Created in COMSOL Multiphysics 6.0

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.

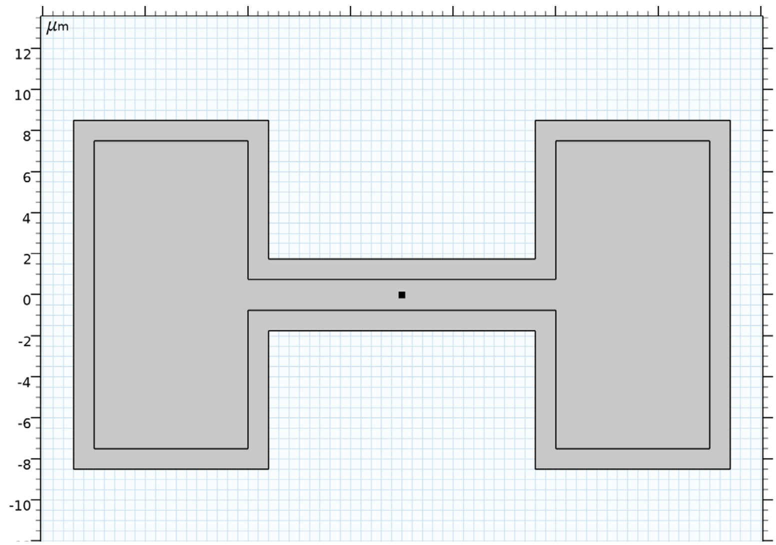


Figure 1: The Model Geometry

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

$$\begin{aligned} \mathbf{u}_{\mathrm{slip}} &= \sigma_s \frac{\lambda}{\mu}(\tau\mathbf{n} - ((\mathbf{n}^T\tau\,\mathbf{n})\mathbf{n})) + \sigma_T \frac{\mu}{\rho T_g}[\nabla T_w - (\mathbf{n}\cdot\nabla T_w)\mathbf{n}] \\ T_w &= T_g - \zeta_T \lambda \mathbf{n}\cdot\nabla T_g \end{aligned} \tag{1}$$

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:

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

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

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

where κ is the thermal conductivity of the gas.

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

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

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

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.

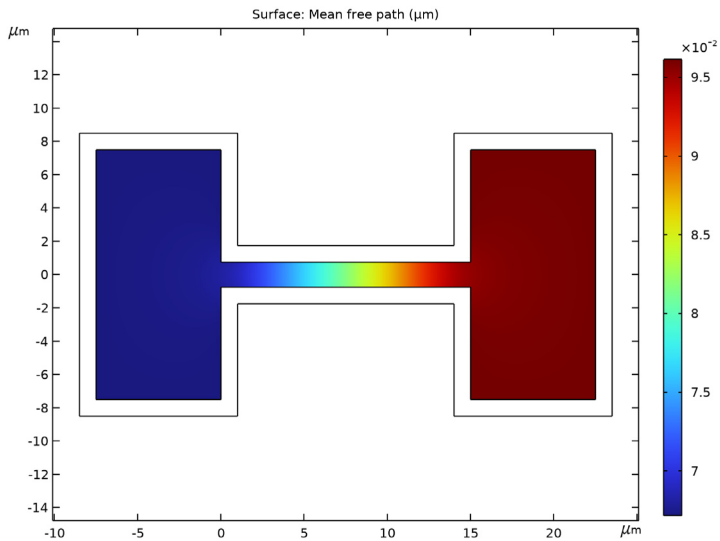


Figure 2: Gas mean free path. The channel width is 1.5 µm*, so the Knudsen number varies between 0.064 and 0.045.*

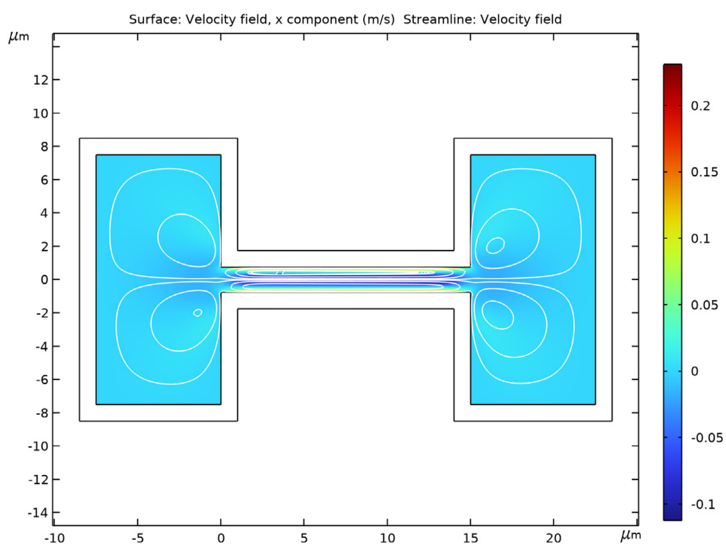


Figure 3: x-velocity (color) and streamlines (white) inside the channel. Flow is driven by thermal creep along the walls of the channel but a back-flow, driven by the pressure difference between the reservoirs, occurs in the center of the channel.

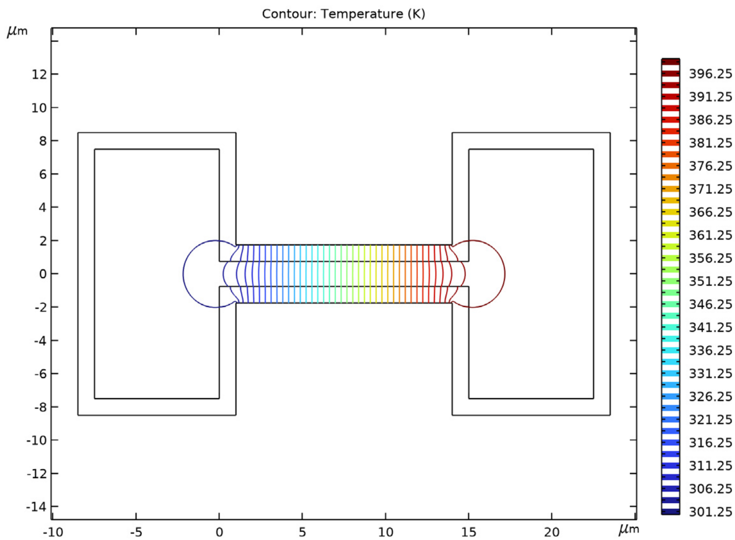


Figure 4: Temperature contours within the model. Note that a temperature jump occurs between the vessel walls and the gas when normal heat fluxes occur into the wall from the gas.

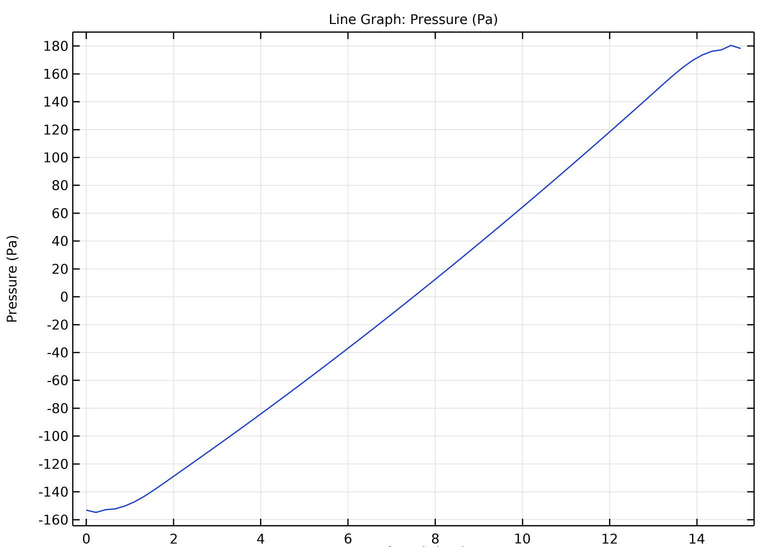


Figure 5: Pressure on the wall of the channel, as a function of position.

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.

Application Library path: `Microfluidics_Module/Rarefied_Flow/slip_flow_benchmark`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

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

MODEL WIZARD

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

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

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Stationary**.

6 Click **Done**.

GEOMETRY 1

Change the length units to µm and specify the geometry.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

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

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

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

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

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

Rectangle 2 (r2)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

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

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

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

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

Rectangle 3 (r3)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

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

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

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

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

Union 1 (uni1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

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

3 In the **Settings** window for **Union**, locate the **Union** section.

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

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

Rectangle 4 (r4)

1 In the **Geometry** toolbar, click **Rectangle**.
2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3 In the **Width** text field, type `9.5`.
4 In the **Height** text field, type `17`.
5 Locate the **Position** section. In the **x** text field, type `-8.5`.
6 In the **y** text field, type `-8.5`.

Rectangle 5 (r5)

1 In the **Geometry** toolbar, click **Rectangle**.
2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3 In the **Width** text field, type `15`.
4 In the **Height** text field, type `3.5`.
5 Locate the **Position** section. In the **y** text field, type `-1.75`.

Rectangle 6 (r6)

1 In the **Geometry** toolbar, click **Rectangle**.
2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3 In the **Width** text field, type `9.5`.
4 In the **Height** text field, type `17`.
5 Locate the **Position** section. In the **x** text field, type `14`.
6 In the **y** text field, type `-8.5`.

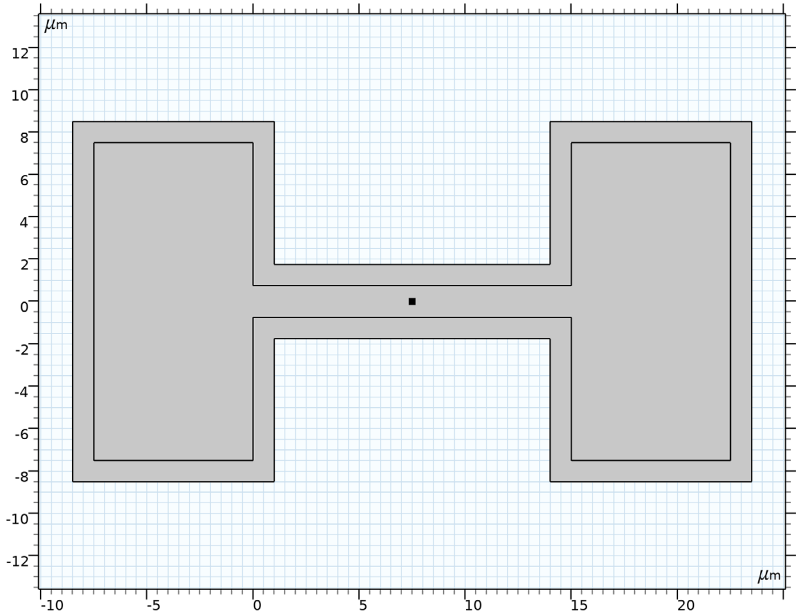
Union 2 (uni2)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.
2 Select the objects **r4**, **r5**, and **r6** only.
3 In the **Settings** window for **Union**, locate the **Union** section.
4 Clear the **Keep interior boundaries** check box.

Point 1 (pt1)

1 In the **Geometry** toolbar, click **Point**.
2 In the **Settings** window for **Point**, locate the **Point** section.
3 In the **x** text field, type `7.5`.
4 Click **Build All Objects**.

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



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

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

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

3 In the tree, select **Built-in>Air**.

4 Click **Add to Component** in the window toolbar.

5 In the tree, select **Built-in>Silicon**.

6 Click **Add to Component** in the window toolbar.

7 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Silicon (mat2)

Select Domain 1 only.

SLIP FLOW (SLPF)

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

Solid 1

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Slip Flow (slpf)** and choose the domain setting **Heat Transfer>Solid**.
2. Select Domain 1 only.

Apply thermal insulation on the boundaries of the connecting duct.

Thermal Insulation 1

1. In 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. In the **Physics** toolbar, click **Boundaries** and choose **Temperature**.
2. Select Boundaries 1–3, 11, and 13 only.
3. In the **Settings** window for **Temperature**, locate the **Temperature** section.
4. In the T_0 text field, type `300[K]`.

Temperature 2

1. In the **Physics** toolbar, click **Boundaries** and choose **Temperature**.
2. Select Boundaries 15–18 and 24 only.
3. In the **Settings** window for **Temperature**, locate the **Temperature** section.
4. In the T_0 text field, type `400[K]`.

Apply slip boundary conditions near and inside the channel.

Slip Wall 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Slip Wall**.
2. In the **Settings** window for **Slip Wall**, 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. In 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 (comp1)** right-click **Mesh 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

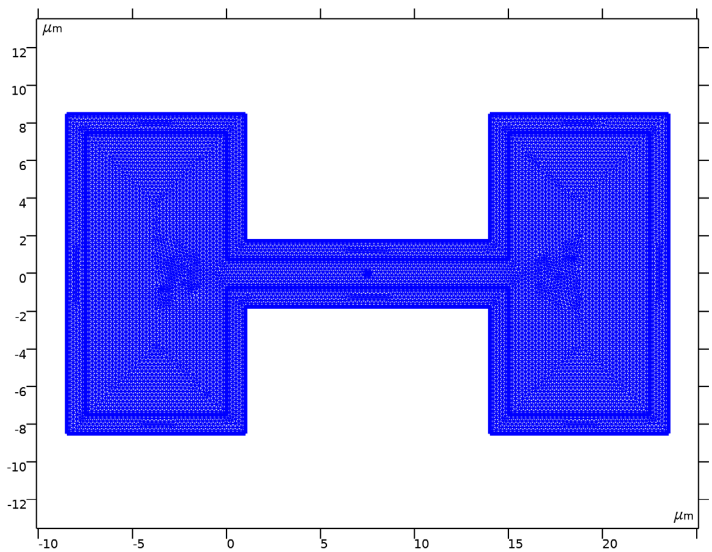
3 From the **Calibrate for** list, choose **Fluid dynamics**.

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

Free Triangular 1

1 In the **Mesh** toolbar, click **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.



STUDY 1

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

RESULTS

Velocity (slpf)

Plot the mean free path number in the domain to check the Knudsen number.

Mean Free Path

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

2 Right-click **2D Plot Group 5** and choose **Rename**.

3 In the **Rename 2D Plot Group** dialog box, type `Mean Free Path` in the **New label** text field.

4 Click **OK**.

Surface 1

1 Right-click **Mean Free Path** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

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

4 In the **Mean Free Path** toolbar, click **Plot**.

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

Compare the resulting plot with Figure 2.

Plot the x-velocity and streamlines in the domain.

x-Velocity, Streamlines

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

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

3 In the **Rename 2D Plot Group** dialog box, type `x-Velocity, Streamlines` in the **New label** text field.

4 Click **OK**.

Streamline 1

1 Right-click **x-Velocity, Streamlines** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

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

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

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **White**.

Surface

1 In the **Model Builder** window, click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `u`.

4 In the **x-Velocity, Streamlines** toolbar, click **Plot**.

Compare the resulting plot with Figure 3.

Plot the Temperature in the domain.

Contour

1 In the **Model Builder** window, expand the **Isothermal Contours (slpf)** node, then click **Contour**.

2 In the **Settings** window for **Contour**, locate the **Levels** section.

3 In the **Total levels** text field, type `40`.

4 In the **Isothermal Contours (slpf)** toolbar, click **Plot**.

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

Compare the resulting plot with Figure 4.

Plot the pressure along the channel wall.

Channel Pressure

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

2 Right-click **1D Plot Group 7** and choose **Rename**.

3 In the **Rename 1D Plot Group** dialog box, type `Channel Pressure` in the **New label** text field.

4 Click **OK**.

Line Graph 1

1 Right-click **Channel Pressure** and choose **Line Graph**.

2 Select Boundary 10 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `p`.

5 In the **Channel Pressure** toolbar, click **Plot**.

Compare the resulting plot with Figure 5.