Molecular Flow Through a Microcapillary

Introduction

Computing molecular flows in arbitrary geometries produces complex integral equations which are very difficult to compute analytically. Analytic solutions are therefore only available for simple geometries. One of the earliest problems solved was that of gas flow through tubes of arbitrary length, which was first treated correctly by Clausing (Ref. 1). Later the integral expressions he derived were computed more accurately by Cole (Ref. 2). These authors derived values for the transmission probability of molecules incident on a tube of arbitrary length, which is independent of the pressure, provided that the Knudsen number is much greater than one (that is in the molecular flow regime).

This model uses COMSOL Multiphysics to compute the transmission probability for molecular flow of molecules through a microcapillary with different ratios of the length to the radius. The results are compared with the accurate solution due to Cole (Ref. 2).

Model Definition

Nitrogen gas flows through a microcapillary tube of diameter 200 μm, from a reservoir at a fixed pressure of 10^{-3} mBar to a reservoir at high vacuum. The flux of molecules entering the tube from the high vacuum end is assumed to be negligible. At this pressure the mean free path of the nitrogen is approximately 100 mm, so the Knudsen number of the flow is much greater than 1. The ratio of the flux of molecules entering the tube to the flux of molecules leaving the tube is computed for tube lengths of 0.4 mm, 0.8 mm, 1.2 mm, 1.6 mm, and 2.0 mm. The model is axially symmetric and is built in the 2D axially symmetric interface. The geometry is shown in Figure 1 for the case of the 2.0 mm long tube. The lower boundary is connected to the reservoir at low vacuum, the upper boundary is connected to the reservoir at high vacuum and the nonaxial vertical boundary is the capillary wall.

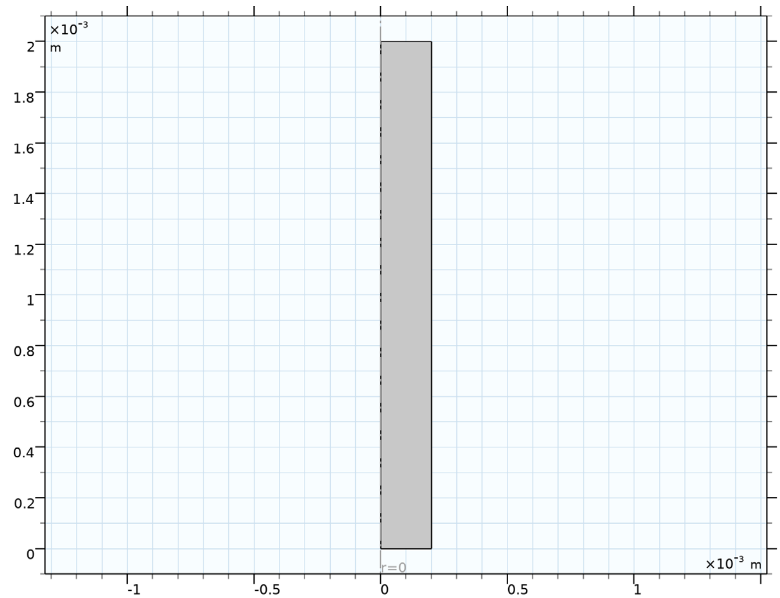


Figure 1: Model geometry.

The probability, χ, of molecules that strike the tube passing through the tube can be computed as the following integral:

$$\chi = \frac{\int_{\mathrm{HV}} 2\pi r G dr}{\int_{\mathrm{RS}} 2\pi r J dr}$$

where J is the outgoing flux, G is the incident flux, r is the radial distance, RS is the boundary adjacent to the reservoir, and HV is the boundary adjacent to high vacuum.

Results and Discussion

The incident flux on the surfaces of the tube is shown in Figure 2 for the case of the 2 mm long tube. A line plot of the pressure along the wall is shown in Figure 3. As expected, the incident flux decreases steadily from the reservoir end to the end at high vacuum, as does the pressure. Note that the incident flux (in contrast with the emitted flux) is not constant along the two reservoir boundaries, as it results from reflections within the geometry. The transmission probability for the tube is plotted against length to radius ratio in Figure 4. Good agreement is obtained between the calculated results and the probabilities calculated by Cole (Ref. 2).

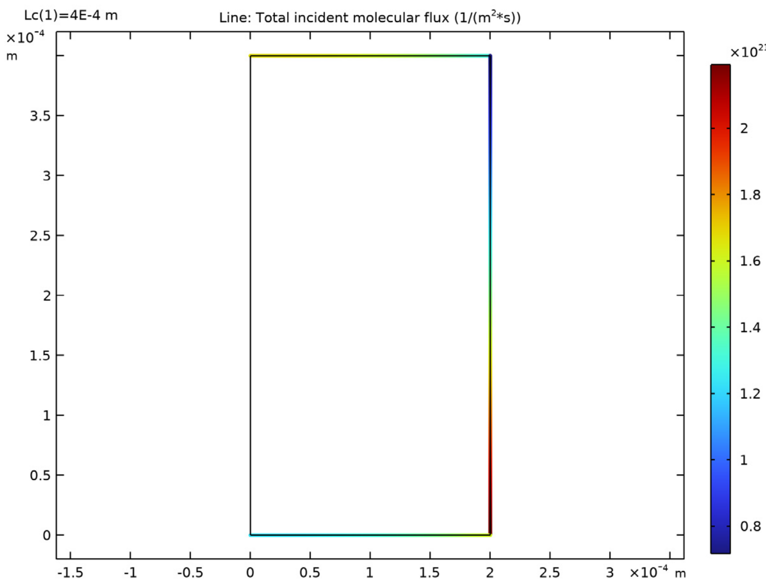


Figure 2: The incident flux inside the tube.

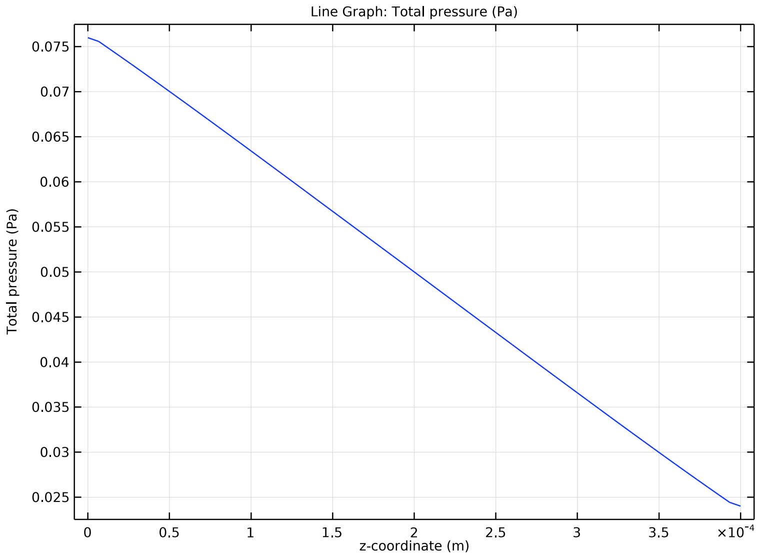


Figure 3: The pressure along the tube wall.

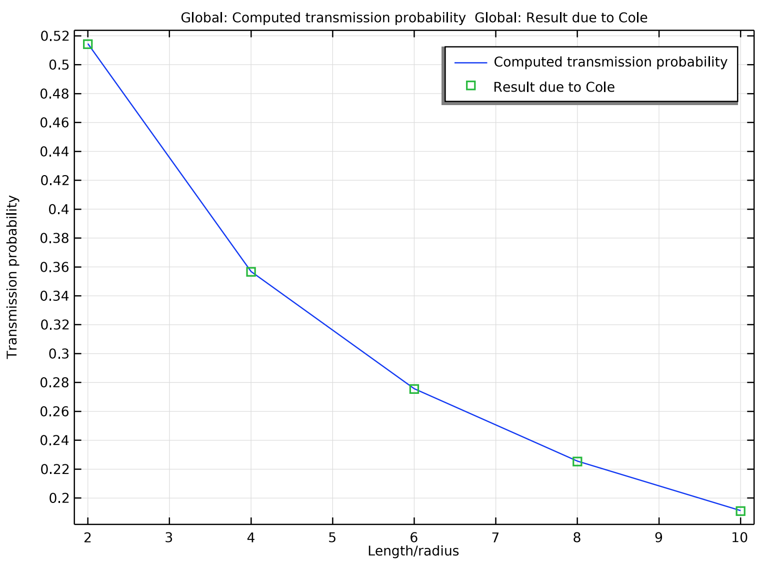


Figure 4: The transmission probability for the pipe as a function of the length to radius ratio. The results due to Cole (Ref. 2) are shown for comparison.

References

1. P. Clausing, "Über die Strömung sehr verdünnter Gase durch Röhren von beliebiger Länge", *Ann. Physik*, vol. 404, no. 8, pp. 961–989, 1932. English translation available as: "The Flow of Highly Rarefied Gases Through Tubes of Arbitrary Length", *J. Vacuum Science and Technology*, vol. 8. no. 5, pp. 636–646, 2009.

2. R.J. Cole, "Complementary Variational Principles for Knudsen Flow Rates", *IMA J. Appl. Math.*, vol. 20, pp. 107–115, 1977.

Notes About the COMSOL Implementation

The model is straightforward to set up using the Molecular Flow interface. The capillary walls are assigned the wall boundary condition, the reservoir boundary condition is used for the bottom opening, and the top opening is assigned the total vacuum boundary condition. The geometry is parameterized, and a parametric solver is used to vary the capillary dimensions.

Application Library path: `Molecular_Flow_Module/Benchmarks/vacuum_capillary`

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 Axisymmetric**.
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**.

Global Definitions

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 In the table, enter the following settings:

Name	Expression	Value	Description
Lc	2[mm]	0.002 m	Capillary length
Rc	0.2[mm]	2E-4 m	Capillary radius
p0	1e-3[mbar]	0.1 Pa	Reservoir pressure

Geometry 1

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 `Rc`.

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

5 Click **Build All Objects**.

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

Free Molecular Flow (FMF)

Set boundary conditions for the tube entrance and exit.

Total Vacuum 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Free Molecular Flow (fmf)** and choose **Total Vacuum**.

2 Select Boundary 3 only.

Reservoir 1

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

2 Select Boundary 2 only.

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

4 In the $p_{0,\mathrm{G}}$ text field, type `p0`.

DEFINITIONS

Define an interpolation function for Cole's solution for the transmission probability as a function of the length-to-radius ratio. You will use it later for comparison with the model result.

Interpolation 1 (int1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Local>Interpolation**.

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

3 In the table, enter the following settings:

t	f(t)
2	0.5142
4	0.3566
6	0.2755
8	0.2253
10	0.1910

Set up integration nonlocal couplings to compute the total flux of molecules through the system.

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 Select Boundary 2 only.

5 Locate the **Advanced** section. Clear the **Compute integral in revolved geometry** check box.

Integration 2 (intop2)

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 Select Boundary 3 only.

5 Locate the **Advanced** section. Clear the **Compute integral in revolved geometry** check box.

Use a mapped mesh for this simple geometry.

MESH 1

Mapped 1

In the **Mesh** toolbar, click **Mapped**.

Distribution 1

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

2 Select Boundaries 2 and 3 only.

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

4 In the **Number of elements** text field, type 15.

Distribution 2

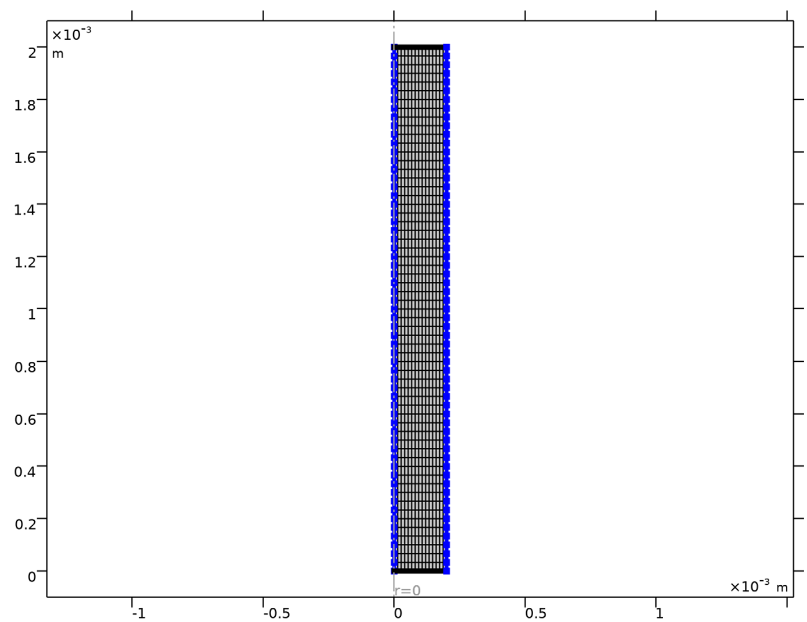
1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1 and 4 only.

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

4 In the **Number of elements** text field, type 60.

5 Click **Build All**.



Set up a parametric sweep over the capillary length.

STUDY 1

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 From the list in the **Parameter name** column, choose **Lc (Capillary length)**.

5 Click **Range**.

6 In the **Range** dialog box, type `0.4[mm]` in the **Start** text field.

7 In the **Stop** text field, type `2[mm]`.

8 In the **Step** text field, type `0.4[mm]`.

9 Click **Add**.

10 In the **Study** toolbar, click **Compute**.

RESULTS

Incident Molecular Flux (fmf)

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

2 From the **Parameter value (Lc (m))** list, choose **4E-4**.

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

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

The default plot shows the incident molecular flux inside the microcapillary tube. Compare with the plot in Figure 2.

Plot the pressure along the tube wall by following these steps.

Total Pressure

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

2 In the **Settings** window for **1D Plot Group**, type `Total Pressure` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

4 From the **Parameter selection (Lc)** list, choose **First**.

Line Graph 1

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

2 Select Boundary 4 only.

3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Free Molecular Flow>Pressure>fmf.ptot - Total pressure - Pa**.

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

Use the z-coordinate for the *x*-axis data.

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

6 In the **Expression** text field, type `z`.

7 In the **Total Pressure** toolbar, click **Plot**.

Compare the resulting plot with that in Figure 3.

Finally, plot the result for the transmission probability versus the length-to-radius ratio and compare with Cole's solution.

1D Plot Group 5

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 1/Parametric Solutions 1 (sol2)**.

Global 1

1 Right-click **1D Plot Group 5** 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
`intop2(2*pi*r*G)/intop1(2*pi*r*fmf.J_G)`		`Computed transmission probability`

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

5 In the **Expression** text field, type `Lc/Rc`.

Transmission Probability

1 In the **Model Builder** window, under **Results** click **1D Plot Group 5**.

2 In the **Settings** window for **1D Plot Group**, type `Transmission Probability` in the **Label** text field.

3 Locate the **Plot Settings** section.

4 Select the **x-axis label** check box. In the associated text field, type `Length/radius`.

5 Select the **y-axis label** check box. In the associated text field, type `Transmission probability`.

Global 2

1 Right-click **Transmission Probability** 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
`int1(Lc/Rc)`		`Result due to Cole`

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

5 In the **Expression** text field, type `Lc/Rc`.

Change the plot style to display only the data points.

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

7 Find the **Line markers** subsection. From the **Marker** list, choose **Square**.

Transmission Probability

1 In the **Model Builder** window, click **Transmission Probability**.

2 In the **Transmission Probability** toolbar, click **Plot**.

Compare with Figure 4.