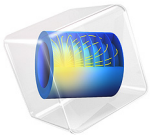

Differential Pumping

Introduction

Differentially pumped vacuum systems use a small orifice or tube to connect two parts of a vacuum system at very different pressures. Such systems are necessary when processes run at higher pressures and are monitored by detectors that require UHV for operation.

In this model, the gas flow through a narrow tube connecting a high vacuum chamber to a chamber held at a lower pressure is approximated using an analytic expression for the flow rate down the tube. The flow is assumed to be isothermal (in practice this may be a rather poor assumption, but it is straightforward to adapt the model to use experimental data directly in place of the analytic expressions).

In the first study, the outgassing wall boundary condition is used at the outlet of the tube (high vacuum side) to solve the problem, meshing only one reservoir. The mass flow rate into the chamber is obtained from an analytical expression developed in Ref. 1. This approach enables the simulation of flows across a range of pressures within the tube, including instances when the flow inside the tube is transitional. It is necessarily an approximation, since, Knudsen's cosine law is assumed to apply at the outlet, whilst in practice there is some focusing of the flow (molecular beaming) as a result of the tube.

The second study treats the case where the pressure in the high pressure reservoir is sufficiently low that flow through the entire tube is in the molecular flow regime. In this case, the tube can be simulated in addition to the high vacuum reservoir. The results obtained are compared with those obtained by the first approach in the appropriate limit.

Model Definition

Figure 1 shows a schematic representation of the model. There are two large reservoirs (named a and b) connected by a small tube of diameter D and length L. Each reservoir has its own steady state pressure defined by variables $p_{a\infty}$ in a and $p_{b\infty}$ in b. Reservoir b is connected to a vacuum pump and has a steady-state pressure $p_{b\infty}$ that is smaller than reservoir a ($p_{a\infty}>p_{b\infty}$). Note that the tube has a finite length and thus, you can expect to see a difference in pressure between the reservoirs and the tube entrances; that is, $p_a>p_{a\infty}$ and $p_b>p_{b\infty}$, where p_a and p_b are the inlet and outlet pressure, respectively.

In the steady state, the mass flow rate is constant in every region of the tube (entrances and central sections). Note that this model also uses the assumption of an isothermal flow (that is, a constant temperature everywhere in the system).

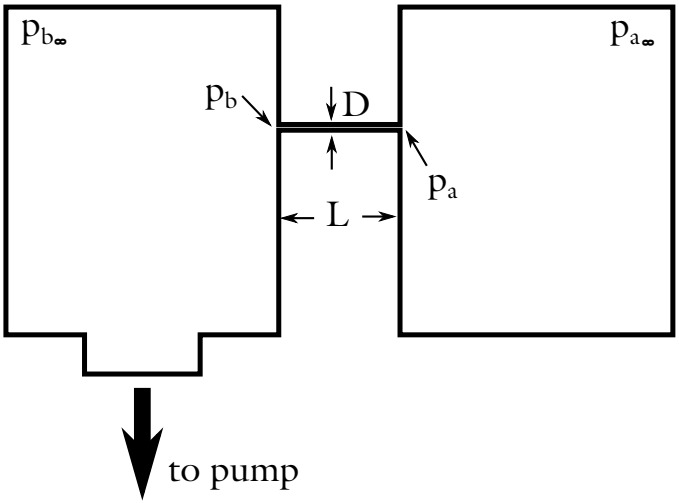

Figure 1: Not-to-scale schematic of the model. It consists of two large reservoirs at different pressures connected by a small tube.

FIRST STUDY

In the first part of the model, the outgassing wall boundary condition is used at the outlet of the tube (on the high vacuum side, or side b) to represent the flow coming out of the tube from the low vacuum reservoir, which is held at pressure $p_{a\infty}>p_{b\infty}$. This approach allows a significant reduction in the problem size at the expense of some simplifying assumptions. The mass flow in the tube is obtained from the analytical expression developed in Ref. 1.

ANALYTICAL EXPRESSION FOR THE MASS FLOW RATE

For finite length tubes, the pressure difference between the two reservoirs differs from that between the corresponding entry regions (inlet/outlet) as a result of entry and exit flows. In order to determine an analytical expression for the mass flow rate, Gallis and Torczynski decomposed the tube into three regions (the inlet, the tube, and the outlet), each of them defining a resistance (B) that can be use to define the mass flow rate by treating the tube as resistances in series (Ref. 1). In terms of mass conductance (inverse of the mass resistance), the mass flow rate can be written as:

$$\dot{M} = \beta A \Delta p$$

where $A = 1/B$ is the mass conductance. δp is the pressure difference, given by $\delta p = p_{i,\infty} - p_i$, Where p_i is either the inlet or outlet tube pressure. Finally, β is given by:

$$\beta = \frac{D^3}{3\pi\mu c^2}$$

where D is the tube diameter, μ is the gas viscosity, and c is the molecular mean thermal speed, given by:

$$c = \sqrt{\frac{8RT}{\pi M_n}}$$

Here M_n is the molar mass, T is the temperature, and R is the ideal gas constant.

Assuming a constant mass flow rate through the tube one can see that the inlet and outlet mass conductances, for all flow regimes, are approximated by summing the corresponding continuum and free-molecular mass conductances. This results in the following equation:

$$\dot{M} = \beta(q_{a\infty}^2 - q_a^2) = \beta(q_b^2 - q_{b\infty}^2) \tag{1}$$

where the variable q is defined by:

$$q = p + 6p_\lambda \tag{2}$$

p_λ is defined as the tube pressure at which the average Knudsen number is unity; that is:

$$p_\lambda = \frac{\pi\mu c}{4D}$$

From Ref. 1, the mass flow rate for an arbitrary-length tube can be approximated by:

$$\dot{M} = \beta F(q_a^2 - q_b^2) \tag{3}$$

with,

$$F \cong F_C\left(1 + \frac{16p_\lambda}{q_{a\infty} + q_{b\infty}}\left(\varpi - \frac{3}{4}\right)\right)$$

$$F_C = \frac{3\pi D}{32L}$$

and

$$\varpi = \frac{2-\alpha}{\alpha}\left\{(1+b_1\alpha)+(\varepsilon b_0-(1+b_1\alpha))\frac{b_2 p_\lambda}{p_{a\infty}-p_{b\infty}}\ln\left(\frac{p_{a\infty}+b_2 p_\lambda}{p_{b\infty}+b_2 p_\lambda}\right)\right\}$$

where α is the accommodation coefficient on the tube walls and where the coefficients b_0, b_1, b_2, and ε are defined as:

$$b_0 = \frac{16}{3\pi}$$

$$b_1 = 0.15$$

$$b_2 = \frac{0.7\alpha}{2-\alpha}$$

$$\varepsilon = \frac{1+\kappa}{\delta+\kappa}$$

where:

$$\kappa = \frac{\delta-1}{\delta}\frac{\alpha L}{D}$$

$$\delta = \frac{4}{3}(2-\alpha)$$

Combining Equation 1 and Equation 3, it is possible to determine the inlet and outlet pressure through Equation 2 and then to define the mass flow rate using

$$q_a = \sqrt{\frac{(1+F)q_{a\infty}^2 + Fq_{b\infty}^2}{1+2F}}$$

and

$$q_b = \sqrt{\frac{(1+F)q_{b\infty}^2 + Fq_{a\infty}^2}{1+2F}}$$

SECOND STUDY: VALIDATION

The second study is intended to simulate the mass flow rate and inlet/outlet pressure at the tube in order to compare the results obtained with the molecular flow interface with the analytical expression from Ref. 1 when the flow within the tube is entirely free molecular. In this case both the high vacuum reservoir and the tube are included in the

model. At the low pressure end of the tube, the reservoir boundary condition, which sets $p_{a,\infty}$, is used.

MODEL GEOMETRY

The model geometry is shown in Figure 2. Note that only the high vacuum chamber is included in the model — the low vacuum chamber geometry does not need to be modeled in detail. In addition, the **Plane Symmetry** boundary condition is used, so the model geometry only shows half of the high vacuum chamber in order to save computational resources.

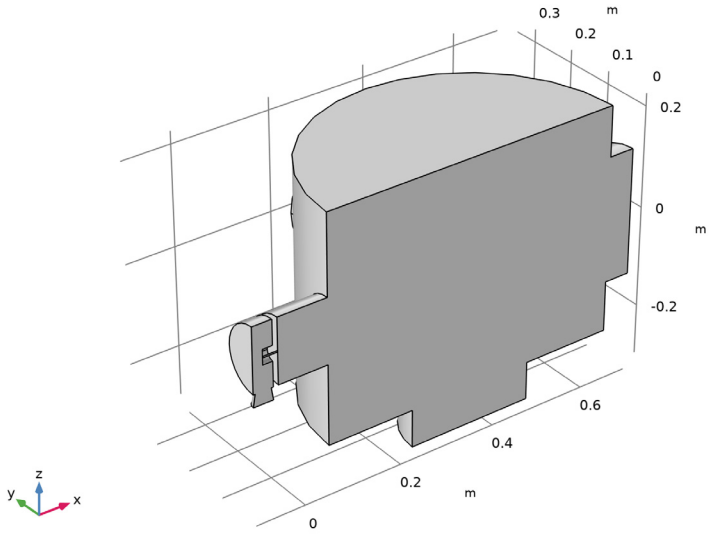

Figure 2: Model geometry. The high vacuum chamber is shown in full detail. The narrow tube that joins the two parts of the system is on the left side of the figure. Only the port connecting to the low vacuum chamber is shown in the figure (on the left side); the low vacuum chamber itself is not included in the geometry or the model.

Results and Discussion

Figure 3 shows the incident molecular flux on the surface of the high vacuum chamber at the lowest applied pressure. The corresponding number density is shown in Figure 4. The flux and number density distributions are similar for all parameters. This is expected since no geometrical changes have been made.

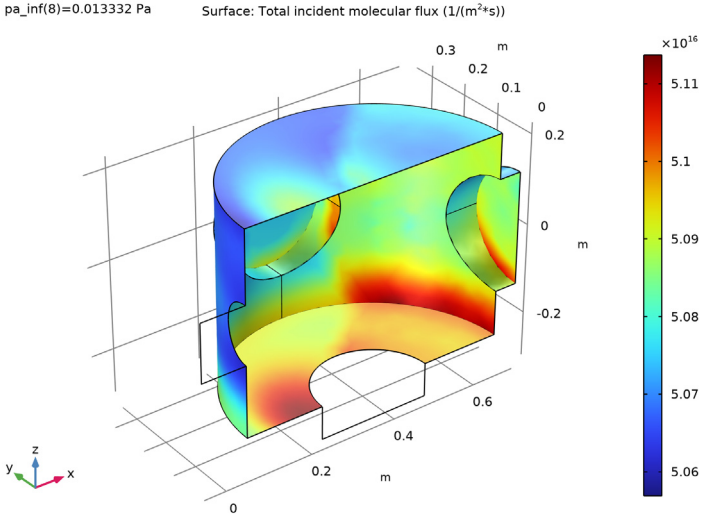

Figure 3: Incident molecular flux on the surface of the high vacuum chamber when the pressure in the low vacuum chamber ($p_{a,inf}$) is 0.1 mTorr. Flow through the tube is modeled using the expressions from Ref. 1 and assuming diffuse emission from the outlet.

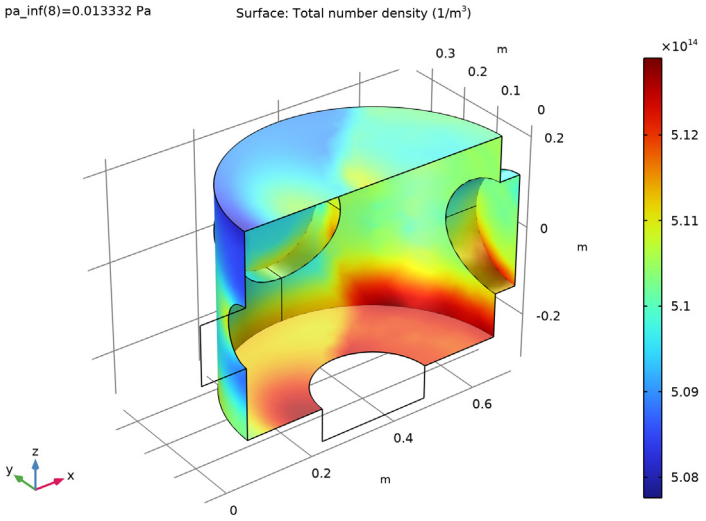

Figure 4: Number density on the surface of the high vacuum chamber when the pressures in the low vacuum chamber ($p_{a,inf}$) is 0.1 mTorr. Flow through the tube is modeled using the expressions from Ref. 1 and assuming diffuse emission from the outlet.

A number of interesting features are apparent in Figure 3 and Figure 4. The shadowing effect of the port to which the tube is attached is apparent. Surfaces with a clear line of sight to the pump have a lower molecular flux and number density than those without a clear line of sight — consider for example the upper and lower surfaces of the port opposite the tube. The variation in the total flux is relatively small, approximately 1% of its absolute magnitude. Note that a higher integration resolution than the default is required to see this fine detail in the number density distribution.

Figure 5 shows the mass flow rate through the tube, as a function of the applied pressure. When the flow rate is normalized to the flow that would occur in an infinite tube (for which entry and exit effects can be neglected) a clear minimum in the flow rate as a function of pressure can be seen (see Figure 6). This is known as Knudsen's minimum. The minimum is not apparent in Figure 5, due to the effect of the pump, which is assumed to have a constant pump speed and consequently produces different pressures on the high vacuum side, depending on the mass flow into this part of the chamber. The free molecular flow in the high vacuum chamber and the flow through the tube (which is potentially transitional) are coupled together by the model in a self consistent manner. Note that the analytic model for the mass flow rate assumes an isothermal flow and in practice there may be significant cooling of the gas as it flows through the tube. However the analytic model for the mass flow rate could straightforwardly be replaced by an interpolation function based on experimental data (note that the temperature of the incoming gas can also be specified arbitrarily in the model).

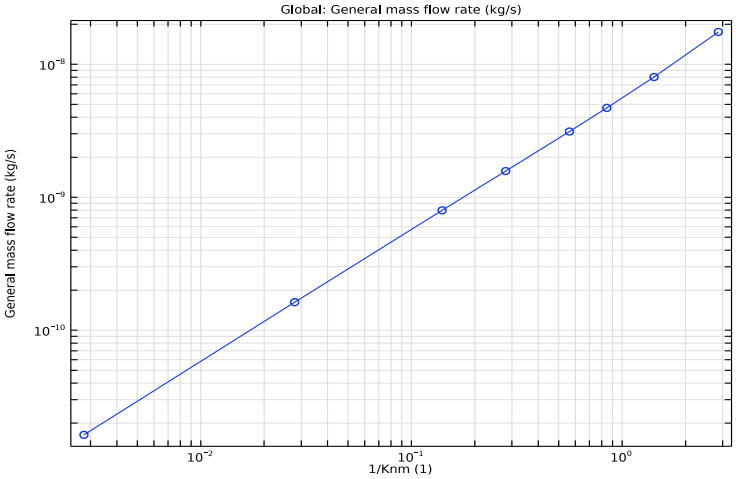

Figure 5: Mass flow rate through the tube as a function of the pressure in the low vacuum reservoir.

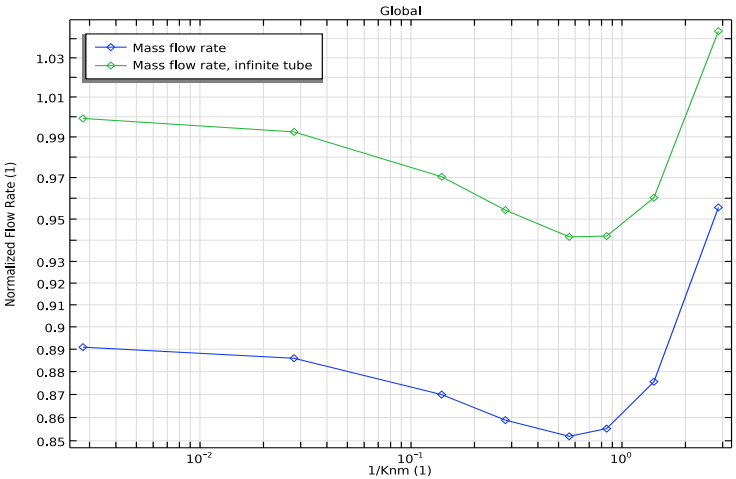

Figure 6: Mass flow rate through the tube, normalized to the flow rate through an infinite tube in the free molecular flow limit. The normalized flow rate through an infinite tube (with no pressure drop at the inlet or outlet) is also shown for comparison.

The second study computes the mass flow rate through the tube using the free molecular flow interface when the pressure on the low vacuum side is at its lowest value (0.1 mTorr).

This is possible since at this low pressure the entire tube is in the free molecular flow regime. Figure 8 and Figure 9 show the pressure and number density within the high vacuum chamber for this study. The distribution of flux and number density is significantly different from those in Figure 3 and Figure 4. Significant molecular beaming effects, which cannot be captured by the diffuse emission boundary condition used in Study 1, are apparent. Molecular beaming occurs since molecules traveling at a small angle to the tube axis are more likely to leave the tube than those traveling at large angles to the axis. The flow from the outlet of the tube becomes more focused as a result of this effect and consequently Knudsen's law does not apply at the tube outlet. However, even with the beaming effect, the number density in the high vacuum chamber varies by at most 2% of its absolute value and the absolute value agrees well with that predicted by the approach adopted in Study 1. So although COMSOL Multiphysics is capable of resolving the differences between these two approaches, they are not significant for practical purposes and the approach adopted in Study 1 is reasonable. Furthermore, the beaming effect is expected to be maximal in the free molecular flow limit so the approach used in Study 1 should be reasonable over the full range of Knudsen numbers.

The mass flow rate into the chamber computed by Study 2 (1.65×10^{-11} kg/s) agrees well with that produced by the analytic expression (1.63×10^{-11} kg/s). Mass conservation in the model is also reasonable — the mass flow out of the pump is 1.66×10^{-11} kg/s, which differs from the mass flow into the system by less than less than 1%. Finally the number density in the tube, which is expected to vary linearly along the tube in the free molecular flow limit (Ref. 1) agrees well with the number density profile predicted by the model, as shown in Figure 7. Note that Ref. 1 defines the pressure in terms of the number density, assuming the ideal gas law. The pressure expressions given in the reference can be reinterpreted as number densities, which is the approach taken in this model (COMSOL Multiphysics defines the pressure as the normal force acting on a surface in the Free Molecular Flow interface).

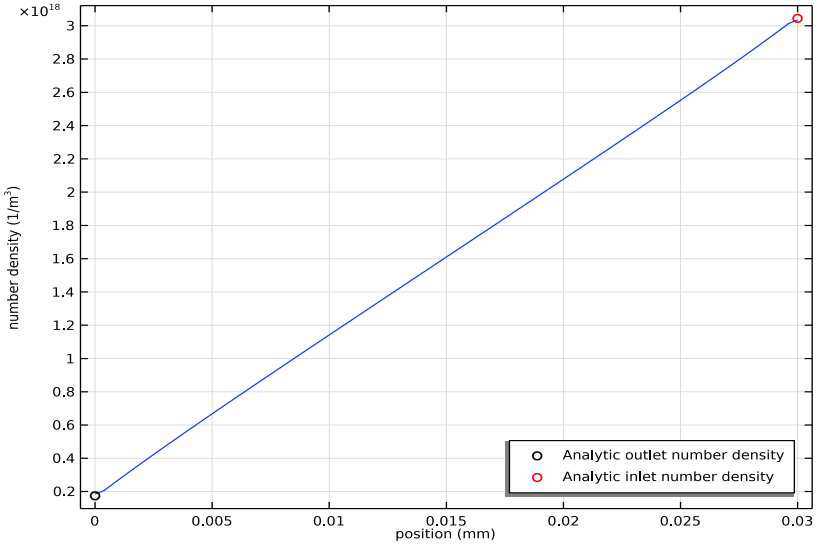

Figure 7: Number density on the inside of the tube computed in study 2 (line) compared with the results from the analytic expression at the entrance and exit from the tube (symbols). A linear variation of the number density in the tube is expected in the free molecular flow limit.

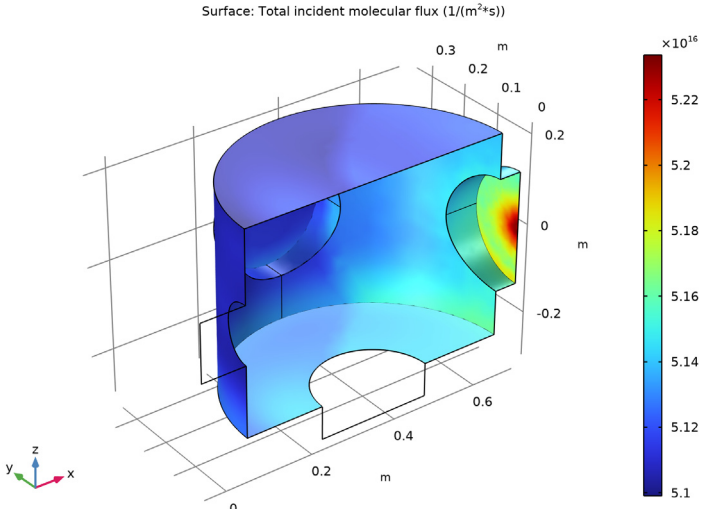

Figure 8: Incident molecular flux on the surface of the high vacuum chamber when the pressures in the low vacuum chamber ($p_{a,inf}$) is 0.1 mTorr. Flow through the tube is modeled using the Free Molecular Flow interface and the reservoir boundary condition. Molecular beaming (focusing of the flow from the outlet) can be seen on the port opposite the tube.

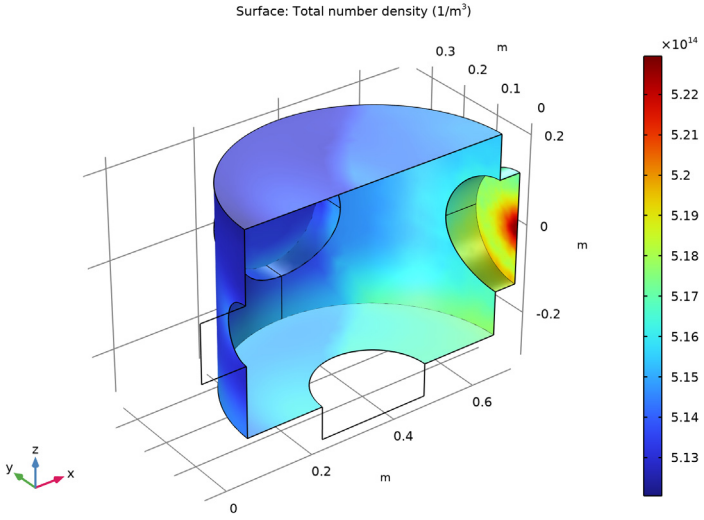

Figure 9: Number density on the surface of the high vacuum chamber when the pressure in the low vacuum chamber ($p_{a,inf}$) is 0.1 mTorr. Flow through the tube is modeled using the Free Molecular Flow interface and the reservoir boundary condition. Molecular beaming (focusing of the flow from the outlet) is apparent.

Application Library path: `Molecular_Flow_Module/Industrial_Applications/differential_pumping`

Reference

1. M.A. Gallis and J.R. Torczynski, "Direct simulation Monte Carlo-based expressions for the gas mass flow rate and pressure profile in a microscale tube", *Phys. Fluids*, vol. 24, pp. 012005, 2012.

Modeling Instructions

Note: This model requires 7.5 GB of RAM to run.

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 In the **Select Physics** tree, select **Fluid Flow>Rarefied Flow>Free Molecular Flow (fmf)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GEOMETRY 1

Insert the prepared geometry sequence from file. You can read the instructions for creating the geometry in the appendix.

1 In the **Geometry** toolbar, click **Insert Sequence** and choose **Insert Sequence**.

2 Browse to the model's Application Libraries folder and double-click the file `differential_pumping_geom_sequence.mph`.

3 In the **Geometry** toolbar, click **Build All**.

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

GLOBAL DEFINITIONS

Import the differential pumping parameters.

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `differential_pumping_parameters.txt`.

5 Click the **Wireframe Rendering** button in the **Graphics** toolbar. Wireframe rendering enables easier visualization of the interior boundaries.

Generate a nonlocal average coupling on the upstream face of the chamber. This coupling will be used to define the pressure at the tube outlet.

DEFINITIONS

Average 1 (aveop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Average**.

2 In the **Settings** window for **Average**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 16 only.

Variables 1

Import the differential pumping variables.

1 In the **Definitions** toolbar, click **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `differential_pumping_variables.txt`.

FREE MOLECULAR FLOW (FMF)

Model free molecular flow in the low pressure chamber only.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free Molecular Flow (fmf)**.

2 In the **Settings** window for **Free Molecular Flow**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Chamber Domain**.

This model primarily focuses on the number density of the molecules so disable the pressure computation to save computation time.

4 Locate the **Compute** section. Clear the **Pressure** check box.

Increase the integration resolution to enable finer details in the flow to be resolved.

5 Locate the **Integration Settings** section. From the **Integration resolution** list, choose **1024**.

Set the gas properties.

Molecular Flow 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Free Molecular Flow (fmf)** click **Molecular Flow 1**.

2 In the **Settings** window for **Molecular Flow**, locate the **Molecular Weight of Species** section.

3 In the $M_{\mathrm{n,G}}$ text field, type `Mn0`.

Define the surface temperature.

Surface Temperature 1

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

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

3 In the T text field, type `T0`.

Specify the boundary conditions. Divide the pump speed and the mass flow rate by two to account for the plane symmetry condition.

Vacuum Pump 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Vacuum Pump**.

2 In the **Settings** window for **Vacuum Pump**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Pump**.

4 Locate the **Vacuum Pump** section. From the **Specify pump flux** list, choose **Pump speed**.

5 In the S_{G} text field, type `Spump/2`.

The **Wall** boundary condition with outgassing is used to represent the tube. This is because the net mass flow through the tube is given by the expressions from Ref. 1.

Wall 2

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

2 In the **Settings** window for **Wall**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

4 Locate the **Wall Type** section. From the **Wall type** list, choose **Outgassing wall**.

5 Locate the **Flux** section. From the **Outgoing flux** list, choose **Total mass flow**.

6 In the $Q_{\mathrm{m,G}}$ text field, type `Mdot/2`.

Symmetry 1

1 In the **Physics** toolbar, click **Global** and choose **Symmetry**.

2 Select Boundary 17 only.

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 **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Outlet**.

5 Locate the **Element Size** section. From the **Predefined** list, choose **Extremely fine**.

Size

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

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

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

Free Triangular 1

1 In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Chamber and Outlet**.

4 Click **Build All**.

STUDY 1

Generate a list of values for the reservoir pressure that you are going to solve for.

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
pa_inf (Reservoir pressure (low vacuum))	1e-1[torr] 5e-2[torr] 3e-2[torr] 2e-2[torr] 1e-2[torr] 5e-3[torr] 1e-3[torr] 1e-4[torr]	Pa

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

RESULTS

Study 1/Solution 1 (sol1)

Add the previously created box selection to enable visualization of a cross section of the chamber.

1 In the **Model Builder** window, expand the **Results>Datasets** node, then click **Study 1/ Solution 1 (sol1)**.

Selection

1 In the **Results** toolbar, click **Attributes** and choose **Selection**.

2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Postprocessing**.

View the incident molecular flux on the surfaces inside the chamber.

Surface

1 In the **Model Builder** window, expand the **Results>Incident Molecular Flux (fmf)** node, then click **Surface**.

2 In the **Incident Molecular Flux (fmf)** toolbar, click **Plot**.

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

Compare the results with Figure 3.

Total Number Density (fmf)

1 In the **Model Builder** window, under **Results** click **Total Number Density (fmf)**.

2 In the **Total Number Density (fmf)** toolbar, click **Plot**.

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

Plot the mass flow rate as a function of the inverse Knudsen number.

Tube mass flow rate

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

2 In the **Settings** window for **1D Plot Group**, type `Tube mass flow rate` in the **Label** text field.

Global 1

1 Right-click **Tube mass flow rate** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`Mdot`	`kg/s`	`General mass flow rate`

4 Click to expand the **Legends** section. Clear the **Show legends** check box.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `1/Knm`.

7 Click to expand the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

8 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.

9 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

10 In the **Tube mass flow rate** toolbar, click  **Plot**.

Plot the normalized mass flow rate in the tube in order to see Knudsen's minimum.

1D Plot Group 4

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

2 In the **Settings** window for **1D Plot Group**, locate the **Legend** section.

3 From the **Position** list, choose **Upper left**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** check box. In the associated text field, type `Normalized Flow Rate (1)`.

Global 1

1 Right-click **1D Plot Group 4** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`Mdot/Mdot_f_inf`	`1`	`Mass flow rate`
`Mdot_inf/Mdot_f_inf`	`1`	`Mass flow rate, infinite tube`

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `1/Knm`.

6 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.

7 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

8 Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Diamond**.

Normalized mass flow rate

1 In the **Model Builder** window, under **Results** click **1D Plot Group 4**.

2 In the **Settings** window for **1D Plot Group**, type `Normalized mass flow rate` in the **Label** text field.

3 In the **Normalized mass flow rate** toolbar, click  **Plot**.

Check the Knudsen number on the high vacuum side is in the free molecular flow regime.

Global Evaluation 1

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

3 In the table, enter the following settings:

Expression	Unit	Description
Knm_b	1	Knudsen number in reservoir b

4 Click **Evaluate**.

TABLE

1 Go to the **Table** window.

The lowest Knudsen number for the outlet is 5. At this low number there is some intramolecular scattering in the flow, but it is very limited. All the other results have Knudsen numbers greater than 10, so the free molecular flow assumption is justified.

Add a second instance of the **Free Molecular Flow** interface for comparison with the results obtained at low pressures when the flow in the entire tube is free molecular.

ADD PHYSICS

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

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

3 In the tree, select **Fluid Flow>Rarefied Flow>Free Molecular Flow (fmf)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Study 1**.

5 Click **Add to Component 1** in the window toolbar.

6 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

FREE MOLECULAR FLOW 2 (FMF2)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free Molecular Flow 2 (fmf2)**.

2 Select Domains 2 and 3 only.

Select the tube in addition to the high vacuum chamber.

3 In the **Settings** window for **Free Molecular Flow**, locate the **Compute** section.

4 Clear the **Pressure** check box.

5 Locate the **Integration Settings** section. From the **Integration resolution** list, choose **2048**.

Molecular Flow 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Free Molecular Flow 2 (fmf2)** click **Molecular Flow 1**.

2 In the **Settings** window for **Molecular Flow**, locate the **Molecular Weight of Species** section.

3 In the $M_{\mathrm{n,G2}}$ text field, type `Mn0`.

Surface Temperature 1

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

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

3 In the T text field, type `T0`.

Add the **Vacuum Pump** boundary condition. Divide the pump speed by two in order to account for the plane symmetry condition.

Vacuum Pump 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Vacuum Pump**.

2 In the **Settings** window for **Vacuum Pump**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Pump**.

4 Locate the **Vacuum Pump** section. From the **Specify pump flux** list, choose **Pump speed**.

5 In the S_{G2} text field, type `Spump/2`.

The **Reservoir** boundary condition is used to represent the low vacuum part of the system.

Reservoir 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Reservoir**.

2 In the **Settings** window for **Reservoir**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Reservoir** section. In the $p_{0,\mathrm{G2}}$ text field, type `pa_inf`.

DEFINITIONS

Define a nonlocal integration coupling at the inlet boundary to compute the total mass flow through the inlet.

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Inlet**.

Add a second integration to check the mass flow out of the pump.

Integration 2 (intop2)

1 Right-click **Integration 1 (intop1)** and choose **Duplicate**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 Click **Clear Selection**.

4 From the **Selection** list, choose **Pump**.

FREE MOLECULAR FLOW 2 (FMF2)

Symmetry 1

1 In the **Physics** toolbar, click **Global** and choose **Symmetry**.

2 Select Boundaries 10 and 17 only.

COMPONENT 1 (COMP1)

Create a new mesh that includes the tube.

MESH 2

In the **Mesh** toolbar, click **Add Mesh** and choose **Add Mesh**.

Size 1

1 Right-click **Mesh 2** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Port**.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

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

This setting refines the mesh on the port opposite the outlet to better capture the molecular beaming from the tube.

Size

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

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

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

Size 2

1 In the **Model Builder** window, right-click **Mesh 2** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Inlet**.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

6 From the **Predefined** list, choose **Extremely fine**.

Free Triangular 1

1 In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Click **Build Selected**.

Mapped 1

1 In the **Mesh** toolbar, click **Boundary** and choose **Mapped**.

2 In the **Settings** window for **Mapped**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Tube**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 In the **Number of elements** text field, type `80`.

4 Select Edge 19 only.

Free Triangular 2

1 In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Chamber**.

Free Triangular 3

1 In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

2 Select Boundary 10 only.

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

In **Study 2** only the **Free Molecular Flow 2** physics interface should be solved for.

STUDY 2

Step 1: Stationary

1 In the **Model Builder** window, under **Study 2** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Free Molecular Flow (fmf)**.

Use mesh 2.

4 Click to expand the **Mesh Selection** section. In the table, enter the following settings:

Component	Mesh
Component 1	Mesh 2

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

RESULTS

Study 2/Solution 2 (3) (sol2)

In the **Model Builder** window, under **Results>Datasets** right-click **Study 2/Solution 2 (sol2)** and choose **Duplicate**.

Selection

1 In the **Results** toolbar, click **Attributes** and choose **Selection**.

2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Postprocessing**.

Surface

1 In the **Model Builder** window, expand the **Results>Incident Molecular Flux (fmf2)** node, then click **Surface**.

2 In the **Incident Molecular Flux (fmf2)** toolbar, click **Plot**.

Compare the resulting plot with Figure 8.

Surface

1 In the **Model Builder** window, expand the **Results>Total Number Density (fmf2)** node, then click **Surface**.

2 In the **Total Number Density (fmf2)** toolbar, click **Plot**.

Compare the resulting plot with Figure 9.

Plot the number density along the tube.

Number density in the tube

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

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 (3) (sol2)**.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** check box. In the associated text field, type `position (mm)`.

6 Select the **y-axis label** check box. In the associated text field, type `number density (1/m<sup>3</sup>)`.

7 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

8 Click to expand the **Title** section. From the **Title type** list, choose **None**.

9 In the **Label** text field, type `Number density in the tube`.

Line Graph 1

1 Right-click **Number density in the tube** and choose **Line Graph**.

2 Select Edge 19 only.

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

4 In the **Expression** text field, type `fmf2.ntot`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Reversed arc length**.

6 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

Global 1

1 In the **Model Builder** window, right-click **Number density in the tube** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
pb/(k_B_const*T0)	1/m^3	

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type 0.

6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

7 From the **Color** list, choose **Black**.

8 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

9 Locate the **y-Axis Data** section. In the **Description** text field, type Analytic outlet number density.

Global 2

1 Right-click **Number density in the tube** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
pa/(k_B_const*T0)	1/m^3	Analytic inlet number density

4 In the **Description** text field, type Analytic inlet number density.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type 30[mm].

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

8 From the **Color** list, choose **Red**.

9 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

Evaluate the mass flow into the system and compare with the analytic value and the flow out of the system. Multiply the nonlocal integration couplings by two in order to account for the plane symmetry condition.

Global Evaluation 2

1 In the **Results** toolbar, click 8.5 **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 (2) (sol2)**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
Mdot	kg/s	Analytic Inflow

5 Click = **Evaluate**.

Global Evaluation 3

1 Right-click **Global Evaluation 2** and choose **Duplicate**.

2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

3 In the table, enter the following settings:

Expression	Unit	Description
2*intop1(fmf2.Jnet_G2)*MnO/N_A_const	kg/s	Numerical Inflow

4 Click ▼ next to = **Evaluate**, then choose **Table 2 - Global Evaluation 2**.

Global Evaluation 4

1 Right-click **Global Evaluation 3** and choose **Duplicate**.

2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

3 In the table, enter the following settings:

Expression	Unit	Description
2*intop2(fmf2.Jnet_G2)*MnO/N_A_const	kg/s	Numerical Outflow

4 Click ▼ next to = **Evaluate**, then choose **Table 2 - Global Evaluation 2**.

TABLE

1 Go to the **Table** window.

There is good agreement between the mass flow predicted by COMSOL and that produced by the analytic expressions. The mass conservation is also reasonable.

Appendix: Geometry Instructions

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

NEW

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

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **3D**.

Combining Cylinders

The geometry consists of several cylinders that are joined together.

Cylinder 1 (cyl1)

1. In the **Geometry** toolbar, click **Cylinder**.
2. In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
3. In the **Radius** text field, type `0.3`.
4. In the **Height** text field, type `0.45`.
5. Locate the **Position** section. In the **x** text field, type `0.35`.
6. In the **z** text field, type `-0.225`.

Cylinder 2 (cyl2)

1. In the **Geometry** toolbar, click **Cylinder**.
2. In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
3. In the **Radius** text field, type `0.125`.
4. In the **Height** text field, type `0.7`.
5. Locate the **Position** section. In the **x** text field, type `0.35`.
6. In the **y** text field, type `-0.35`.
7. Locate the **Axis** section. From the **Axis type** list, choose **y-axis**. By changing the axis, the cylinder is oriented accordingly.

Cylinder 3 (cyl3)

1. In the **Geometry** toolbar, click **Cylinder**.
2. In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
3. In the **Radius** text field, type `0.125`.
4. In the **Height** text field, type `0.075`.
5. Locate the **Position** section. In the **x** text field, type `0.35`.
6. In the **z** text field, type `-0.3`.

Cylinder 4 (cyl4)

1. In the **Geometry** toolbar, click **Cylinder**.
2. In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.

3 In the **Radius** text field, type `0.065`.

4 In the **Height** text field, type `0.4`.

5 Locate the **Position** section. In the **x** text field, type `-0.05`.

6 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Cylinder 5 (cyl5)

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

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

3 In the **Radius** text field, type `0.125`.

4 In the **Height** text field, type `0.35`.

5 Locate the **Position** section. In the **x** text field, type `0.35`.

6 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Union 1 (uni1)

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

2 Click the  **Select All** button in the **Graphics** toolbar.

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

4 Clear the **Keep interior boundaries** check box. This combines the selected cylinders into an object with a single domain.

Cylinder 6 (cyl6)

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

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

3 In the **Radius** text field, type `0.065`.

4 In the **Height** text field, type `0.04`.

5 Locate the **Position** section. In the **x** text field, type `-0.1`.

6 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Cone 1 (cone1)

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

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

3 In the **Bottom radius** text field, type `20[mm]`.

4 In the **Height** text field, type `27[mm]`.

5 In the **Top radius** text field, type `15.5[mm]`.

6 Locate the **Position** section. In the **x** text field, type `-0.08`.

7 In the **z** text field, type `-0.09`.

Union 2 (uni2)

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

2 Select the objects **cone1** and **cyl6** only.

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

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

Cylinder 7 (cyl7)

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

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

3 In the **Radius** text field, type `0.015`.

4 In the **Height** text field, type `0.02`.

5 Locate the **Position** section. In the **x** text field, type `-0.08`.

6 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Difference 1 (dif1)

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

2 Select the object **uni2** only.

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

4 Find the **Objects to subtract** subsection. Click to select the **Activate Selection** toggle button.

5 Select the object **cyl7** only.

Cylinder 8 (cyl8)

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

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

3 In the **Radius** text field, type `1.5[mm]`.

4 In the **Height** text field, type `0.03`.

5 Locate the **Position** section. In the **x** text field, type `-0.08`.

6 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Using Symmetry

The geometry and the physics are symmetrical with respect to the *zx*-plane. The geometry can therefore be partitioned to save mesh elements and computation resources.

Work Plane 1 (wp1)

1 In the **Geometry** toolbar, click **Work Plane**.

2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 From the **Plane** list, choose **zx-plane**.

Partition Objects 1 (par1)

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

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

3 In the **Settings** window for **Partition Objects**, locate the **Partition Objects** section.

4 From the **Partition with** list, choose **Work plane**.

Delete Entities 1 (del1)

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

2 In the **Settings** window for **Delete Entities**, locate the **Entities or Objects to Delete** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select all **Domains** in the $-y$ half of the geometry.

5 On the object **par1(1)**, select Domain 1 only.

6 On the object **par1(2)**, select Domain 1 only.

7 On the object **par1(3)**, select Domain 1 only.

8 Click **Build Selected**.

Form Union (fin)

1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

Add Named Selections to the Geometry

Chamber Domain

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Chamber Domain` in the **Label** text field.

3 On the object **fin**, select Domain 3 only.

Chamber and Outlet

1 In the **Geometry** toolbar, click **Selections** and choose **Adjacent Selection**.

2 In the **Settings** window for **Adjacent Selection**, type `Chamber and Outlet` in the **Label** text field.

3 Locate the **Input Entities** section. Click + **Add**.

4 In the **Add** dialog box, select **Chamber Domain** in the **Input selections** list.

5 Click **OK**.

Outlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Outlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 Click the **Wireframe Rendering** button in the **Graphics** toolbar.

5 On the object **fin**, select Boundary 19 only.

Chamber

1 In the **Geometry** toolbar, click **Selections** and choose **Difference Selection**.

2 In the **Settings** window for **Difference Selection**, type `Chamber` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click + **Add**.

5 In the **Add** dialog box, select **Chamber and Outlet** in the **Selections to add** list.

6 Click **OK**.

7 In the **Settings** window for **Difference Selection**, locate the **Input Entities** section.

8 Click + **Add**.

9 In the **Add** dialog box, select **Outlet** in the **Selections to subtract** list.

10 Click **OK**.

Inlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Inlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 9 only.

Tube

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Tube` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select the **Group by continuous tangent** check box.

5 On the object **fin**, select Boundaries 11 and 12 only.

Pump

1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Pump` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 25 only.

Port

1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Port` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 35 only.

Box Selection 1 (boxsel1)

1 In the **Geometry** toolbar, click  **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, locate the **Geometric Entity Level** section.

3 From the **Level** list, choose **Boundary**.

4 Locate the **Box Limits** section. In the **y minimum** text field, type `-0.1[mm]`.

5 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.

Cylinder Selection 1 (cylsel1)

1 In the **Geometry** toolbar, click  **Selections** and choose **Cylinder Selection**.

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

3 In the **Outer radius** text field, type `0.1`.

4 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

5 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.

6 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

Cylinder Selection 2 (cylsel2)

1 In the **Geometry** toolbar, click **Selections** and choose **Cylinder Selection**.

2 In the **Settings** window for **Cylinder Selection**, locate the **Geometric Entity Level** section.

3 From the **Level** list, choose **Boundary**.

4 Locate the **Size and Shape** section. In the **Outer radius** text field, type `0.2`.

5 Locate the **Position** section. In the **x** text field, type `0.35`.

6 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.

Postprocessing

1 In the **Geometry** toolbar, click **Selections** and choose **Difference Selection**.

2 In the **Settings** window for **Difference Selection**, type `Postprocessing` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click **Add**.

5 In the **Add** dialog box, select **Box Selection 1** in the **Selections to add** list.

6 Click **OK**.

7 In the **Settings** window for **Difference Selection**, locate the **Input Entities** section.

8 Click **Add**.

9 In the **Add** dialog box, in the **Selections to subtract** list, choose **Cylinder Selection 1** and **Cylinder Selection 2**.

10 Click **OK**.