\[ \text{File} \rightarrow \text{Write} \rightarrow \text{Case & Data...} \]

**Summary**

In this tutorial, you studied the setup and solution for a fluid flow problem involving solidification for the Czochralski growth process.

The solidification model in ANSYS FLUENT can be used to model the continuous casting process where a solid material is continuously pulled out from the casting domain. In this tutorial, you patched a constant value and a custom field function for the pull velocities instead of computing them. This approach is used for cases where the pull velocity is not changing over the domain, as it is computationally less expensive than having ANSYS FLUENT compute the pull velocities during the calculation.

For more information about the solidification/melting model, see Chapter 25 in the separate User’s Guide.

**Further Improvements**

This tutorial guides you through the steps to reach an initial set of solutions. You may be able to obtain a more accurate solution by using an appropriate higher-order discretization scheme and by adapting the mesh. Mesh adaption can also ensure that the solution is independent of the mesh. These steps are demonstrated in Tutorial 1.