Slip Flow Benchmark

Introduction

As the absolute pressure in a gas flow is reduced, the mean free path of the gas molecules begins to approach the size of the vessel through which the flow occurs. Such rarefied flows are characterized by a parameter known as the Knudsen number, which is the ratio of the mean free path to the characteristic length of the geometry. In a rarefied flow the gas cannot be treated as a continuum and the kinetic nature of the flow must be considered. However, at moderate Knudsen numbers between approximately 0.01 and 0.1, the flow can be modeled using the Navier-Stokes equations, except in a thin region adjacent to the walls, termed the Knudsen layer. This regime is termed the slip flow regime. In the slip flow regime the Knudsen layer can be replaced by alternative boundary conditions for the Navier-Stokes equations. A slip velocity along the geometry walls develops, and the temperature at the walls of the structure becomes discontinuous at this level of approximation. Phenomena such as viscous slip and thermal creep or transpiration become important.

This model is a benchmark model for COMSOL's Slip Flow interface. It is based on analytic and numeric calculations presented in Ref. 1. Air at atmospheric pressure flows through a conducting microchannel connecting two reservoirs maintained at different temperatures. A flow between the two reservoirs develops as a result of thermal creep along the channel wall, which in turn produces a pressure gradient. At steady state the net flow through the channel is zero, but a pressure gradient exists between the hot and cold sides of the reservoir and a circulating flow occurs.

Model Definition

The model consists of two chambers 7.5 µm by 15 µm, with a depth significantly larger than either of these dimensions (this means that the simulation can be performed using the 2D XY interface). The chambers are linked by a narrow channel of the same depth with width 1.5 µm and length 15 µm. The chamber and channel walls are fabricated from silicon and have a thickness of 1 µm. The walls of the two chambers are in thermal contact with heat sinks maintained at 300 K and 400 K, respectively. The channel walls are thermally insulated. Figure 1 shows the model geometry. The gas in the center of the channel is at a pressure of 1 atmosphere.

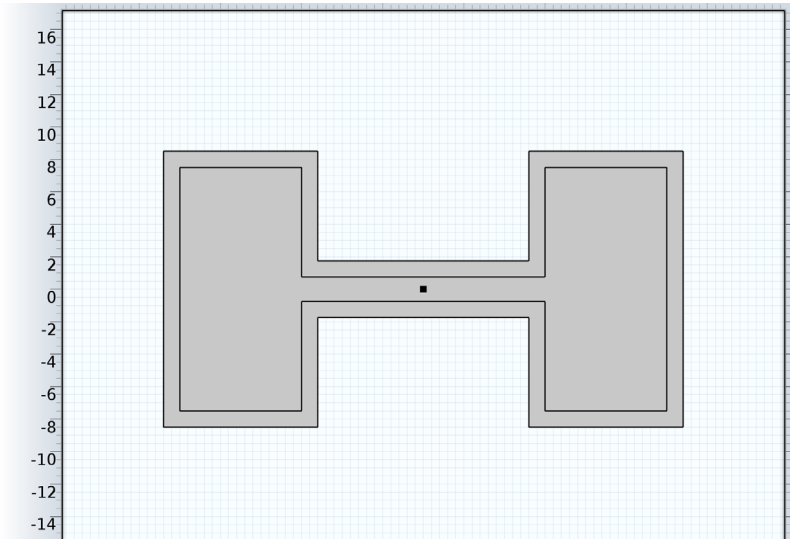


Figure 1: The Model Geometry

For channels of micron scale dimensions the Knudsen number becomes greater than 0.01 even at atmospheric pressure. It is therefore necessary to use a slip condition on the surfaces of walls in the vicinity of the channel.

SLIP WALL BOUNDARY CONDITION

The slip velocity, $\mathbf{u}_{\text{slip}}$, along the walls of the channel is given by (Ref. 2):

$$\mathbf{u}_{\text{slip}} = \sigma_s \frac{\lambda}{\mu}(\boldsymbol{\tau}\mathbf{n} - ((\mathbf{n}^T\boldsymbol{\tau}\,\mathbf{n})\mathbf{n})) + \sigma_T \frac{\mu}{\rho T_g}[\nabla T_w - (\mathbf{n}\cdot\nabla T_w)\mathbf{n}]$$
$$T_w = T_g - \zeta_T \lambda \mathbf{n}\cdot\nabla T_g \qquad (1)$$

where λ is the mean free path of the gas, $\mathbf{n}$ is the boundary normal, τ is the viscous stress tensor, T_w is the wall temperature, T_g is the temperature of the gas, μ is its viscosity, and ρ is its density. The slip coefficients: σ_s (the viscous slip coefficient), σ_T (the thermal slip coefficient), and ζ_T (the temperature jump coefficient) can be defined by material properties and the tangential momentum accommodation coefficient, a_v, within a generalized form of Maxwell's original slip model (see Ref. 2 and Ref. 3). For a model in which the surface reflects some molecules diffusely and some specularly, a_v is the fraction of molecules which are reflected diffusely. Within Maxwell's model the slip coefficients are:

$$\sigma_s = 2C_0\frac{2-a_v}{a_v}$$

$$\sigma_T = \frac{3}{4}$$

$$\zeta_T = 4C_0\frac{2-a_v}{a_v}\frac{\gamma}{\gamma+1}\frac{\kappa}{\mu C_p}$$

where κ is the thermal conductivity of the gas, and C_0 is a constant derived from kinetic theory ($C_0 = 0.499$ for hard elastic spheres; see Ref. 2).

The mean free path can be computed from the gas properties using the following equation (Ref. 2):

$$\lambda = \frac{1}{C_0\rho}\frac{\mu}{\langle c\rangle}$$

$$\langle c\rangle = \left(\frac{8RT}{\pi M_n}\right)^{1/2} = \left(\frac{8p}{\pi\rho}\right)^{1/2}$$

Results and Discussion

Figure 2 shows the mean free path of the gas throughout the simulation domain. Since the channel width is 1.5 µm, a mean free path of 75 nm corresponds to a Knudsen number of 0.05. This value is comparable to the Knudsen number of the gas in the channel and is within the slip flow regime.

The velocity of the gas in the x-direction is shown in Figure 3, together with the velocity streamlines. In the steady state there is no net flow through the channel, but a flow parallel to the walls, in the direction of the thermal gradient (cold to hot), develops due to thermal creep. To compensate for this flow a back flow develops in the center of the channel, which is driven by a pressure gradient in the gas.

The temperature distribution in the channels is shown in Figure 4. The thermal gradient is predominately parallel to the walls, however there are some normal thermal gradients in the vicinity of the opening to the channel, which result in a temperature jump between the gas and the wall, according to Equation 1. This temperature jump simulates the effect of the Knudsen layer, which is not captured by the continuum Navier-Stokes equations.

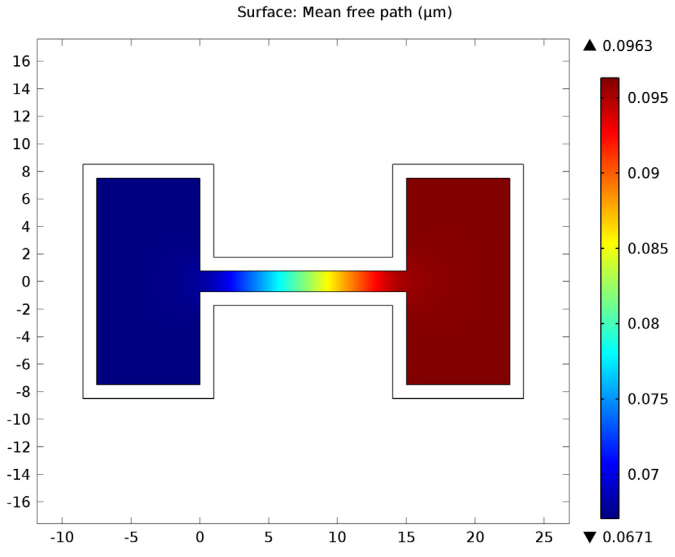


Figure 2: Gas mean free path. The channel width is 1.5 μm, so the Knudsen number varies between 0.064 and 0.045.

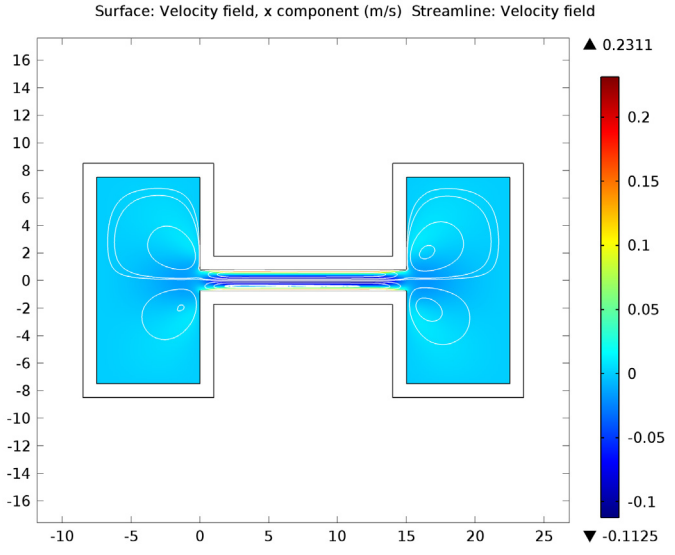


Figure 3: x-velocity (color) and streamlines (white) inside the channel. Flow is driven by thermal creep along the walls of the channel but a back-flow, driven by the pressure difference between the reservoirs, occurs in the center of the channel.

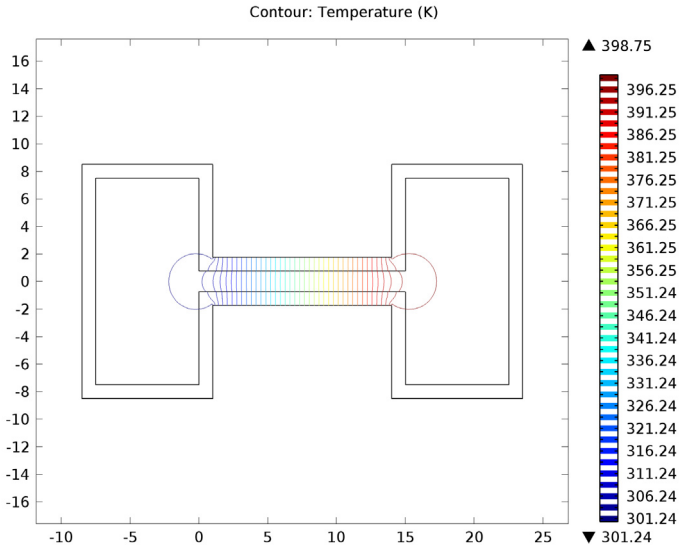


Figure 4: Temperature contours within the model. Note that a temperature jump occurs between the vessel walls and the gas when normal heat fluxes occur into the wall from the gas.

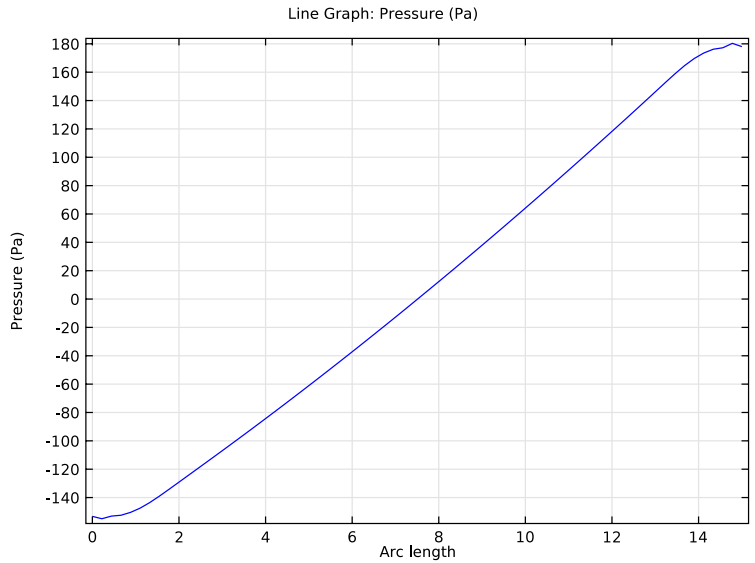


Figure 5: Pressure on the wall of the channel, as a function of position.

Figure 5 shows the relative pressure acting on the channel wall, as a function of position along the wall. The pressure is lowest in the coolest chamber, at 151 Pa below atmospheric, and highest in the warmer chamber, at 179 Pa above atmospheric pressure. The asymmetry of the pressure distribution about the center of the channel results from changes in the number density of the gas in the two reservoirs. The total pressure difference of 330 Pa is similar to the value predicted in Ref. 1 for a numerical simulation of an equivalent problem (336 Pa), and is also in good agreement with the value predicted by the analytic model of Ref. 1, which is (335 Pa). This model therefore serves as a benchmark for the Slip Flow interface.

References

1. G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

2. E.H. Kennard, *Kinetic Theory of Gases*, McGraw-Hill, New York, 1938.

3. J.C. Maxwell, "On Stresses in Rarefied Gases Arising from Inequalities of Temperature," *Phil. Trans. R. Soc. Lond.* vol. 170, pp. 231–256, 1879.

Model Library path: `Microfluidics_Module/Rarefied_Flow/slip_flow_benchmark`

Modeling Instructions

NEW

1 In the **New** window, click the **Model Wizard** button.

MODEL WIZARD

1 In the **Model Wizard** window, click the **2D** button.

2 In the **Select physics** tree, select **Fluid Flow>Rarefied Flow>Slip Flow (slpf)**.

3 Click the **Add** button.

4 Click the **Study** button.

5 In the tree, select **Preset Studies>Stationary**.

6 Click the **Done** button.

GEOMETRY 1

Change the length units to μm and specify the geometry.

1 In the **Model Builder** window, under **Component 1** click **Geometry 1**.

2 In the **Geometry** settings window, locate the **Units** section.

3 From the **Length unit** list, choose **μm**.

Rectangle 1

1 Right-click **Component 1>Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `15`.

4 In the **Height** edit field, type `1.5`.

5 Locate the **Position** section. In the **y** edit field, type `-0.75`.

6 Click the **Build Selected** button.

Rectangle 2

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `7.5`.

4 In the **Height** edit field, type `15`.

5 Locate the **Position** section. In the **x** edit field, type `-7.5`.

6 In the **y** edit field, type `-7.5`.

7 Click the **Build Selected** button.

Rectangle 3

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `7.5`.

4 In the **Height** edit field, type `15`.

5 Locate the **Position** section. In the **x** edit field, type `15`.

6 In the **y** edit field, type `-7.5`.

7 Click the **Build Selected** button.

Union 1

1 On the **Geometry** toolbar, click **Union**.

2 Click in the **Graphics** window and then press Ctrl+A to select all objects.

3 In the **Union** settings window, locate the **Union** section.

4 Clear the **Keep interior boundaries** check box.

5 Click the **Build Selected** button.

6 Click the **Zoom Extents** button on the Graphics toolbar.

Rectangle 4

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `9.5`.

4 In the **Height** edit field, type `17`.

5 Locate the **Position** section. In the **x** edit field, type `-8.5`.

6 In the **y** edit field, type `-8.5`.

7 Click the **Build Selected** button.

Rectangle 5

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `15`.

4 In the **Height** edit field, type `3.5`.

5 Locate the **Position** section. In the **y** edit field, type `-1.75`.

6 Click the **Build Selected** button.

Rectangle 6

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `9.5`.

4 In the **Height** edit field, type `17`.

5 Locate the **Position** section. In the **x** edit field, type `14`.

6 In the **y** edit field, type `-8.5`.

7 Click the **Build Selected** button.

Union 2

1 On the **Geometry** toolbar, click **Union**.

2 Select the objects **r4**, **r5**, and **r6** only.

3 In the **Union** settings window, locate the **Union** section.

4 Clear the **Keep interior boundaries** check box.

5 Click the **Build Selected** button.

Point 1

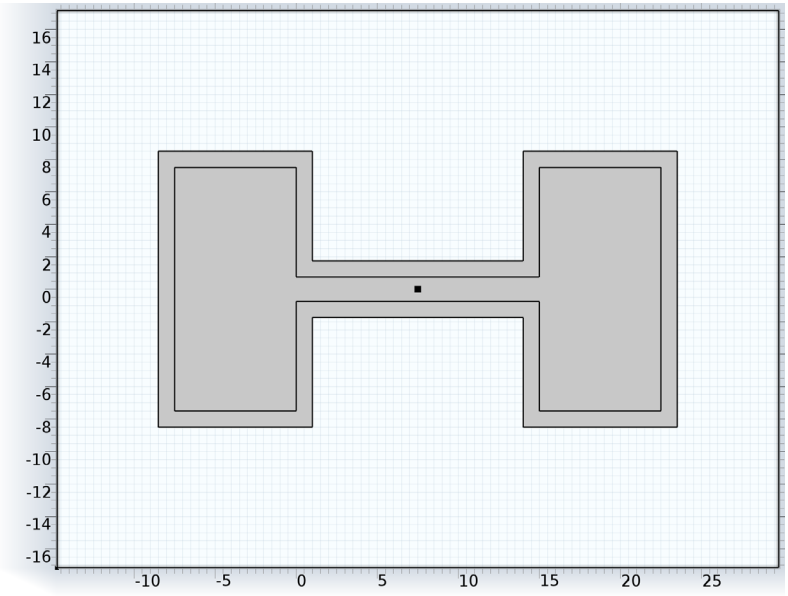
1 Right-click **Geometry 1** and choose **Point**.

2 In the **Point** settings window, locate the **Point** section.

3 In the **x** edit field, type `7.5`.

4 Click the **Build All Objects** button.

5 Click the **Zoom Extents** button on the Graphics toolbar.



Specify the material properties for the cavity walls and the gas.

MATERIALS

On the **Home** toolbar, click **Add Material**.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Built-In>Air**.

3 In the **Add material** window, click **Add to Component**.

MATERIALS

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Built-In>Silicon**.

3 In the **Add material** window, click **Add to Component**.

MATERIALS

Silicon

1 In the **Model Builder** window, under **Component 1>Materials** click **Silicon**.

2 Select Domain 1 only.

SLIP FLOW

Set the physics for the solid regions to be the heat transfer equation.

Heat Transfer in Solids 1

1 On the **Physics** toolbar, click **Domains** and choose **Heat Transfer in Solids**.

2 Select Domain 1 only.

Apply thermal insulation on the boundaries of the connecting duct.

Thermal Insulation 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Thermal Insulation**.

2 Select Boundaries 12 and 14 only.

Fix the temperature on the walls of the two reservoirs.

Temperature 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 Select Boundaries 1–3, 11, and 13 only.

3 In the **Temperature** settings window, locate the **Temperature** section.

4 In the T_0 edit field, type `300[K]`.

Temperature 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 Select Boundaries 15–18 and 24 only.

3 In the **Temperature** settings window, locate the **Temperature** section.

4 In the T_0 edit field, type `400[K]`.

Apply slip boundary conditions near and inside the channel.

Slip Wall 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Slip Wall**.

2 In the **Slip Wall** settings window, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All boundaries**.

Apply a pressure constraint in the center of the channel.

Pressure Point Constraint 1

1 On the **Physics** toolbar, click **Points** and choose **Pressure Point Constraint**.

2 Select Point 13 only.

Set up the mesh.

MESH 1

Size 1

1 In the **Model Builder** window, under **Component 1** right-click **Mesh 1** and choose **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

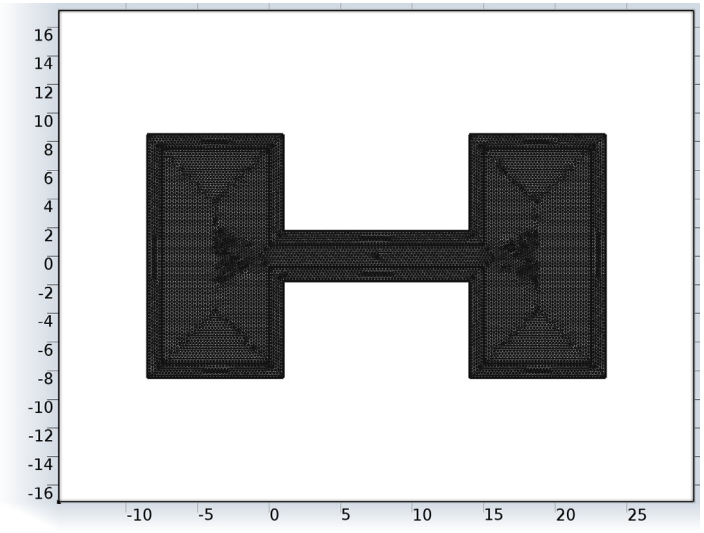
3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Extra fine**.

Free Triangular 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 Right-click **Free Triangular 1** and choose **Build All**.



STUDY 1

On the **Home** toolbar, click **Compute**.

RESULTS

Velocity (slpf)

Plot the mean free path number in the Domain to check the Knudesn number.

2D Plot Group 3

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 3** and choose **Rename**.

3 Go to the **Rename 2D Plot Group** dialog box and type `Mean Free Path` in the **New name** edit field.

4 Click **OK**.

Mean Free Path

1 Right-click **Results>2D Plot Group 3** and choose **Surface**.

2 In the **Surface** settings window, locate the **Expression** section.

3 In the **Expression** edit field, type `slpf.lambda`.

4 On the **2D plot group** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the Graphics toolbar.

Compare the resulting plot with Figure 2.

Plot the x-velocity and streamlines in the domain.

Velocity (slpf) 1

1 In the **Model Builder** window, under **Results** right-click **Velocity (slpf)** and choose **Duplicate**.

2 Right-click **Velocity (slpf) 1** and choose **Rename**.

3 Go to the **Rename 2D Plot Group** dialog box and type `x-Velocity, Streamlines` in the **New name** edit field.

4 Click **OK**.

x-Velocity, Streamlines

1 Right-click **Results>Velocity (slpf) 1** and choose **Streamline**.

2 In the **Streamline** settings window, locate the **Streamline Positioning** section.

3 From the **Positioning** list, choose **Magnitude controlled**.

4 In the **Density** edit field, type `12`.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **White**.

6 In the **Model Builder** window, under **Results>x-Velocity, Streamlines** click **Surface 1**.

7 In the **Surface** settings window, locate the **Expression** section.

8 In the **Expression** edit field, type `u`.

9 On the **2D plot group** toolbar, click **Plot**.

Compare the resulting plot with Figure 3.

Plot the Temperature in the domain.

Pressure (slpf) 1

1 In the **Model Builder** window, under **Results** right-click **Pressure (slpf)** and choose **Duplicate**.

2 Right-click **Pressure (slpf) 1** and choose **Rename**.

3 Go to the **Rename 2D Plot Group** dialog box and type `Temperature` in the **New name** edit field.

4 Click **OK**.

Temperature

1 In the **Model Builder** window, expand the **Results>Temperature** node, then click **Contour 1**.

2 In the **Contour** settings window, locate the **Expression** section.

3 In the **Expression** edit field, type `T`.

4 On the **2D plot group** toolbar, click **Plot**.

Compare the resulting plot with Figure 4.

Plot the pressure along the channel wall.

1D Plot Group 6

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Model Builder** window, under **Results** right-click **1D Plot Group 6** and choose **Rename**.

3 Go to the **Rename 1D Plot Group** dialog box and type `Channel Pressure` in the **New name** edit field.

4 Click **OK**.

Channel Pressure

1 On the **1D plot group** toolbar, click **Line Graph**.

2 In the **Line Graph** settings window, locate the **Selection** section.

3 Select the **Activate Selection** toggle button.

4 Select Boundary 10 only.

5 Locate the **y-Axis Data** section. In the **Expression** edit field, type `p`.

6 On the **1D plot group** toolbar, click **Plot**.

Compare the resulting plot with Figure 5.