Chapter 24: Modeling Solidification

This tutorial is divided into the following sections:

24.1. 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.

24.2. Prerequisites

This tutorial is written with the assumption that you have completed *Introduction to Using ANSYS FLUENT: Fluid Flow and Heat Transfer in a Mixing Elbow* (p. 111), 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.

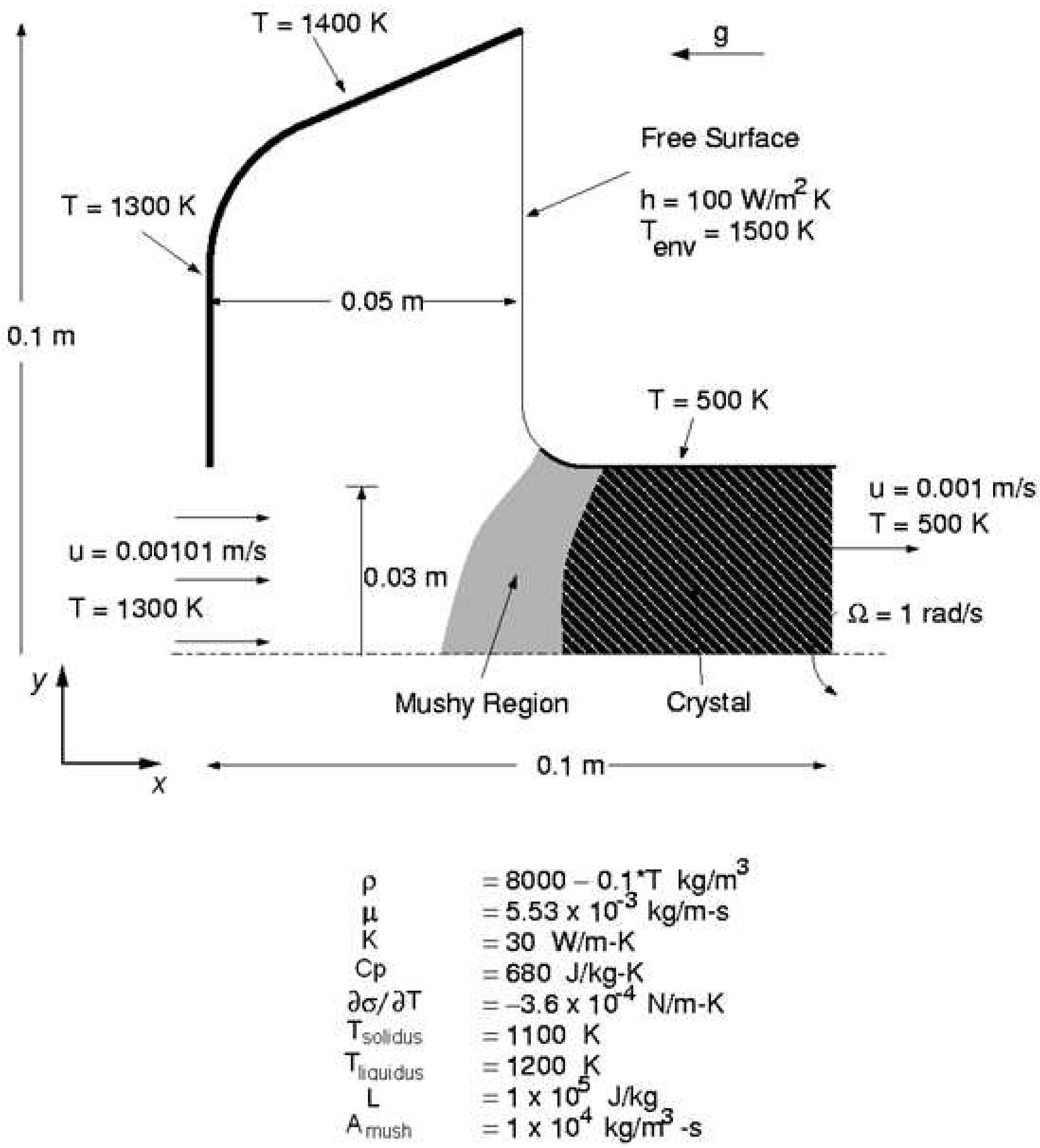
24.3. Problem Description

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 24.1* (p. 890)), 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 24.1* (p. 890).

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.

Figure 24.1 Solidification in Czochralski Model



ρ	=	8000 - 0.1 $\times$ T kg/m^3
μ	=	5.53 $\times 10^{-3} kg/m-s$
k	=	30 $W/m-K$
C_p	=	680 $J/kg-K$
$\partial\sigma/\partial T$	=	-3.6 $\times 10^{-4} N/m-K$
$T_{solidus}$	=	1100 K
$T_{liquidus}$	=	1200 K
L	=	1 $\times 10^5 J/kg$

A_{mush}	=	$1 \times 10^5 kg/m^3 - s$

A_{mush} is the mushy zone constant. For details refer to section Momentum Equations for modeling the solidification/melting process, in the Theory Guide.

24.4. Setup and Solution

The following sections describe the setup and solution steps for this tutorial:

24.4.1. Preparation

1. Download `solidification.zip` from the ANSYS Customer Portal or the User Services Center to your working folder (as described in *Preparation* (p. 4) of *Introduction to Using ANSYS FLUENT in ANSYS Workbench: Fluid Flow and Heat Transfer in a Mixing Elbow* (p. 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 Launcherflauncher;, see Starting ANSYS FLUENT Using FLUENT Launcher in the 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.

24.4.2. Step 1: Mesh

1. Read the mesh file `solid.msh`.

   File → **Read** → **Mesh...**

   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.

24.4.3. Step 2: General Settings

General

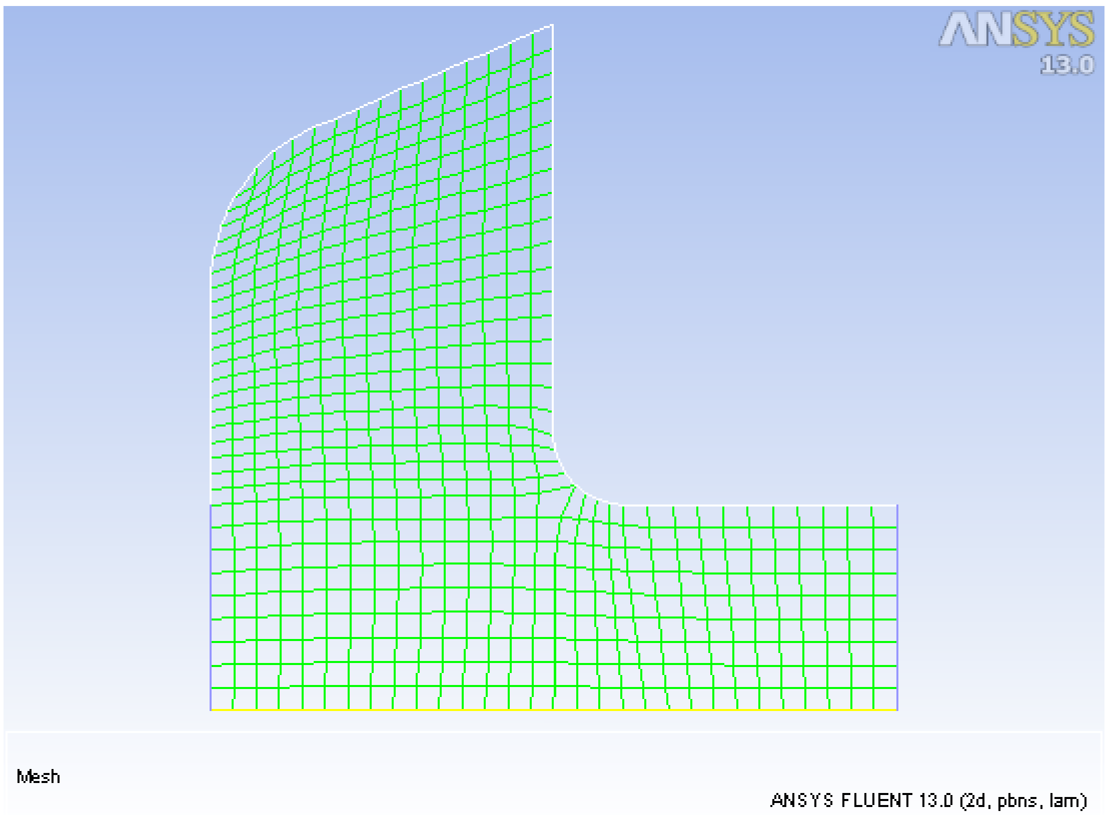
1. Check the mesh.

   General → **Check**

   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.

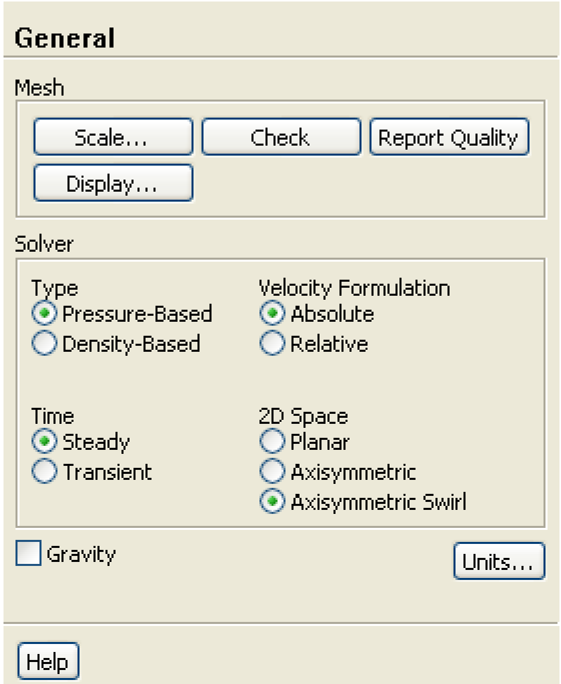
2. Examine the mesh (*Figure 24.2* (p. 892)).

   Figure 24.2 Mesh Display



3. Select **Axisymmetric Swirl** from the **2D Space** list.

   General

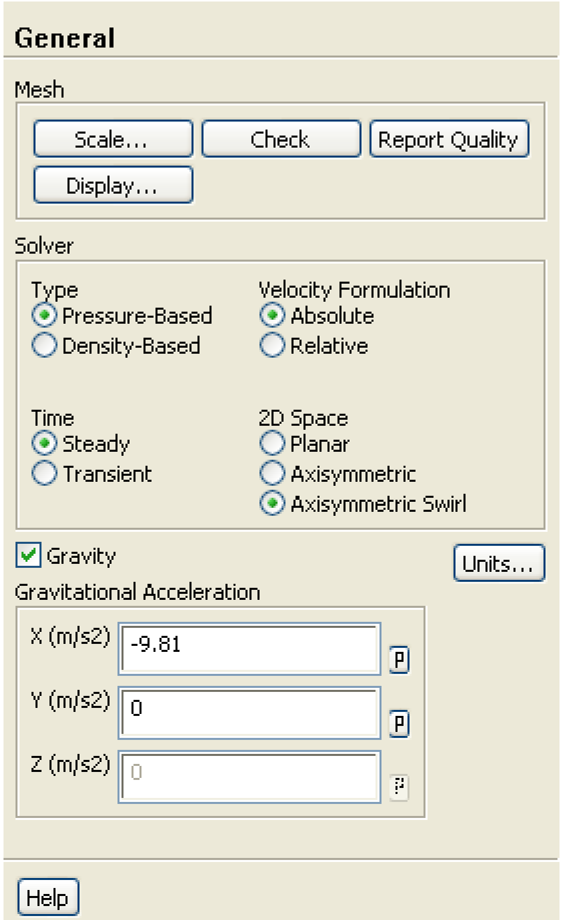


*The geometry comprises an axisymmetric bowl. Furthermore, swirling flows are considered in this problem, so the selection of **Axisymmetric Swirl** best defines this geometry.*

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**.

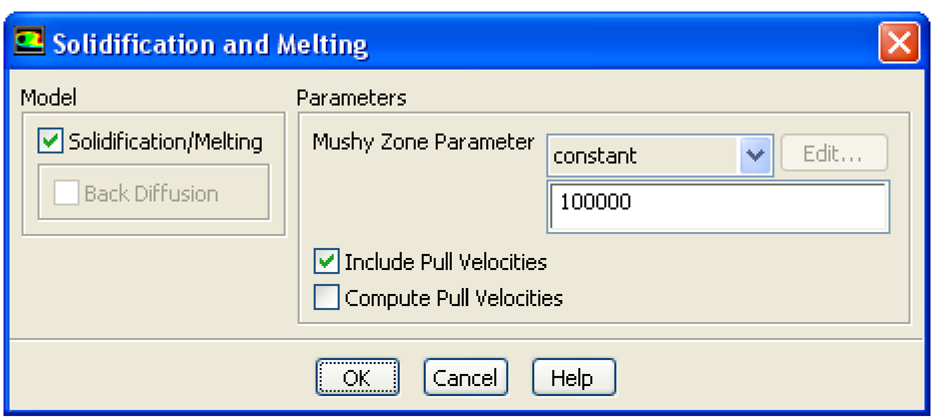
b. Enter `-9.81` m/s^2 for **X** in the **Gravitational Acceleration** group box.

24.4.4. 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.

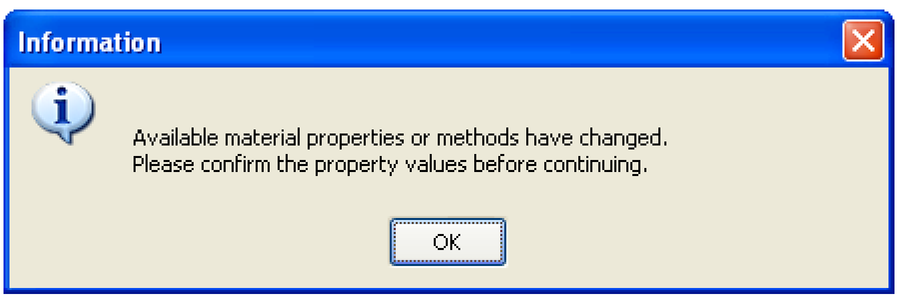
   By including the pull velocities, you will account for the movement of the solidified material as it is continuously withdrawn from the domain in the continuous casting process.

   *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 Setup Procedure in the 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.

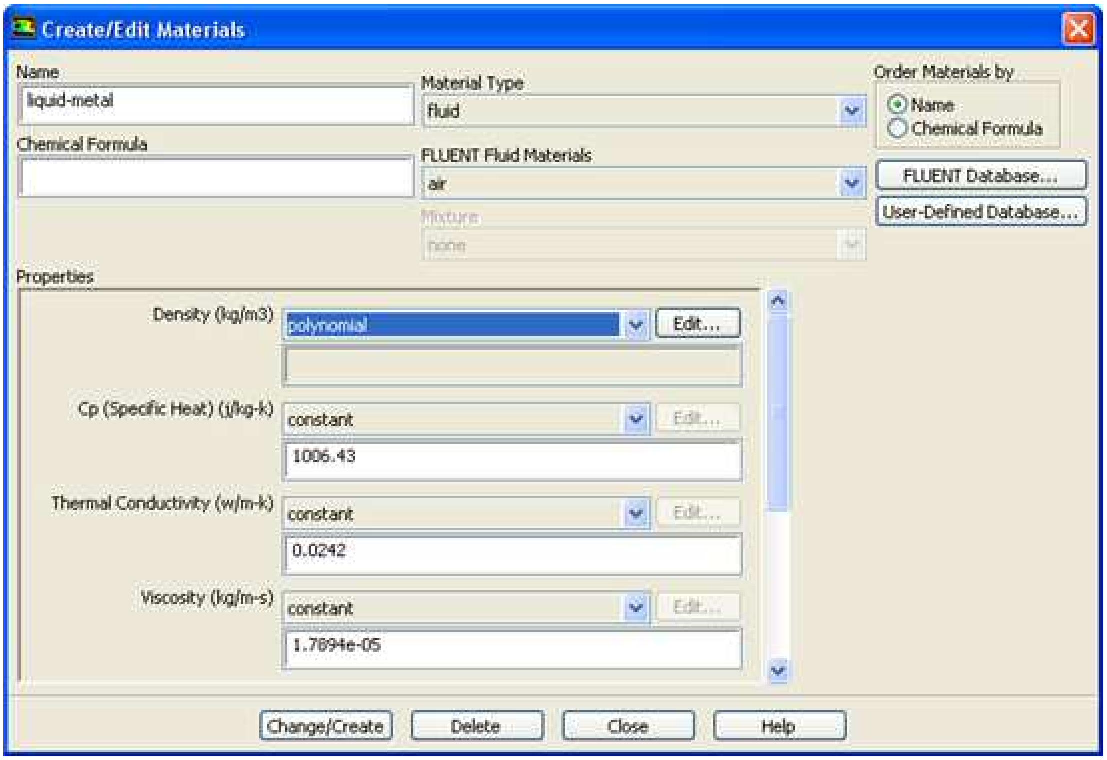
24.4.5. Step 4: Materials

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.

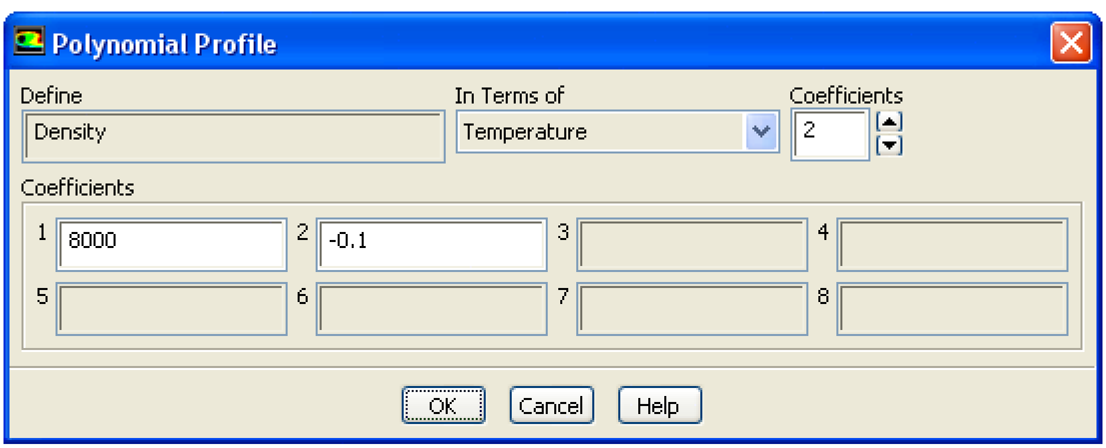
Materials → **Fluid** → **Create/Edit...**



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**.*



   i. Set **Coefficients** to 2.

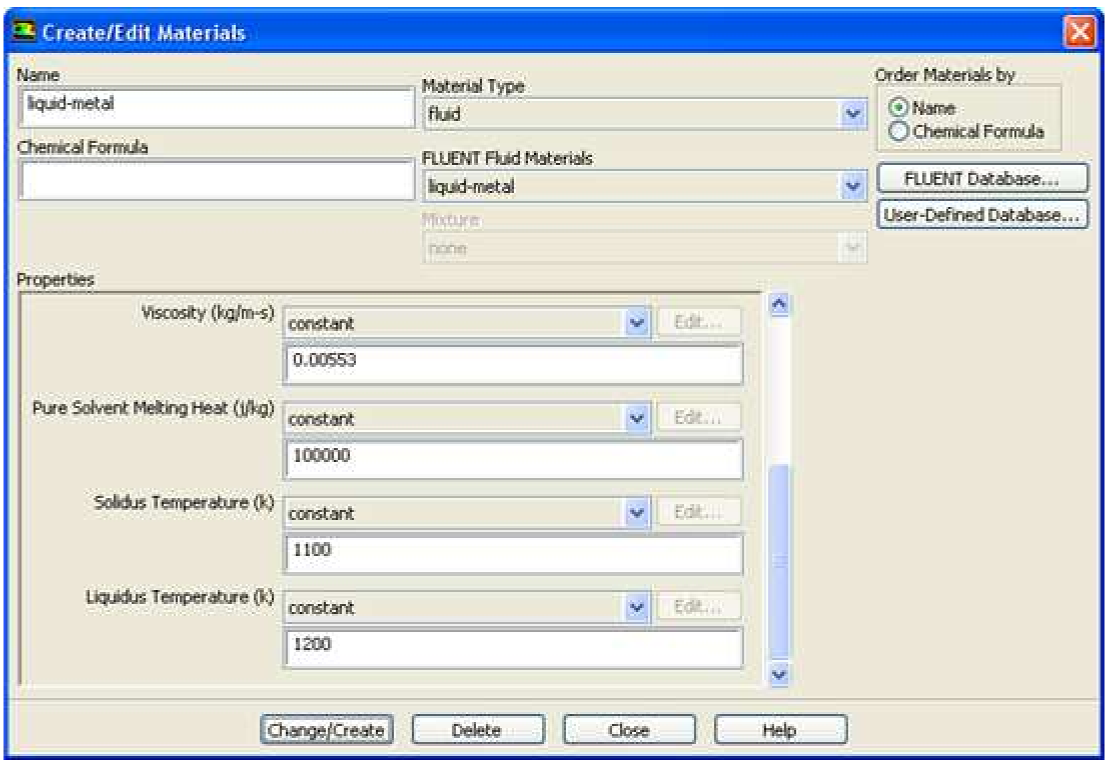
   ii. Enter `8000` for **1** and `-0.1` for **2** in the **Coefficients** group box.

   As shown in Figure 24.1 (p. 890), 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 **Cp (Specific Heat)**.

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.*

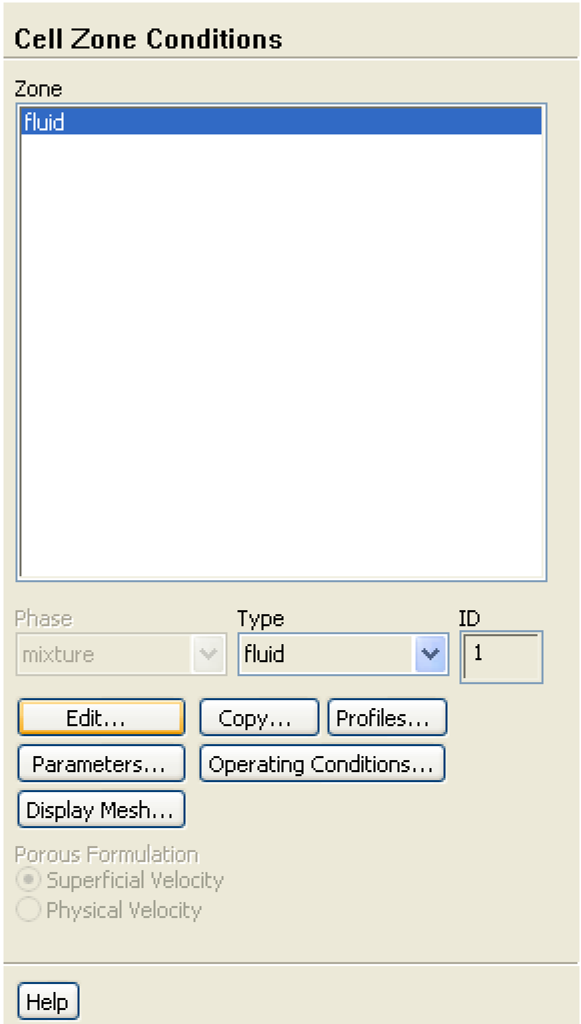
h. Enter `1100` K for **Solidus Temperature**.

i. Enter `1200` K for **Liquidus Temperature**.

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

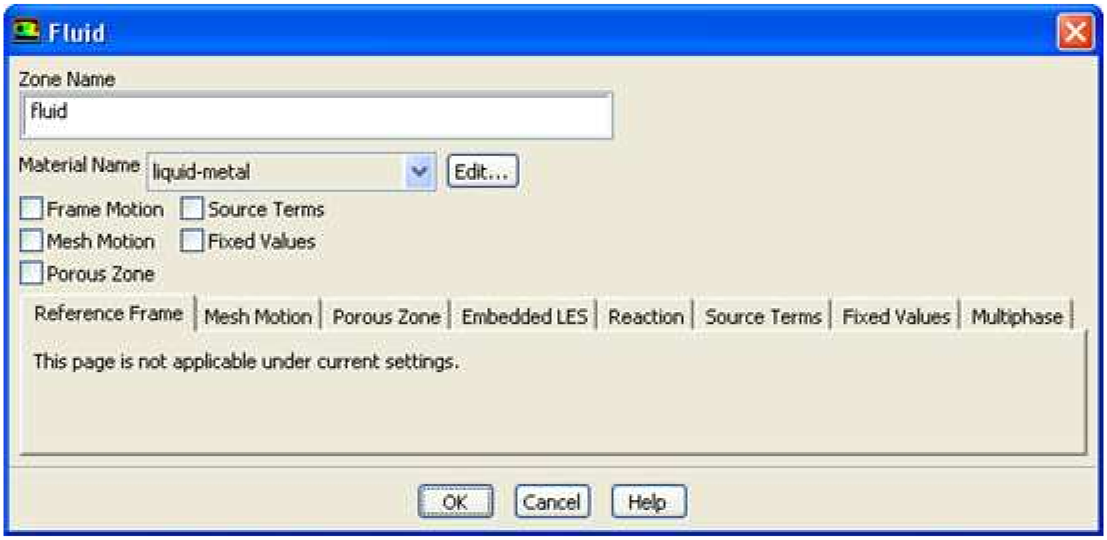
24.4.6. Step 5: Cell Zone Conditions

Cell Zone Conditions



1. Set the boundary conditions for the fluid (**fluid**).

   Cell Zone Conditions → **fluid** → **Edit...**

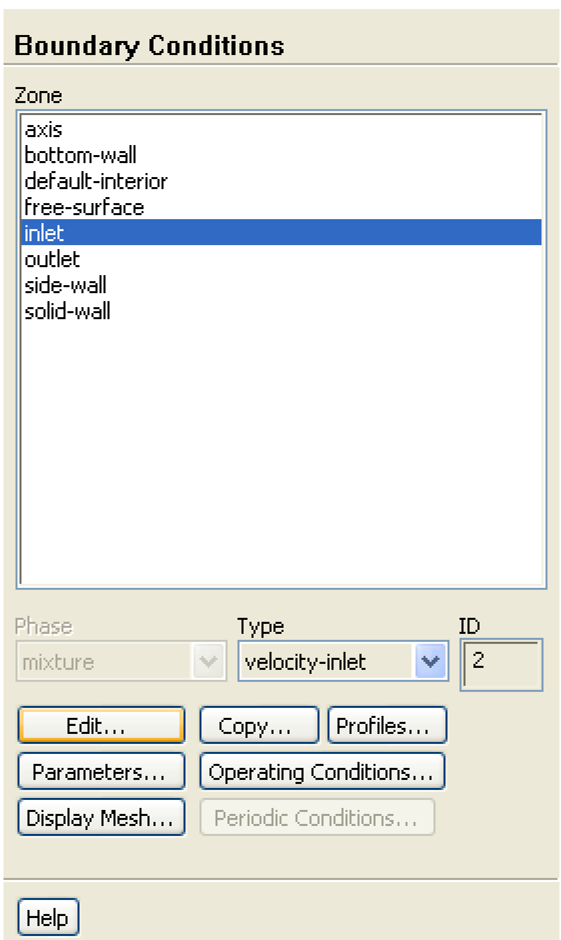


a. Select **liquid-metal** from the **Material Name** drop-down list.

b. Click **OK** to close the **Fluid** dialog box.

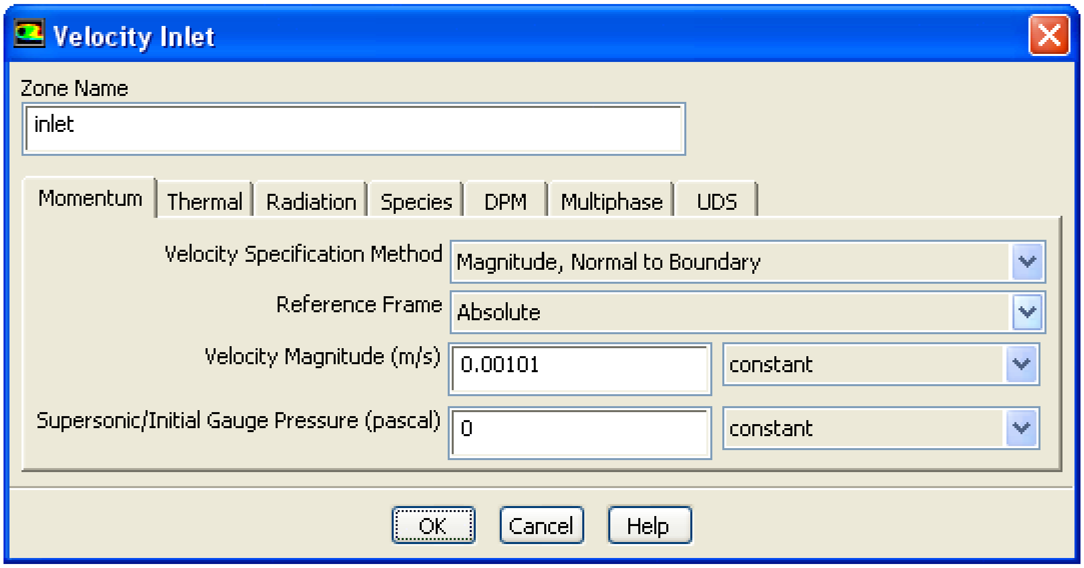
24.4.7. Step 6: Boundary Conditions

Boundary Conditions



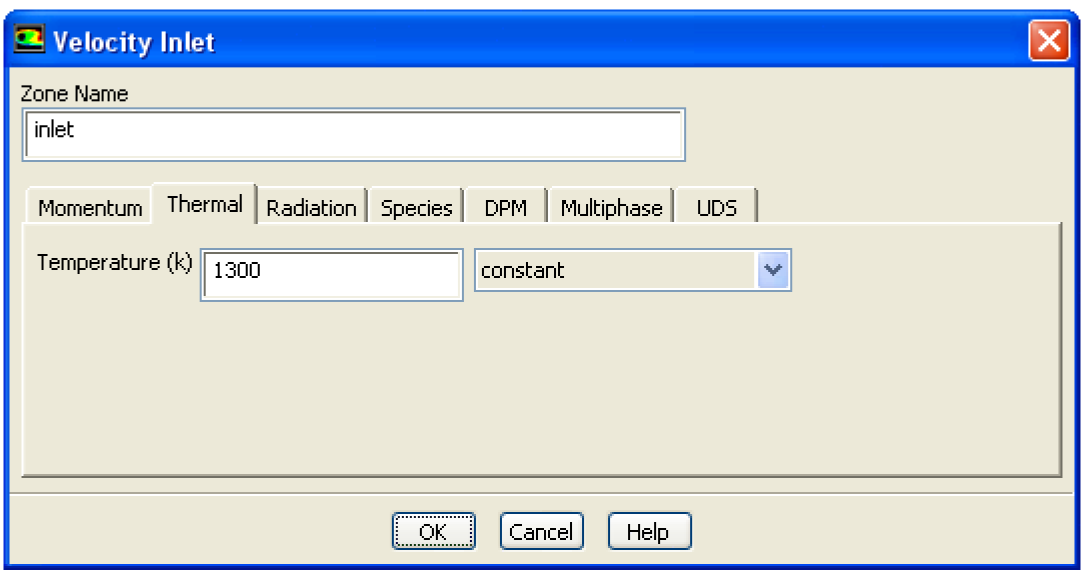
1. Set the boundary conditions for the inlet (**inlet**).

Boundary Conditions → **inlet** → **Edit...**



a. Enter `0.00101` m/s for **Velocity Magnitude**.

b. Click the **Thermal** tab and enter `1300` K for **Temperature**.

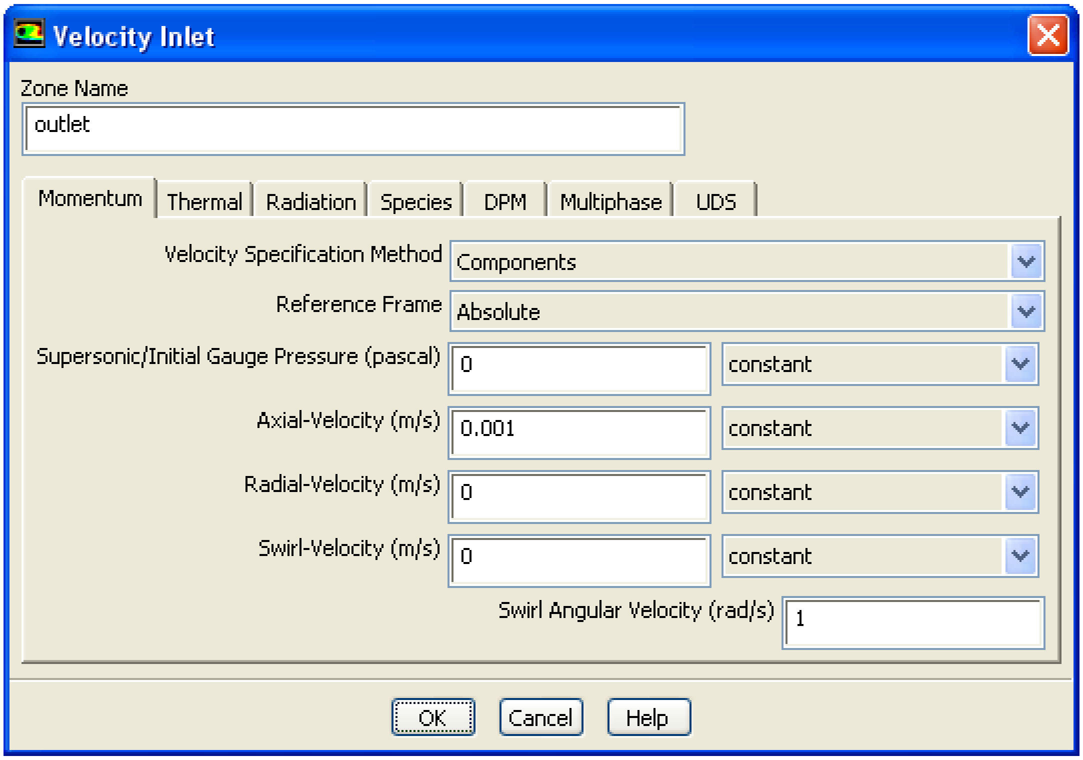


c. Click **OK** to close the **Velocity Inlet** dialog box.

2. Set the boundary conditions for the outlet (**outlet**).

Boundary Conditions → **outlet** → **Edit...**

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



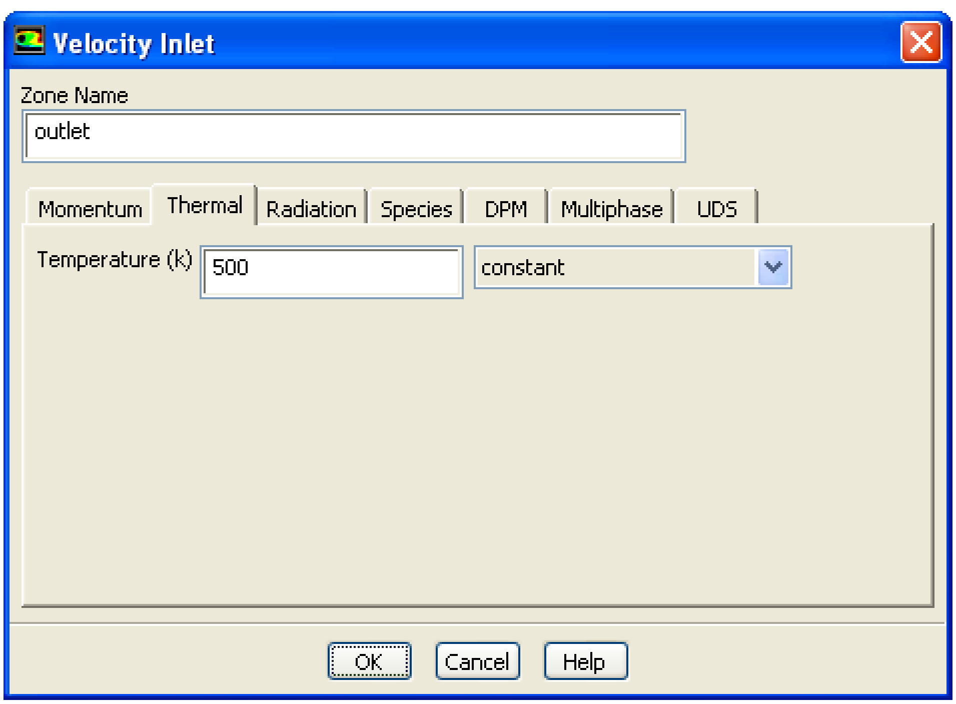
a. Select **Components** from the **Velocity Specification Method** drop-down list.

   *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**.

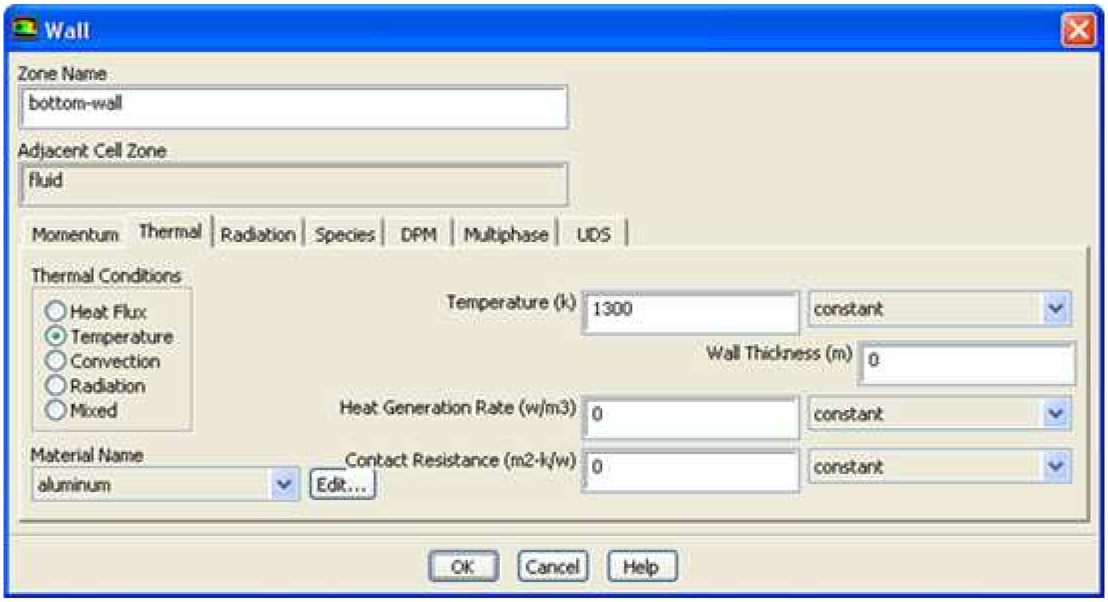


e. Click **OK** to close the **Velocity Inlet** dialog box.

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

Boundary Conditions → **bottom-wall** → **Edit...**

a. Click the **Thermal** tab.



i. Select **Temperature** from the **Thermal Conditions** group box.

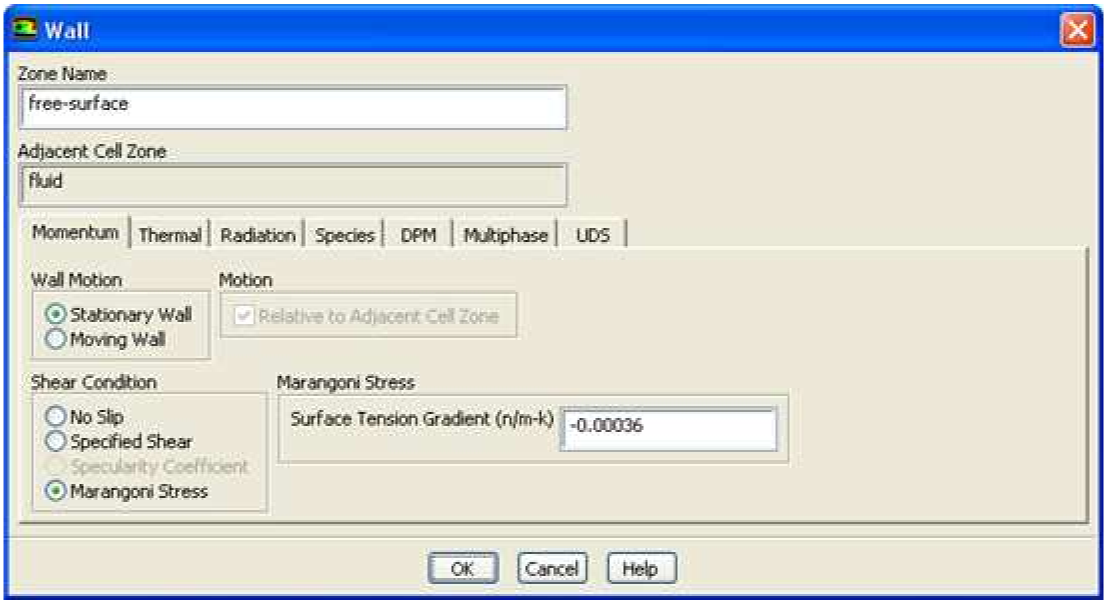
ii. Enter `1300` K for **Temperature**.

b. Click **OK** to close the **Wall** dialog box.

4. Set the boundary conditions for the free surface (**free-surface**).

Boundary Conditions → **free-surface** → **Edit...**

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.

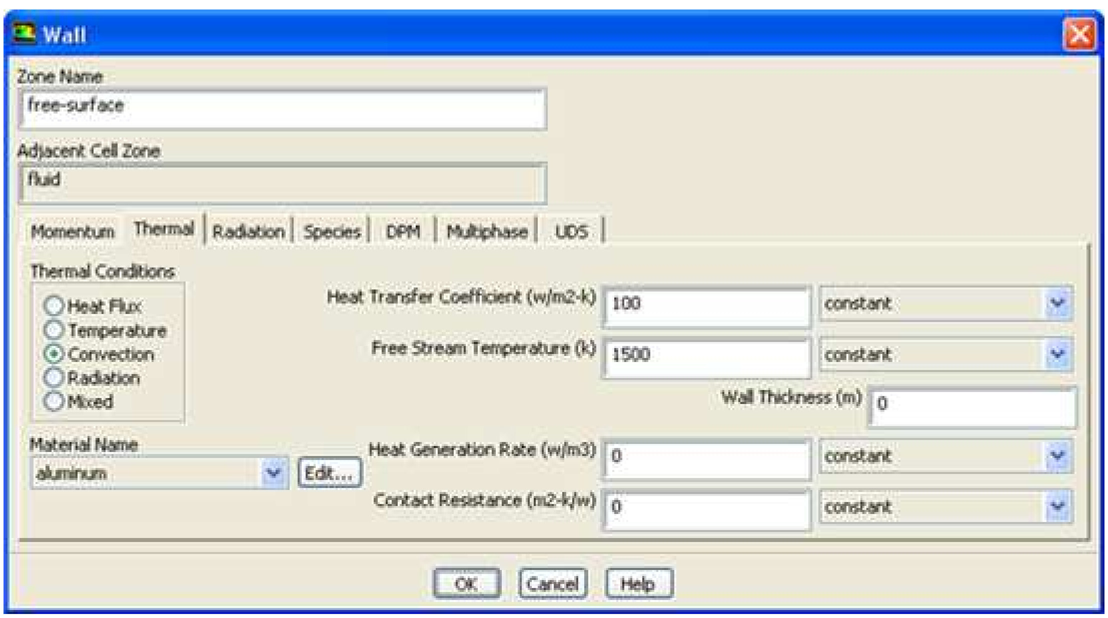


a. Select **Marangoni Stress** from the **Shear Condition** group box.

*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/m^2-k for **Heat Transfer Coefficient**.

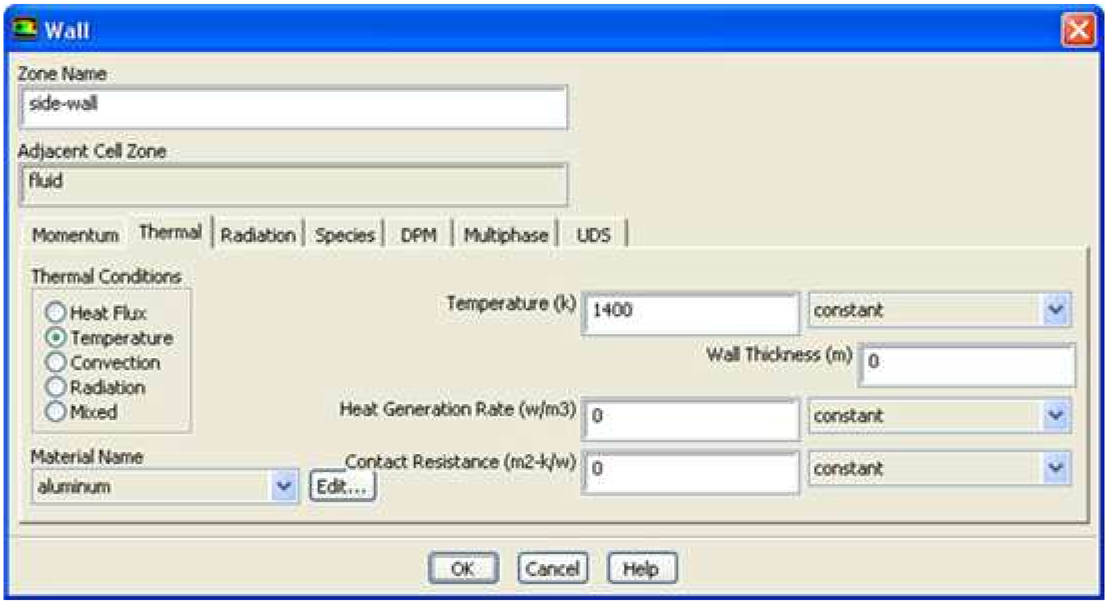
iii. Enter `1500` K for **Free Stream Temperature**.

d. Click **OK** to close the **Wall** dialog box.

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

Boundary Conditions → **side-wall** → **Edit...**

a. Click the **Thermal** tab.



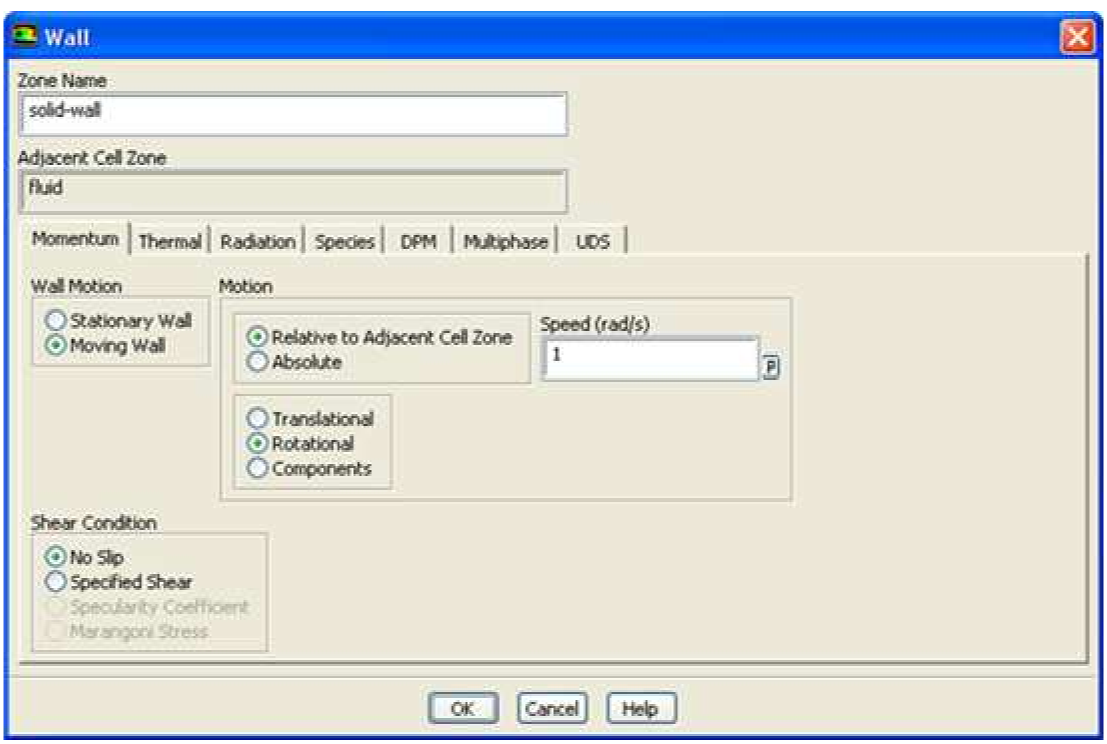
i. Select **Temperature** from the **Thermal Conditions** group box.

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**).

Boundary Conditions → **solid-wall** → **Edit...**



a. Select **Moving Wall** from the **Wall Motion** group box.

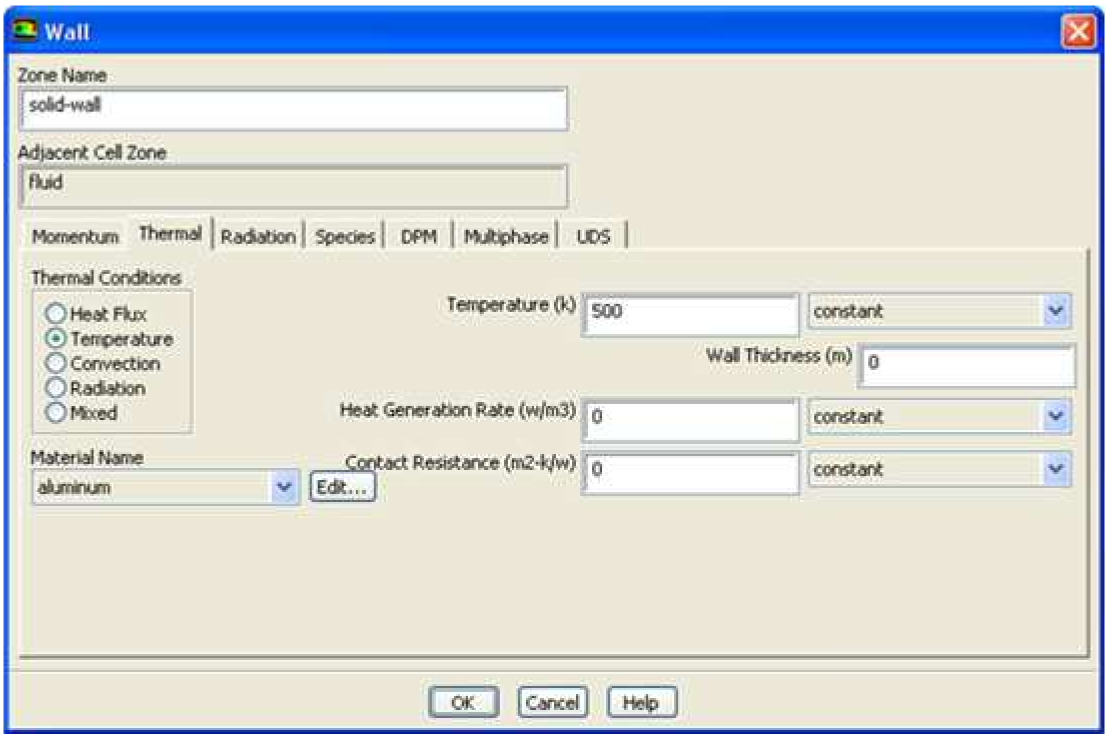
   *The **Wall** dialog box will expand to show additional parameters.*

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.



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

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

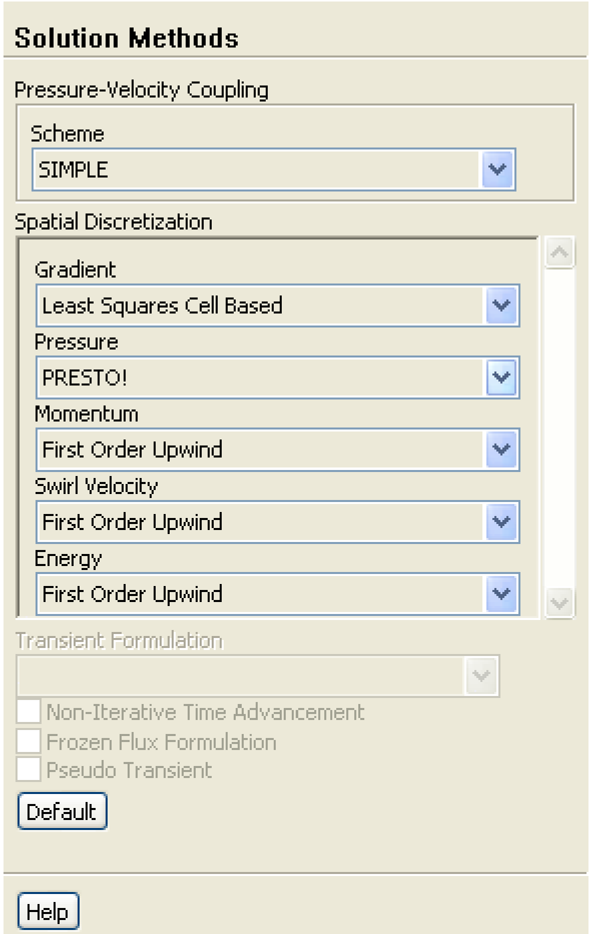
e. Click **OK** to close the **Wall** dialog box.

24.4.8. 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



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

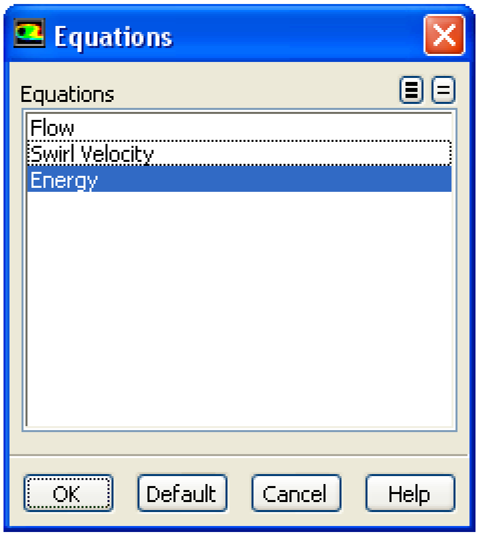
b. Select **PRESTO!** from the **Pressure** drop-down list in the **Spatial Discretization** group box.

   *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 → **Equations...**

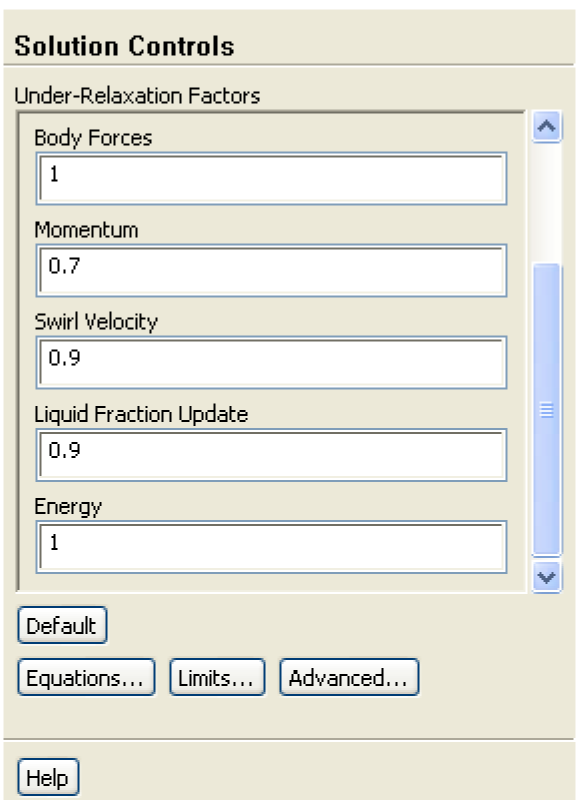


a. Deselect **Flow** and **Swirl Velocity** from the **Equations** selection list to disable the calculation of flow and swirl velocity equations.

b. Click **OK** to close the **Equations** dialog box.

3. Set the **Under-Relaxation Factors**.

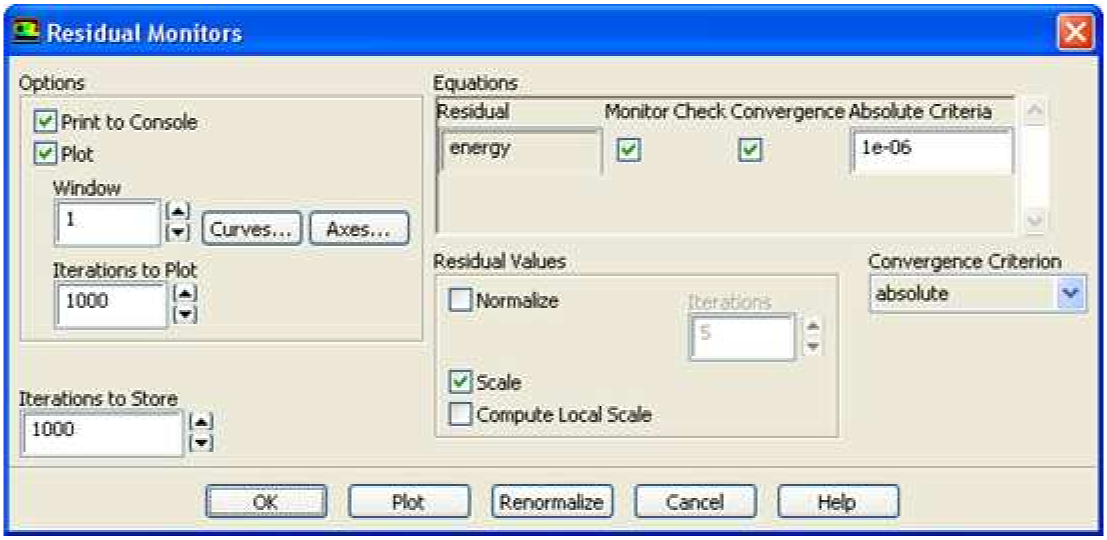
Solution Controls



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. Select **Hybrid Initialization** from the **Initialization Methods** group box.

b. Click **Initialize**.

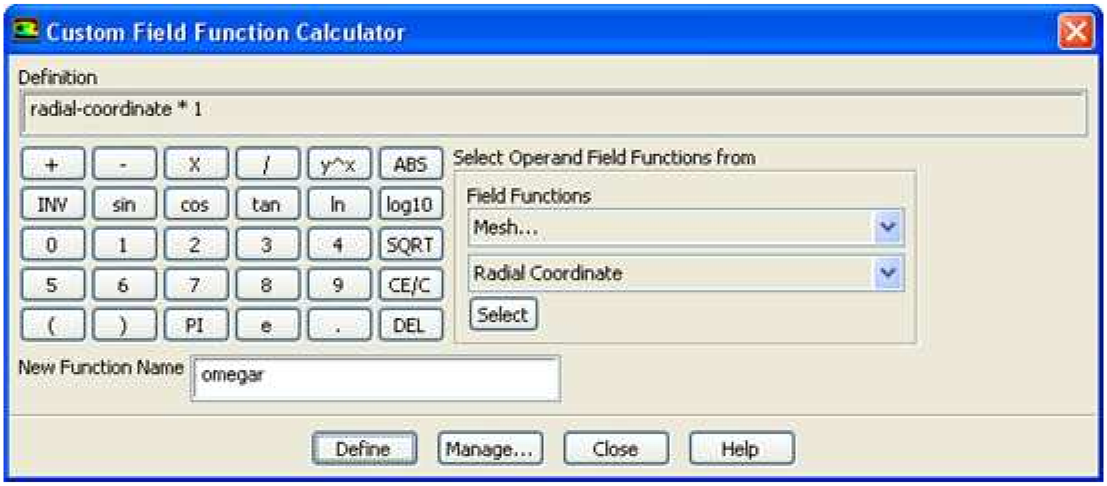
Note

For flows in complex topologies, hybrid initialization will provide better initial velocity and pressure field than standard initialization. This in general will help in improving the convergence behavior of the solver.

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 Ωr*, where* Ω *is the angular velocity and* r *is the radial* *coordinate. Since Ω = 1 rad/s, you can simplify the equation to simply r. In this example, the value of Ω is included for demonstration purposes.*



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 × button on the calculator pad.

d. Click the **1** button.

e. Enter `omegar` for **New Function Name**.

f. Click **Define**.

Note

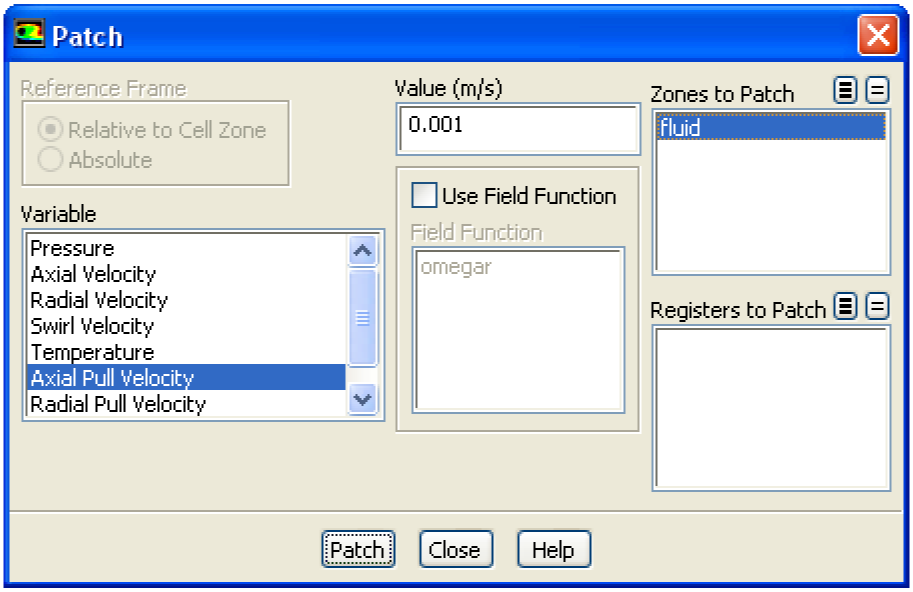
To check the function definition, you can click **Manage...** to open the **Field Function Definitions** dialog box. Then select **omegar** from the **Field Functions** selection list to view the function definition.

g. Close the **Custom Field Function Calculator** dialog box.

7. Patch the pull velocities.

   Solution Initialization → **Patch...**

   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.



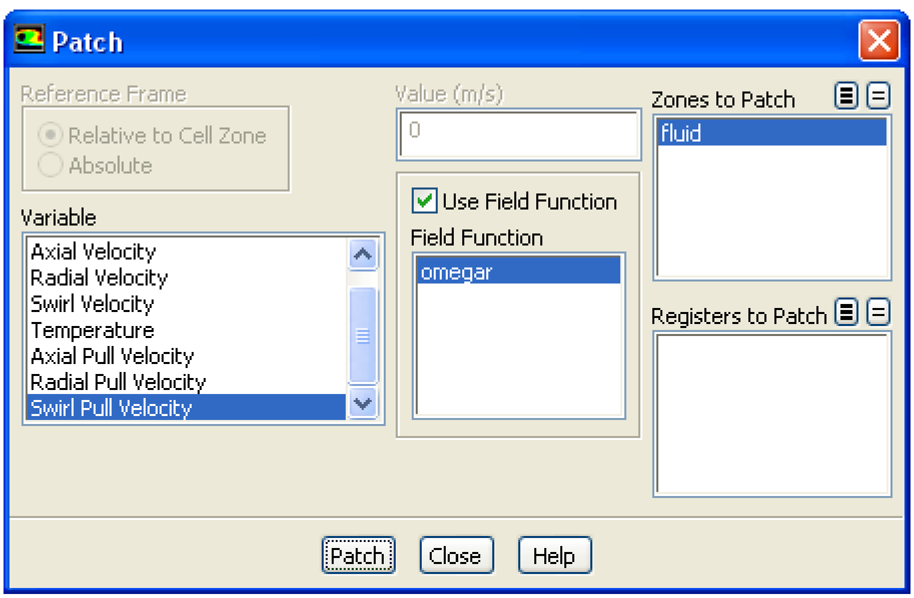
a. Select **Axial Pull Velocity** from the **Variable** selection list.

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 **omegar** from the **Field Function** selection list.

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

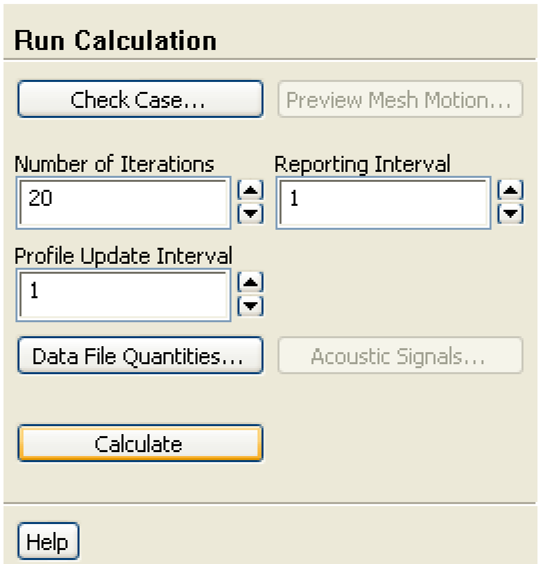
i. Click **Patch** and close the **Patch** dialog box.

8. Save the initial case and data files (`solid0.cas.gz` and `solid0.dat.gz`).

   File → **Write** → **Case & Data...**

9. Start the calculation by requesting 20 iterations.

   Run Calculation



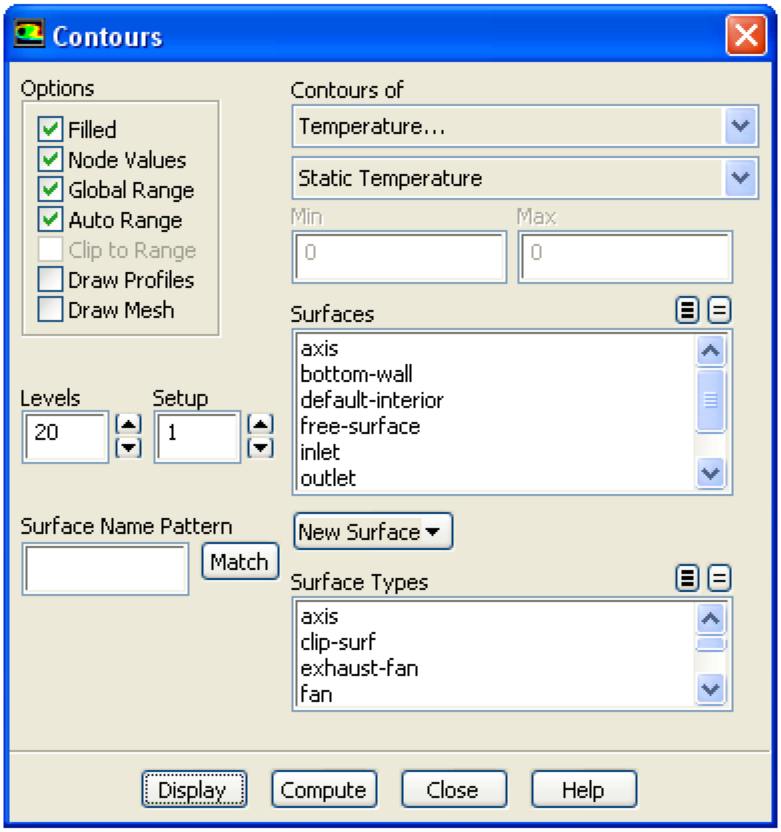
   a. Enter `20` for **Number of Iterations**.

   b. Click **Calculate**.

   The solution will converge in approximately 8 iterations.

10. Display filled contours of temperature (*Figure 24.3* (p. 913)).

    Graphics and Animations → **Contours** → **Set Up...**

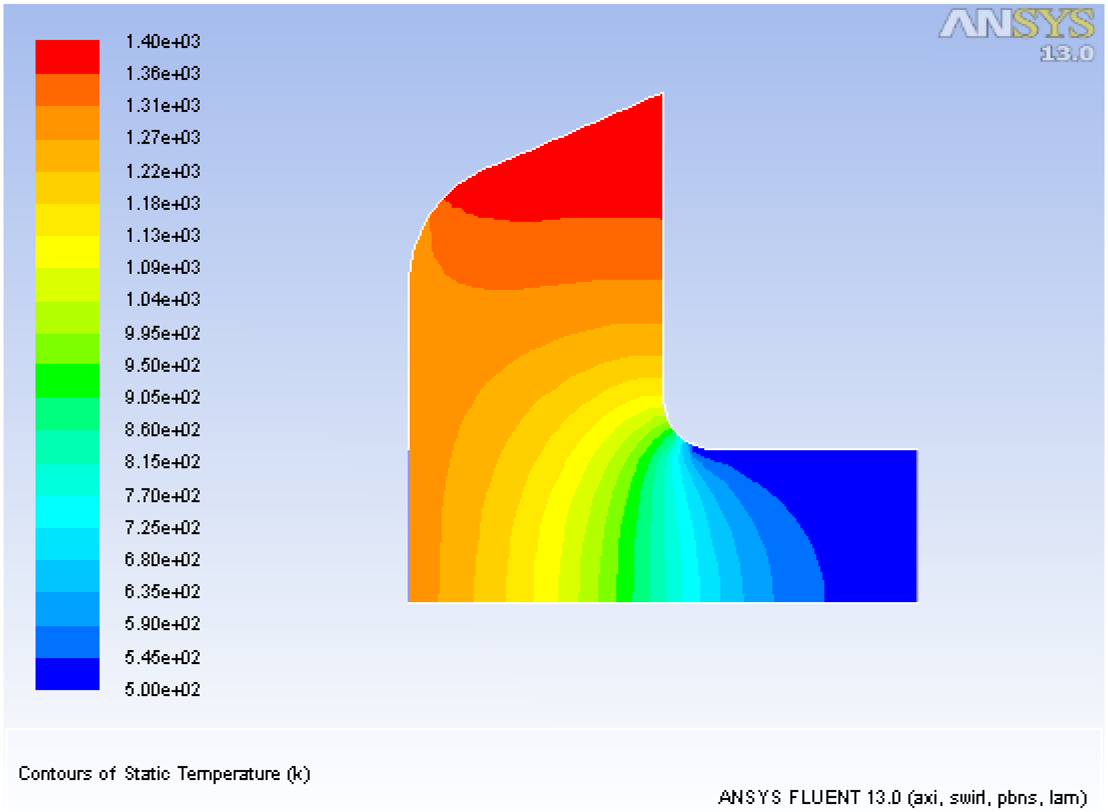


a. Enable the **Filled** option.

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

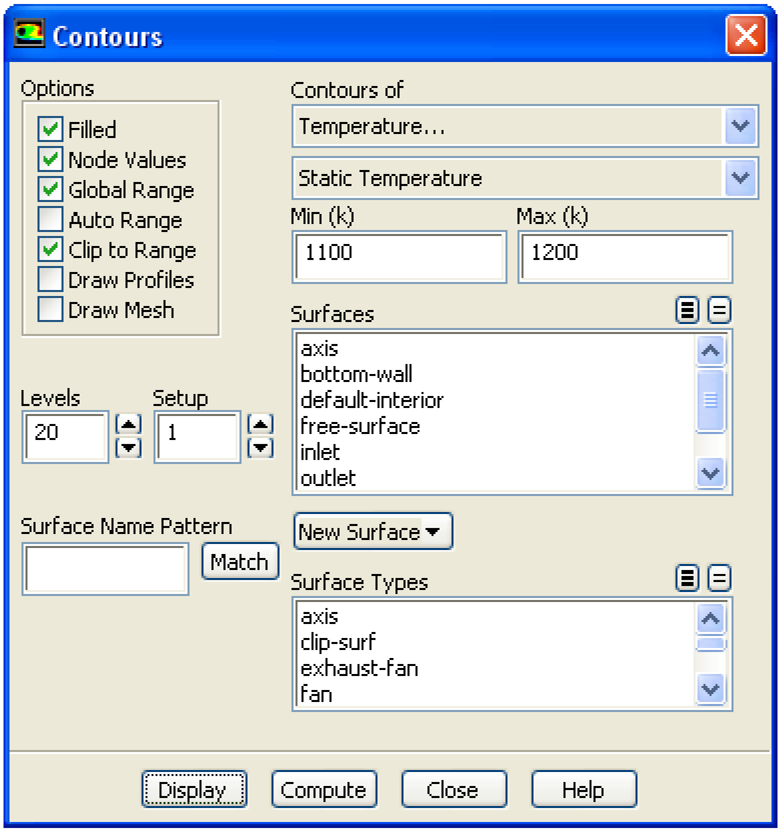
c. Click **Display** (*Figure 24.3* (p. 913)).

Figure 24.3 Contours of Temperature for the Steady Conduction Solution



11. Display filled contours of temperature to determine the thickness of mushy zone.

 Graphics and Animations → **Contours** → **Set Up...**



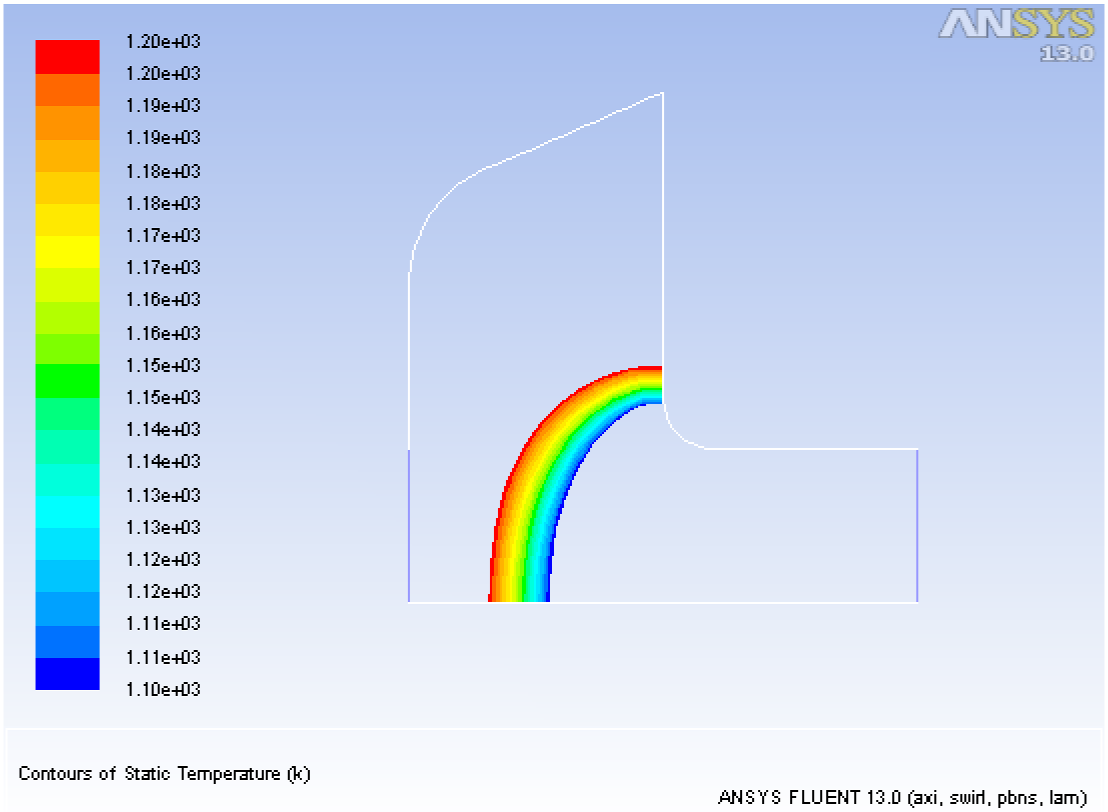
a. Disable **Auto Range** in the **Options** group box.

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

b. Enter `1100` for **Min** and `1200` for **Max**.

c. Click **Display** (See *Figure 24.4* (p. 915)) and close the **Contours** dialog box.

Figure 24.4 Contours of Temperature (Mushy Zone) for the Steady Conduction Solution



12. Save the case and data files for the steady conduction solution (`solid.cas.gz` and `solid.dat.gz`).

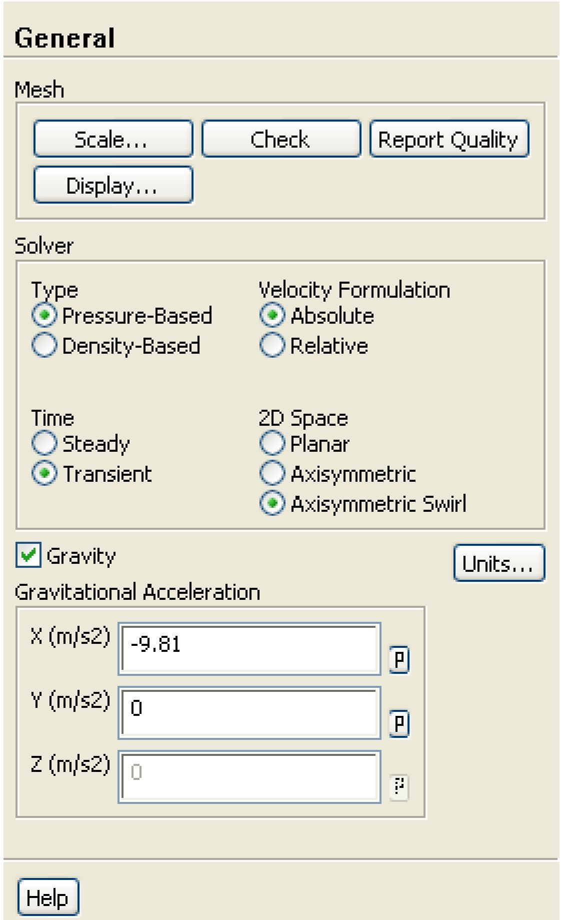
    File → **Write** → **Case & Data...**

24.4.9. 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.

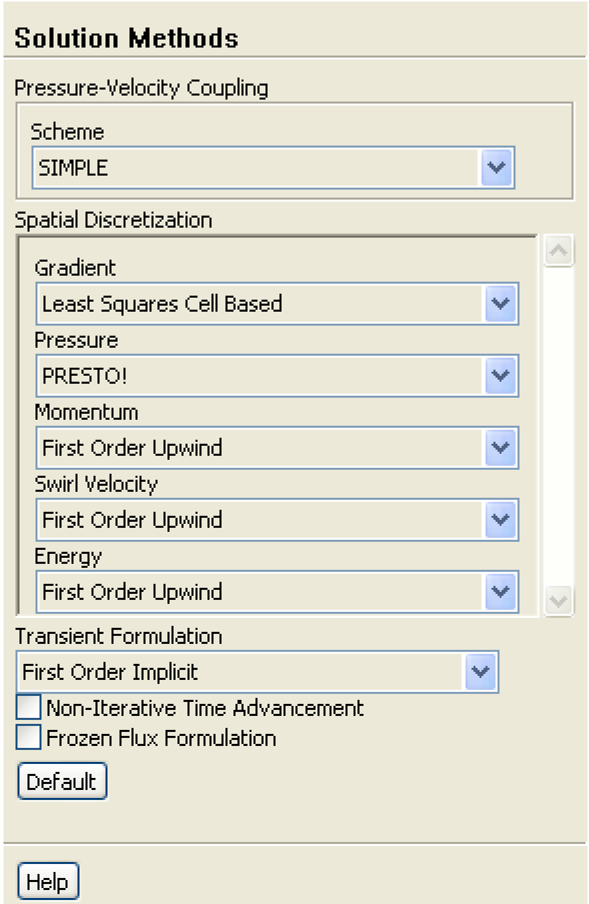
   General



a. Select **Transient** from the **Time** list.

2. Set the solution parameters.

Solution Methods

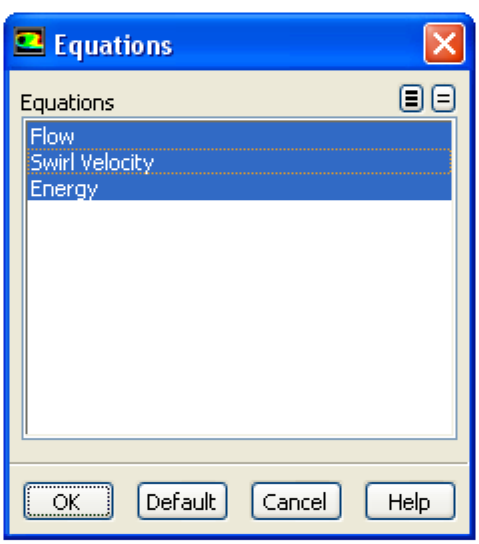


a. Retain the default selection of **First Order Implicit** from the **Transient Formulation** drop-down list.

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.

Solution Controls → **Equations...**



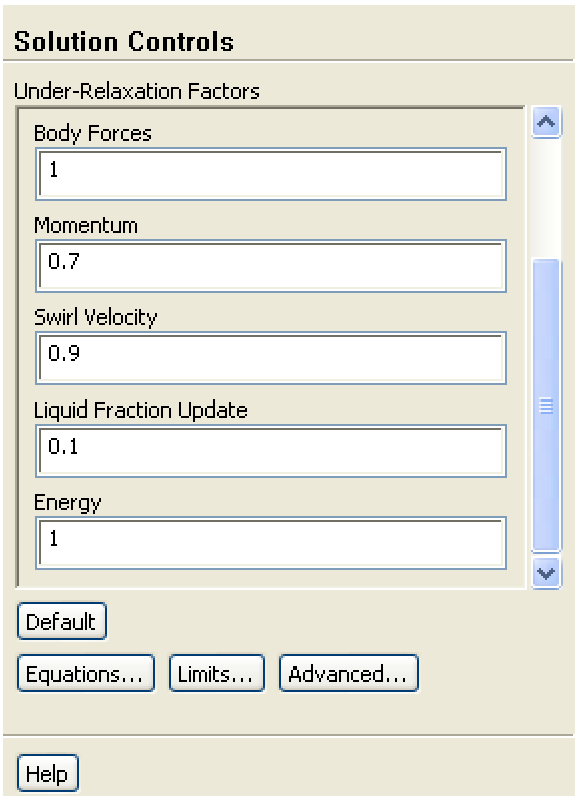
a. Select **Flow** and **Swirl Velocity** and ensure that **Energy** is selected from the **Equations** selection list.

*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**.

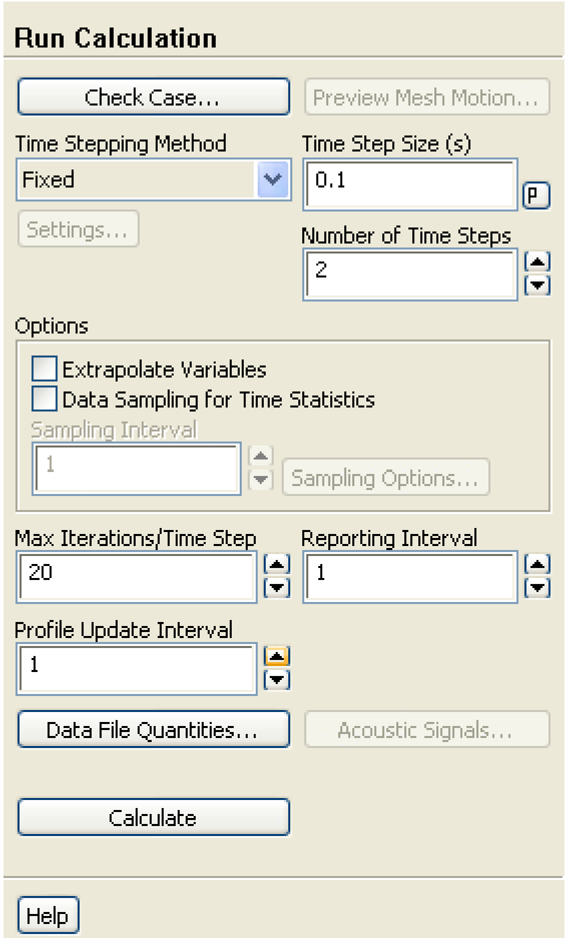
b. Retain the default values for other **Under-Relaxation Factors.**

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



a. Enter `0.1` s for **Time Step Size**.

b. Set the **Number of Time Steps** to 2.

c. Retain the default value of `20` for **Max Iterations/Time Step**.

d. Click **Calculate**.

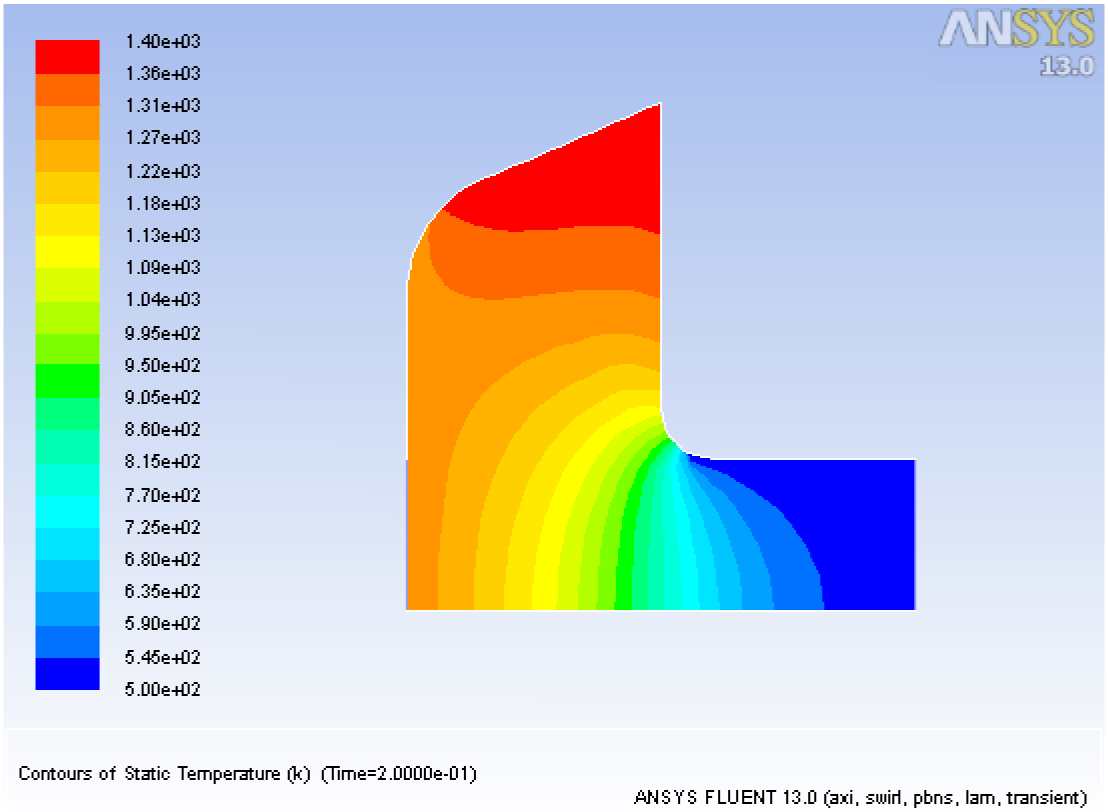
7. Display filled contours of the temperature after 0.2 seconds.

Graphics and Animations → **Contours** → **Set Up...**

a. Make sure that **Temperature...** and **Static Temperature** are selected from the **Contours of** drop-down lists.

b. Click **Display** (See *Figure 24.5* (p. 920)).

Figure 24.5 Contours of Temperature at t=0.2 s



8. Display contours of stream function (*Figure 24.6* (p. 921)).

Graphics and Animations → **Contours** → **Set Up...**

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 24.6 Contours of Stream Function at t=0.2 s

As shown in Figure 24.6 (p. 921), 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 24.7* (p. 922)).

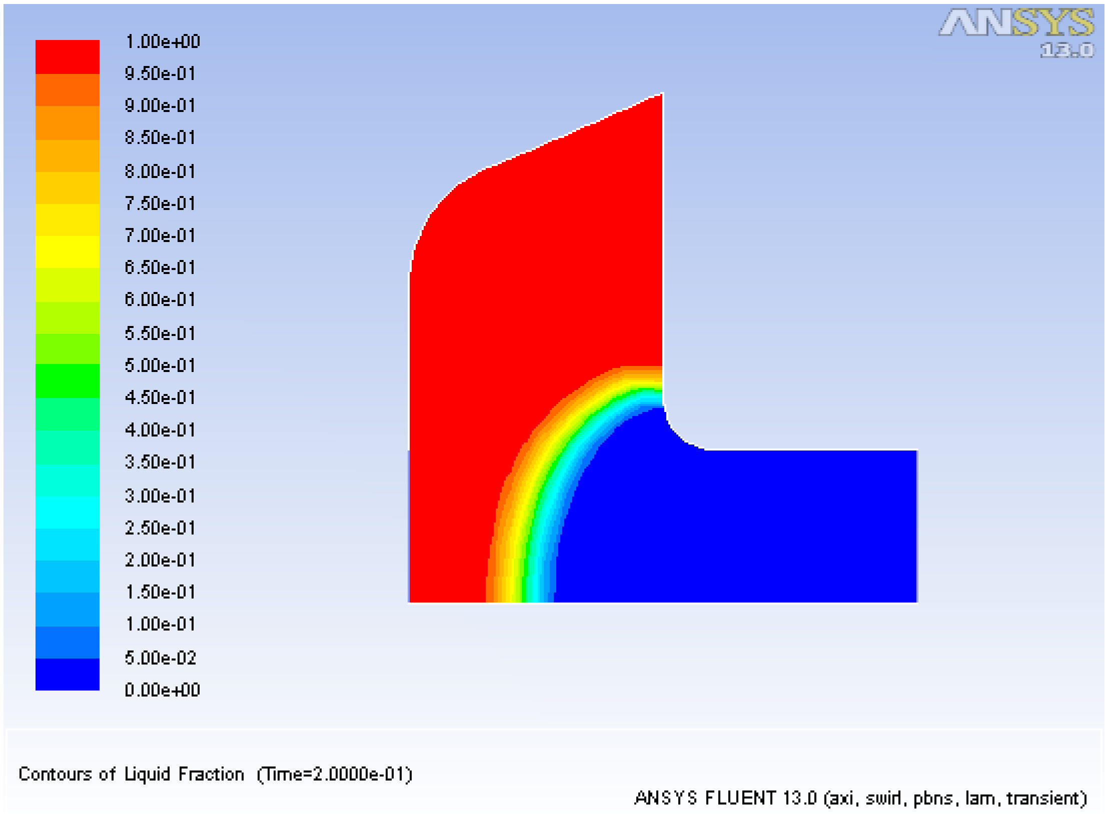
   Graphics and Animations → **Contours** → **Set Up...**

   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.

Figure 24.7 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 24.7 (p. 922), the mushy zone divides the liquid and solid regions roughly in half.

10. Continue the calculation for 48 additional time steps.

Run Calculation

a. Enter 48 for **Number of Time Steps**.

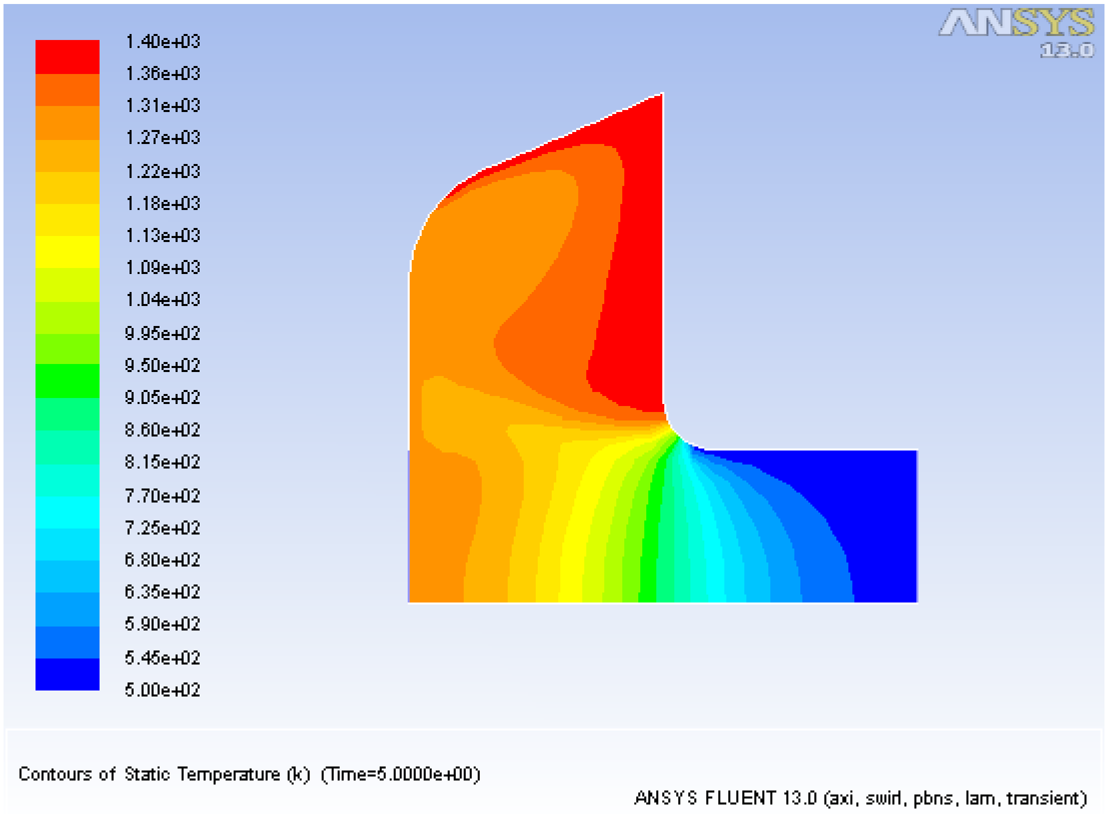
b. Click **Calculate**.

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 24.8* (p. 923)).

Graphics and Animations → **Contours** → **Set Up...**

Figure 24.8 Contours of Temperature at t=5 s



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 24.8 (p. 923), 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 24.9* (p. 924)).

Graphics and Animations → **Contours** → **Set Up...**

a. Disable **Filled** in the **Options** group box.

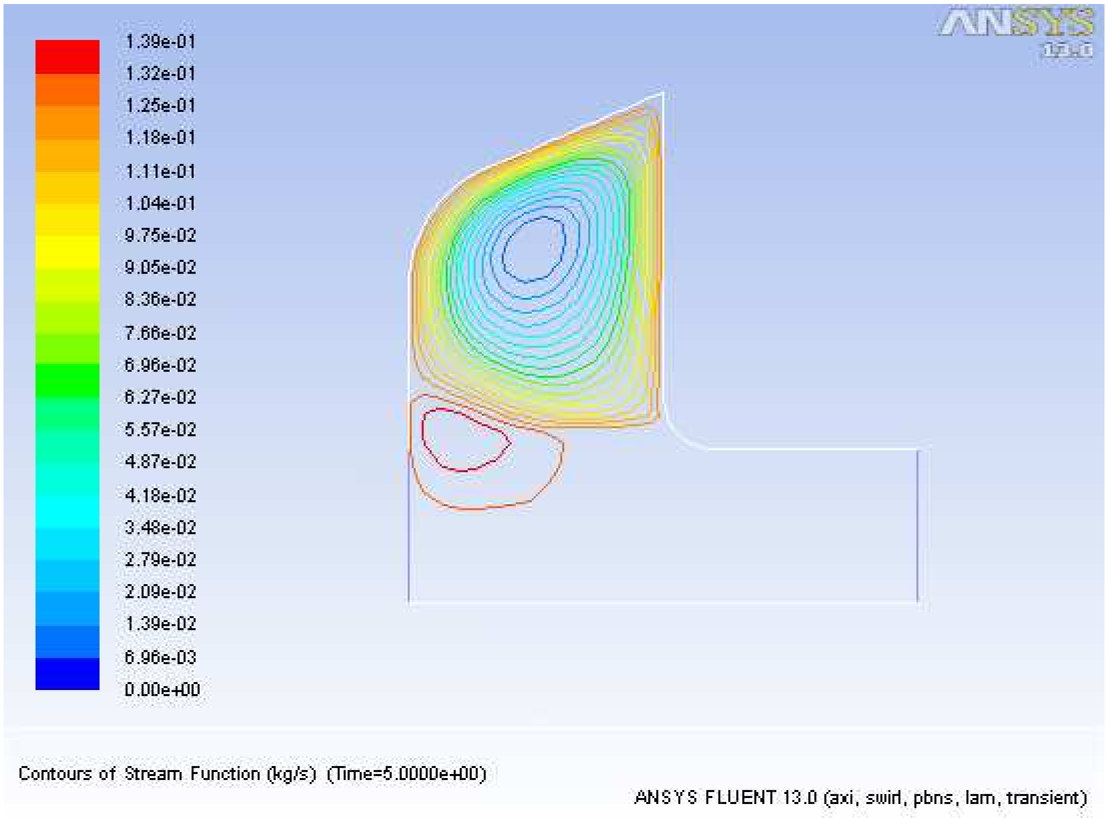
b. Select **Velocity...** and **Stream Function** from the **Contours** of drop-down lists.

c. Click **Display**.

As shown in Figure 24.9 (p. 924), the flow has developed more fully by 5 seconds, as compared with Figure 24.6 (p. 921) 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.

Figure 24.9 Contours of Stream Function at t=5 s



13. Display filled contours of liquid fraction (*Figure 24.10* (p. 925)).

Graphics and Animations → **Contours** → **Set Up...**

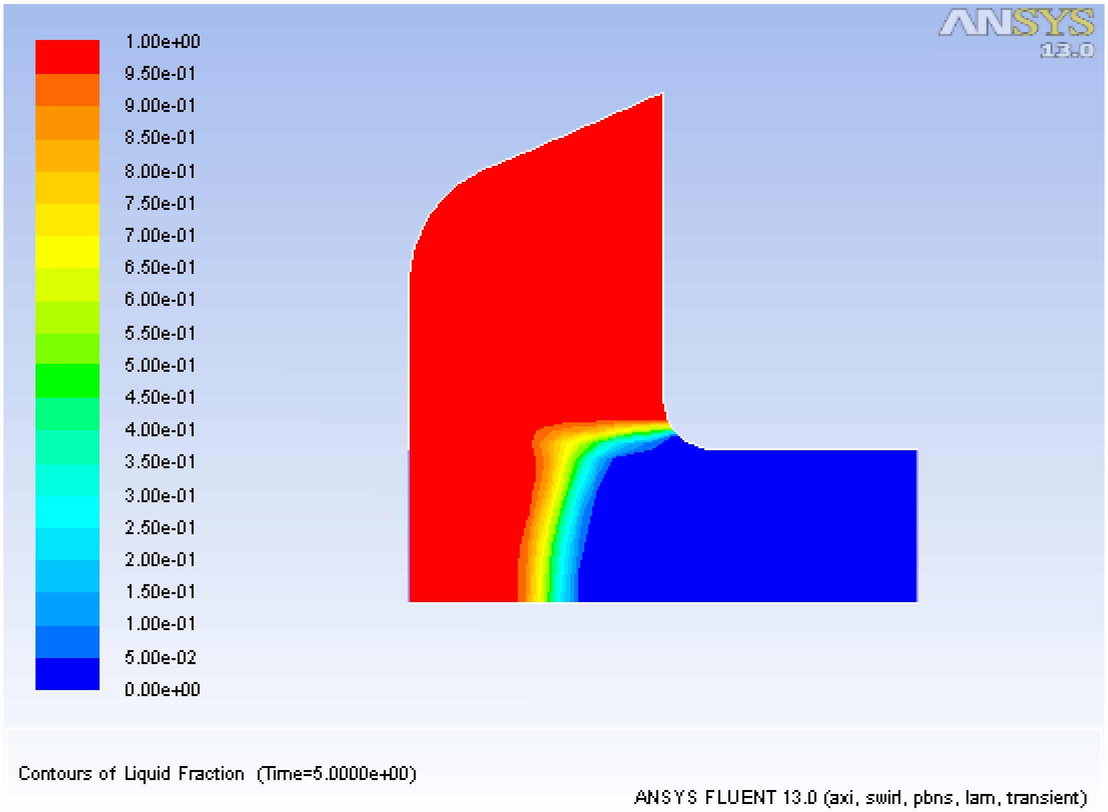
a. Enable **Filled** in the **Options** group box.

b. Select **Solidification/Melting...**and **Liquid Fraction** from the **Contours of** drop-down lists.

c. Click **Display** and close the **Contours** dialog box.

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 24.10 (p. 925)).

Figure 24.10 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`).

    File → **Write** → **Case & Data...**

24.5. 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 "Modeling Solidification and Melting" in the User's Guide.

24.6. 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 *Introduction to Using ANSYS FLUENT: Fluid Flow and Heat Transfer in a Mixing Elbow* (p. 111).