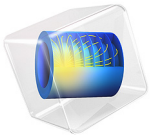

Model created in COMSOL Multiphysics 6.4

Molecular Flow Through an S-Bend

Introduction

Computing molecular flows in arbitrary geometries produces complex integral equations that are very difficult to compute analytically. There are two widely used methods for modeling molecular flows, the Monte Carlo method (which computes the trajectories of large numbers of randomized particles through the system) and the angular coefficient method. The Free Molecular Flow interfaces uses the angular coefficient method, which computes the molecular flow by summing the flux arriving at a surface from all other surfaces in its line of sight. The macroscopic variables in the vicinity of the surface can be derived from kinetic theory. The Particle Tracing Module can be used to implement the Monte Carlo method for molecular flows.

Note: This model requires the Particle Tracing Module.

Model Definition

This model compares the transmission probability, computed by two different methods of a gas through an s-bend geometry. The model geometry is shown in Figure 1.

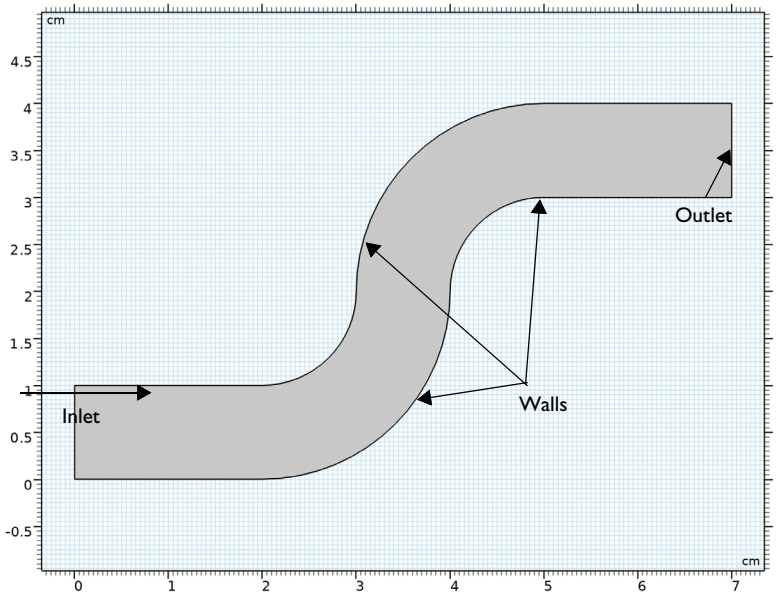

Figure 1: Model geometry for the s-bend. The dimensions are in centimeters.

Particle trajectories are computed using Newton's law of motion:

$$\frac{d}{dt}\left(m\frac{d\mathbf{q}}{dt}\right) = 0$$

The particle velocity is given by:

$$\mathbf{v} = \frac{d\mathbf{q}}{dt}$$

When the particles encounter a boundary, they scatter according to Knudsen's law.

$$v_t = c\sin\theta$$

$$v_n = c\cos\theta$$

where the subscript t denotes the tangential component of the velocity and n the normal. In addition, c is the particle speed and θ is the angle between the wall normal and the particle velocity. The particle speed is sampled from the following probability density function:

$$\rho(c) = \sqrt{\frac{2}{\pi}}\left(\frac{m}{k_B T}\right)^{3/2} c^2 \exp\left(-\frac{mc^2}{2k_B T}\right)$$

This is accomplished using the normally distributed random function, which is used to assign a new normally distributed random speed to each particle at each time step. The angle, θ is a random angle:

$$\theta = \operatorname{asin}(\Gamma)$$

where Γ is a uniformly distributed random number between 0 and 1. Furthermore, it is unique for each particle at each time step. In all 10,000 particles are released into the modeling domain. The number of particles that reaches the outlet boundary determines the transmission probability.

The transmission probability for the molecular flow interface is given by the following:

$$\chi = \frac{\int_{\text{outlet}} (J - G)dl}{\int_{\text{inlet}} (J - G)dl} \tag{1}$$

One of the most important features of the Free Molecular Flow interface is its ability to reconstruct the number density on domains. This is done by evaluating an integral equation for each mesh element. Denoting the distance vector between the boundary and the centroid of each mesh element in the domain by $\mathbf{r}$ the number density can be defined as:

$$n = -\int_{l'} \frac{J'(\mathbf{n}' \cdot \mathbf{r})}{2r} \left\langle \frac{1}{c'} \right\rangle dl' \tag{2}$$

where the integration is carried out over all boundaries in the model. The expression changes slightly for the 3D case. The quantity J' is the rate of emission of molecules per unit area $\mathbf{n}'$ is the boundary normal, and $\langle 1/c' \rangle$ is the inverse mean speed of the gas molecules. For more information, see the "Theory for the Free Molecular Flow Interface" in the *Molecular Flow Module User's Guide*.

Results and Discussion

The incident molecular flux on the exterior boundaries is shown in Figure 2. Using Equation 2 the reconstructed number density is shown in Figure 3.

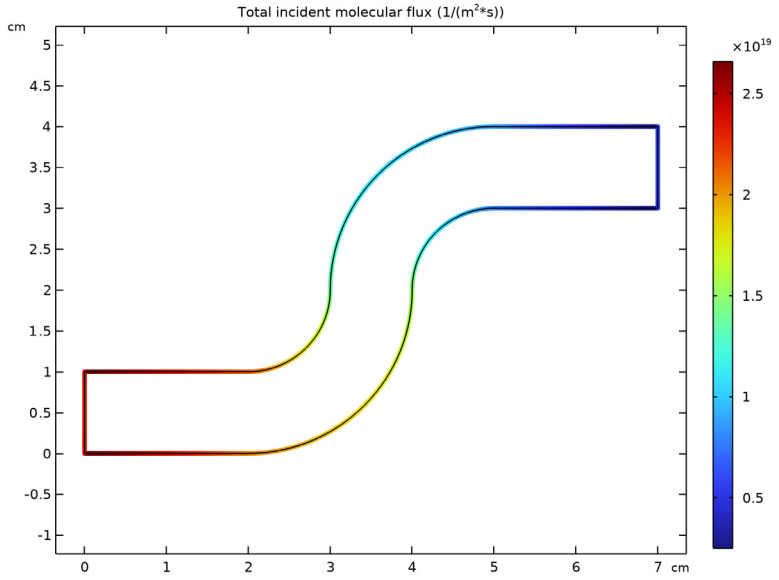

Figure 2: Plot of the incident molecular flux in the s-bend.

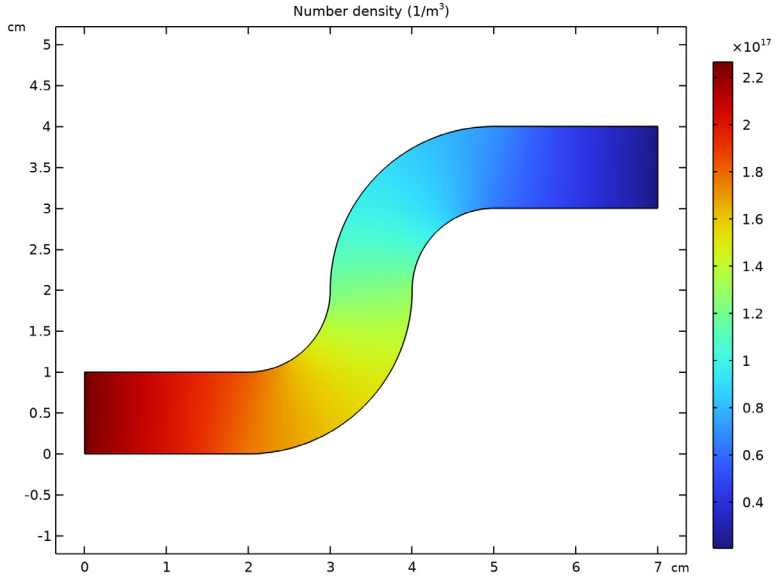

Figure 3: Plot of the reconstructed number density inside the s-bend.

The transmission probability for the molecular flow interface is 0.19676 and 0.1992 for the particle tracing. The two computed values are in close agreement. Note that slightly different results may be obtained for the particle tracing model each time the model is solved because random numbers are used so heavily in the computation.

When a Monte Carlo method is used to estimate the number density in the modeling domain, the results are in agreement with the reconstructed number density of Figure 3, as shown in Figure 4.

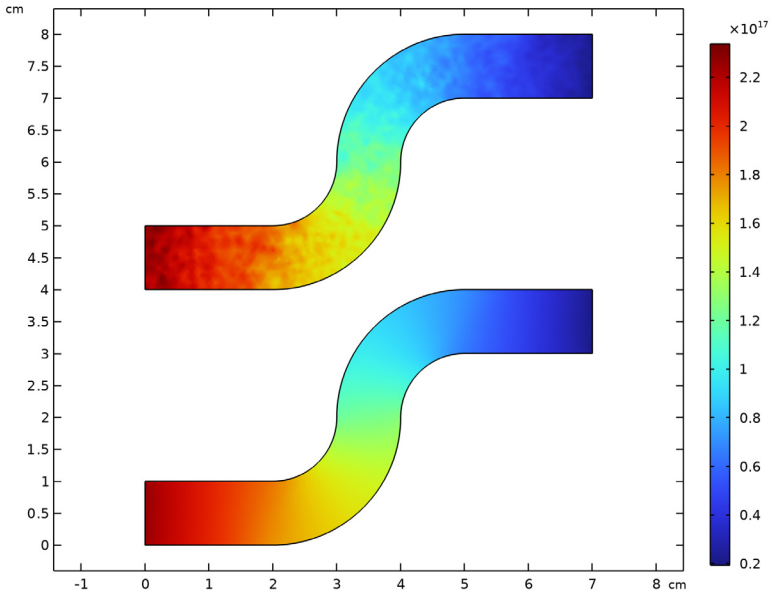

Figure 4: Comparison of the number density from the Molecular Flow and Particle Tracing Modules.

Notes About the COMSOL Implementation

The model is solved in two stages. First, the Free Molecular Flow interface is used to compute the transmission probability using a Stationary study. Subsequently, the Mathematical Particle Tracing interface is used to compute the transmission probability with a Time Dependent study using a Monte Carlo approach. An Accumulator feature is applied to the domain to estimate the number density of particles.

Application Library path: `Molecular_Flow_Module/Benchmarks/s_bend_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** > **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

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 **cm**.

Rectangle 1 (r1)

Each bend in the geometry is the annular region between two concentric circles, created using the boolean **Difference** operation.

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 2.

4 Click **Build Selected**.

Circle 1 (c1)

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

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

3 In the **Sector angle** text field, type 90.

4 Locate the **Position** section. In the **x** text field, type 2.

5 In the **y** text field, type 2.

6 Locate the **Rotation Angle** section. In the **Rotation** text field, type 270.

7 Click **Build Selected**.

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

Circle 2 (c2)

1 Right-click **Circle 1 (c1)** and choose **Duplicate**.

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

3 In the **Radius** text field, type 2.

4 Click **Build Selected**.

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

Difference 1 (dif1)

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

2 Select the object **c2** only.

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

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

5 Select the object **c1** only.

6 Click **Build Selected**.

Circle 3 (c3)

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

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

3 In the **Sector angle** text field, type 90.

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

5 In the **y** text field, type 2.

6 Locate the **Rotation Angle** section. In the **Rotation** text field, type 90.

7 Click **Build Selected**.

Circle 4 (c4)

1 Right-click **Circle 3 (c3)** and choose **Duplicate**.

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

3 In the **Radius** text field, type 2.

4 Click **Build Selected**.

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

Difference 2 (dif2)

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

2 Select the object **c4** only.

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

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

5 Select the object **c3** only.

6 Click **Build All Objects**.

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 2.

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

5 In the **y** text field, type 3.

6 Click **Build All Objects**.

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

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** checkbox.

5 Click **Build All Objects**.

The built geometry should appear as in Figure 1.

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

Now add some parameters for the gas temperature and molecular weight.

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
T0	293.15[K]	293.15 K	Temperature
Mw	0.028[kg/mol]	0.028 kg/mol	Molecular weight
p_in	1E-3[Pa]	0.001 Pa	Inlet pressure

FREE MOLECULAR FLOW (FMF)

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 $M_{n,G}$ text field, type Mw.

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.

Reservoir 1

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

2 Select Boundary 1 only.

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

4 In the $p_{0,G}$ text field, type p_in.

Total Vacuum 1

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

2 Select Boundary 6 only.

The number density inside the domain can be reconstructed by adding the **Number Density Reconstruction** feature.

Number Density Reconstruction 1

1 In the **Physics** toolbar, click **Domains** and choose **Number Density Reconstruction**.

2 Select Domain 1 only.

In order to compute the transmission probability, only the molecular flux needs to be computed. To save some computation time, specify in the physics interface not to compute the pressure.

3 In the **Model Builder** window, click **Free Molecular Flow (fmf)**.

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

5 Clear the **Pressure** checkbox.

6 Locate the **Integration Settings** section. From the **Integration resolution** list, choose **512**.

Add **Integration** component couplings on the inlet and outlet.

DEFINITIONS

Integration 1 (intop1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node.

2 Right-click **Definitions** and choose **Nonlocal Couplings** > **Integration**.

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

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

5 Select Boundary 1 only.

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 6 only.

Add expressions to compute the transmission probability using Equation 1.

Variables 1

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

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
Jin	intop1(fmf.J_G)	1/(m·s)	Influx
Jout	intop2(G)	1/(m·s)	Outflux
alpha	Jout/Jin		Transmission probability

MESH 1

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

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extremely fine**.

4 Click **Build All**.

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

STUDY 1

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

RESULTS

Incident Molecular Flux (fmf)

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

Number Density (fmf)

1 In the **Results** toolbar, click **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Number Density (fmf)` in the **Label** text field.

Surface 1

1 Right-click **Number Density (fmf)** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Free Molecular Flow** > **Number density** > **fmf.n_G - Number density - 1/m³**.

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

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

Now evaluate the transmission probability.

Global Evaluation 1

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

2 In the **Settings** window for **Global Evaluation**, click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **alpha - Transmission probability - 1**.

3 Click **Evaluate**.

Now add the Mathematical Particle Tracing interface to compute the transmission probability and number density using a Monte Carlo approach.

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 **Mathematics** > **Mathematical Particle Tracing (pt)**.

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

5 Click the **Add to Component 1** button 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** > **Time Dependent**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Free Molecular Flow (fmf)**.

5 Click the **Add Study** button in the window toolbar.

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

MATHEMATICAL PARTICLE TRACING (PT)

1 In the **Settings** window for **Mathematical Particle Tracing**, locate the **Particle Release and Propagation** section.

2 In the **Maximum number of secondary particles** text field, type `0`.

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
M	Mw/N_A_const	4.6495E-26 kg	Particle Mass
J_in	p_in*N_A_const/ sqrt(2*R_const*T0*Mw* pi)	2.9082E19 1/(m²·s)	Emitted molecular flux
L	0.01[m]	0.01 m	Inlet length
Np	10000	10000	Number of particles

MATHEMATICAL PARTICLE TRACING (PT)

Thermal Reemission 1

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

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

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

4 Locate the **Wall** section. In the T text field, type `T0`.

Outlet 1

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

2 Select Boundary 6 only.

Inlet 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Inlet**, locate the **Initial Position** section.

4 From the **Initial position** list, choose **Density**.

5 In the N text field, type `Np`.

6 Locate the **Initial Velocity** section. From the **Velocity specification** list, choose **Thermal**.

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

Wall 2

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Wall**, locate the **Wall Condition** section.

4 From the **Wall condition** list, choose **Disappear**.

Particle Counter 1

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

2 Select Boundary 6 only.

3 In the **Settings** window for **Particle Counter**, locate the **Particle Counter** section.

4 From the **Release feature** list, choose **Inlet 1**.

Particle Properties 1

1 In the **Model Builder** window, click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Mass** section.

3 In the m_p text field, type `M`.

Accumulator 1

1 In the **Physics** toolbar, click **Domains** and choose **Accumulator**.

2 Select Domain 1 only.

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

4 From the **Accumulate over** list, choose **Elements and time**.

5 In the **Accumulated variable name** text field, type `Nd`.

6 Locate the **Units** section. Click **Select Quantity**.

7 In the **Physical Quantity** dialog, type `numberdensity` in the text field.

8 In the tree, select **Transport** > **Number density (1/m^3)**.

9 Click **OK**.

10 In the **Settings** window for **Accumulator**, locate the **Accumulator Settings** section.

11 In the R text field, type `J_in*L/Np`.

STUDY 2

Step 1: Time Dependent

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

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 Click **Range**.

4 In the **Range** dialog, choose **Number of values** from the **Entry method** list.

5 In the **Stop** text field, type `0.006`.

6 In the **Number of values** text field, type 30.

7 Click **Replace**.

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

RESULTS

Global Evaluation 2

1 In the **Model Builder** window, expand the **Results** > **Datasets** node.

2 Right-click **Results** > **Derived Values** and choose **Global Evaluation**.

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

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

5 From the **Time selection** list, choose **Last**.

6 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)** > **Mathematical Particle Tracing** > **Particle Counter 1** > **pt.pcnt1.alpha - Transmission probability - 1**.

7 Click **Evaluate**.

TABLE 2

1 Go to the **Table 2** window.

The transmission probability from the particle tracing approach agrees very well with the result from the **Free Molecular Flow** interface.

RESULTS

Number Density Comparison

1 In the **Model Builder** window, right-click **Number Density (fmf)** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Number Density Comparison` in the **Label** text field.

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

4 Click to expand the **Plot Array** section. From the **Array type** list, choose **Linear**.

5 From the **Array axis** list, choose **y**.

6 In the **Relative padding** text field, type `0`.

Surface 2

1 Right-click **Number Density Comparison** and choose **Surface**.

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

3 From the **Dataset** list, choose **Particle 1**.

4 Locate the **Expression** section. In the **Expression** text field, type `pt.Nd`.

5 Click to expand the **Quality** section. From the **Evaluation settings** list, choose **Manual**.

6 From the **Resolution** list, choose **No refinement**.

7 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

8 In the **Number Density Comparison** toolbar, click **Plot**.

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

The results from the **Mathematical Particle Tracing** interface agree with the number density computed using the **Free Molecular Flow** interface.