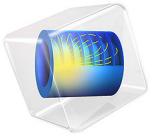

Quasi-2D Turbomolecular Pump

Introduction

Turbomolecular pumps are widely used in vacuum system design. A turbomolecular pump is a bladed molecular turbine that compresses gases by momentum transfer from the rapidly rotating blades of the rotor to the gas molecules. In the free molecular flow range (typically < 10^{-1} Pa), the particles collide primarily with the rotor resulting in an efficient pumping process. The following assumptions are made:

- Intermolecular collisions are negligible
- The molecules follow a Maxwellian velocity distribution
- The gas temperature is constant
- The particles experience diffuse scattering at the blade walls, following the distribution called *Lambert's cosine law* or *Knudsen's cosine law*

The Mathematical Particle Tracing interface can be used to evaluate the performance of a simple turbomolecular pump in the free molecular flow regime. While the Molecular Flow Module provides access to efficient and deterministic calculation of gas density in the free molecular flow regime, it uses the angular coefficient method which is only applicable for molecules or atoms that are moving much faster than any object in the model geometry. For turbopumps, where the blades move over similar time scales as the atoms or molecules themselves, this requirement is not satisfied, so a Monte Carlo approach is used instead.

This example is formulated as a quasi-2D model. That is, each turbine blade is very large compared to the root-to-tip distance, so it is a fair approximation to treat part of the turbine as an inertial frame of reference in which the blades are parallel, neglecting the effects of blade rotation.

The example Turbomolecular Pump shows how to set up a complete 3D model of a pump stage, complete with the centrifugal and Coriolis forces that arise when tracing particles in a noninertial frame of reference.

Model Definition

Modern turbomolecular pumps contain a large number of blades organized into stages, with adjacent stages sometimes rotating in opposite directions, or as rotor-stator pairs.

For a series of compression stages at zero flow, the overall compression ratio is approximately the product of the compression ratios for each stage (Ref. 1), so the overall performance of the pump can be investigated using a numerical model of a single stage. Thus, in this example only a single row of blades is considered. Furthermore, because of sector symmetry only the space between a single pair of adjacent blades is considered.

BLADE GEOMETRY

Typical cross sections of a pump stage are shown for three different radii of curvature in Figure 1. The empty space where molecules are free to propagate is in yellow, and solid domains are in gray. The blades (shown as thin gray rectangles) appear straight in such a cross section taken from above or below the stage, but a side view would reveal them to be inclined.

In the leftmost image, the blade radius (the distance from the center of rotation to the blade root, or the beginning of the empty space) is larger than the blade spacing, but not immensely so. In a co-rotating coordinate system, the centrifugal and Coriolis forces for this stage would be quite significant.

In the middle image, a sector from a pump stage with a much larger radius is shown. The curvature of this section is still evident, but not as greatly so as in the left image.

In the rightmost image, the radius of the pump stage has been taken to be arbitrarily large. Then the ring of blades takes on the appearance of an infinite straight row of blades having only translational velocity.

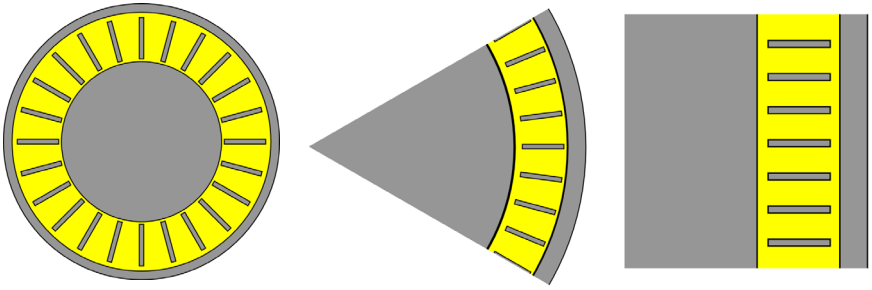

Figure 1: Cross sections of a single stage pump for varying radii of curvature.

This example uses the approximation of a pump stage with a large radius as an infinite row of blades, so that the co-moving frame of reference attached to the blades can be treated as inertial. The main advantage of this approximation is that molecules travel in straight lines in the co-moving frame, allowing the **Time-Dependent Solver** to accurately resolve the molecule trajectories even when taking very large time steps.

THE FREE MOLECULAR FLOW REGIME

As illustrated in Figure 2, a turbomolecular pump causes a pressure difference between the domains on either side, depending on the angle, spacing, and speed of the moving blades. In the numerical model used here, the length scales are assumed to follow the relation

$$L_1 \gg \lambda \gg L_2$$

where

- L_1 is a characteristic length scale of either domain adjacent to the pump
- L_2 is a characteristic length scale within a stage of the pump
- λ (SI unit: m) is the molecular mean free path

Because the mean free path is much smaller than length scales outside the pump, it is reasonable to assume that the gas in each adjacent domain is Maxwellian. This can be used to prescribe appropriate initial conditions for entering molecules. Because the mean free path is much larger than the length scales in each pump stage, it is also reasonable to neglect intermolecular collisions within the stage.

If the gas density were higher, so that the pump stage operates in the *transitional flow regime* instead of the *free molecular flow* regime, then it would still be possible to compute the transmission probability, but this would require intermolecular collisions to be included in the modeling domain, most likely with a Monte Carlo approach.

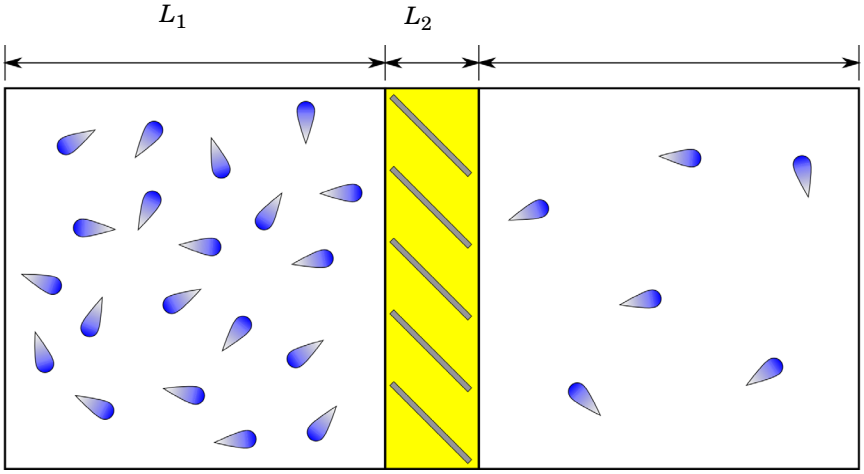

Figure 2: A single stage of a turbomolecular pump, consisting of a row of inclined blades, creates a pressure difference between the two adjacent domains. Not drawn to scale.

MODEL PARAMETERS

The blade geometry is characterized by the blade length B (SI unit: m), blade spacing S (SI unit: m), and blade angle α (SI unit: rad), as shown in Figure 3.

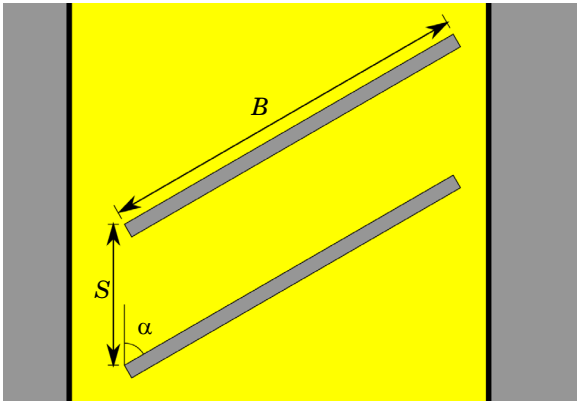

Figure 3: Geometry parameters for the single-stage turbomolecular pump (side view).

In order to compute these transmission probabilities, the model uses an **Inlet** feature defined on at one end of the space between two blades, and uses the **Outlet** and **Particle Counter** to gather information about particles that reach the opposite side. The overall transmission probability is the ratio of the number of molecules that reach the **Outlet** boundary to the total number of released molecules.

Hydrogen gas molecules (H_2) are released using an **Inlet** feature with the built-in **Thermal** velocity distribution. Similarly, the blade surfaces use a dedicated boundary condition called **Thermal Re-Emission** that randomly changes the particle's speed and direction. Both the release feature and boundary condition launch molecules into the modeling domain with a distribution of directions following Knudsen's cosine law, and with speeds sampled from the distribution

$$f(v) = \left(\frac{m_\mathrm{p}}{k_\mathrm{B}T}\right)^2 \frac{v^3}{2} \exp\left(-\frac{m_\mathrm{p}v^2}{2k_\mathrm{B}T}\right)$$

It is convenient to express the model parameters as dimensionless quantities. The blade length and spacing are related by a dimensionless blade aspect ratio S_0,

$$S = BS_0$$

The blade speed is expressed in terms of the dimensionless speed factor C,

$$v_\mathrm{b} = v_\mathrm{p}C$$

where v_p (SI unit: m/s) is the most probable speed of particles in the Maxwellian distribution,

$$v_p = \frac{2k_B T}{m_p}$$

$$m_p = \frac{M}{N_A}$$

where

- $k_B = 1.380649 \times 10^{-23}$ J/K is the Boltzmann constant
- T = 300 K is the ambient temperature
- M = 2 g/mol is the approximate molar mass of the hydrogen gas
- $N_A = 6.02214076 \times 10^{23}$ 1/mol is the Avogadro constant

For hydrogen gas, this gives a most probable speed of approximately $v_p = 1579.3$ m/s.

Results and Discussion

The model includes three studies, each with a separate **Parametric Sweep**. The parameter values used in these three studies are shown in Table 1 below. These values are almost identical to the values used to produce Figures 5-7 in Ref. 2.

TABLE 1: PARAMETER VALUES USED IN EACH PARAMETRIC SWEEP.

Study	Velocity factor	Blade angle (deg)	Blade aspect ratio
Sweep Over Speeds	`range(-10,0.5,10)`	35	1
Sweep Over Angles	1	`range(5,5,55)`	1
Sweep Over Aspect Ratios	1	35	`range(0.5,0.1,1.5)`

The transmission probability as a function of speed factor C is shown in Figure 4. Compare this to Figure 5 in Ref. 2. Two curves are shown, the transmission probability M_{12} and the direct transmission probability m_{12} (both dimensionless). Particles only contribute to the direct transmission probability if they pass through the blades without ever hitting them, hence it reaches a maximum around $C = 1$ when the blade speed and most probable molecule speed are equal.

The transmission probability as a function of the blade angle, α, is shown in Figure 5. Compare this to Figure 6 in Ref. 2. In both figures, the direct transmission probability

reaches a maximum at about $\alpha = 35°$, whereas the overall transmission probability reaches a maximum at the steeper angle $\alpha = 45°$.

The transmission probability as a function of blade aspect ratio is shown in Figure 6. Compare this to Figure 7 in Ref. 2. (Note that, in the reference, the blade angle has been changed to 30°, whereas in this example it is maintained at 35° to be consistent with the first study.) When the blades are placed closer together, the overall transmission probability is decreased, and the direct transmission probability even more so, because it becomes very likely for a molecule to pass through without hitting the closely spaced blades.

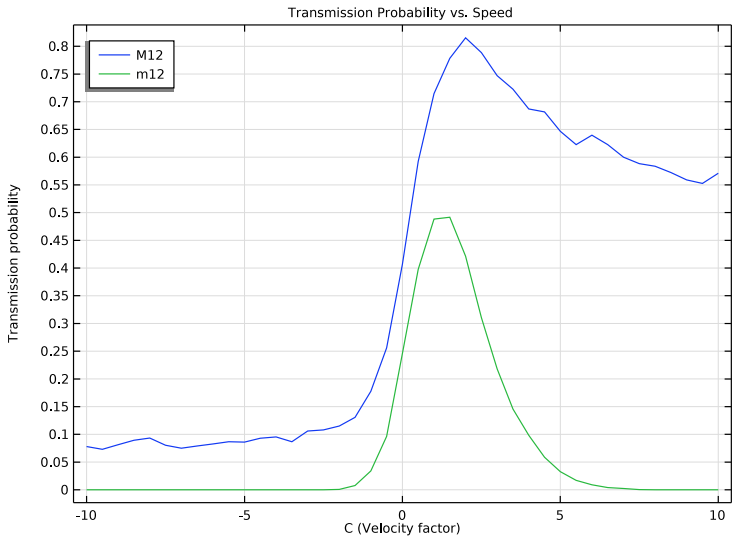

Figure 4: Transmission probability of a single-stage pump as a function of the dimensionless velocity factor C.

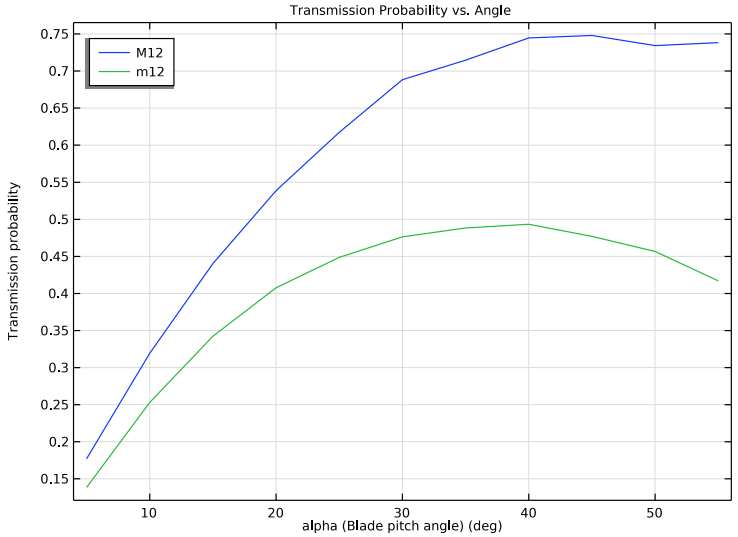

Figure 5: Transmission probability of a single-stage pump as a function of the blade angle α.

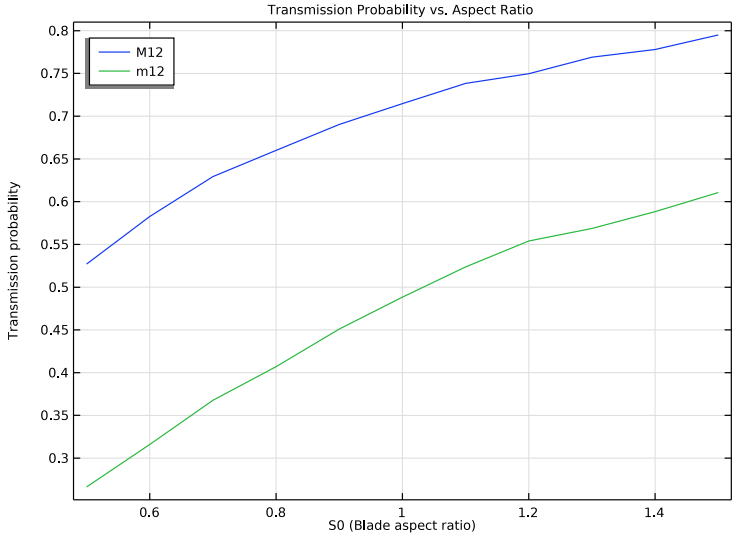

Figure 6: Transmission probability of a single-stage pump as a function of the blade aspect ratio S_0.

References

1. J.F. O'Hanlon, *A user's guide to vacuum technology*, John Wiley & Sons, 2005.

2. S. Katsimichas, A.J.H. Goddard, R. Lewington, and C.R.E. De Oliveira, "General geometry calculations of one-stage molecular flow transmission probabilities for turbomolecular pumps," *J. Vac. Sci. Technol. A: Vac. Surf. Films*, vol. 13, no. 6, pp. 2954–2961, 1995.

3. Y. Li, X. Chen, Y. Jia, M. Liu, and Z. Wang, "Numerical investigation of three turbomolecular pump models in the free molecular flow range," *Vacuum*, vol. 101, pp. 337–344, 2014.

Application Library path: `Particle_Tracing_Module/Vacuum_Systems/turbomolecular_pump_quasi_2d`

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 **3D**.

2 In the **Select Physics** tree, select **Mathematics>Mathematical Particle Tracing (pt)**.

3 Click **Add**.

4 Click **Study**.

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

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 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `turbomolecular_pump_quasi_2d_parameters.txt`.

DEFINITIONS

Define some variables that will be used later for results analysis.

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
M12	`pt.sum(if(bndenv(pt.pcnt1.Ob)==1,1,0))/Np`		Transmission probability
m12	`pt.sum(if(bndenv(pt.pcnt1.Ob)==1,noCollision,0))/Np`		Direct transmission probability

The transmission probability is the fraction of molecules that reach the other side of the turbomolecular pump stage. The direct transmission probability is the fraction of molecules that cross the stage without hitting any of the blades.

At this point, the variable definitions will give a warning indicating an unknown variable. Any unknown variables will be defined later while setting up the physics.

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**.

The model geometry is an extrusion of a 2D polygon.

Work Plane 1 (wp1)

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

The default work plane orientation is used. With this orientation, the direction across the pump stage is the x direction, consecutive blades in the stage are offset in the y direction, and the geometry is considered uniform in the z direction.

Work Plane 1 (wp1)>Plane Geometry

In the **Model Builder** window, click **Plane Geometry**.

Work Plane 1 (wp1)>Polygon 1 (pol1)

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

2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

3 In the table, enter the following settings:

xw (cm)	yw (cm)
0	0
B*sin(alpha)	B*cos(alpha)
B*sin(alpha)	S+B*cos(alpha)
0	S

4 In the **Work Plane** toolbar, click **Build All**.

Extrude 1 (ext1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** right-click **Work Plane 1 (wp1)** and choose **Extrude**.

2 In the **Settings** window for **Extrude**, click **Build All Objects**.

MATHEMATICAL PARTICLE TRACING (PT)

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Mathematical Particle Tracing (pt)** 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 `mp_H2`.

Before setting up the particle releases and boundary conditions, define an additional dependent variable that will be used to identify particles that pass through the stage without ever hitting a blade.

Auxiliary Dependent Variable 1

1 In the **Physics** toolbar, click **Global** and choose **Auxiliary Dependent Variable**.

2 In the **Settings** window for **Auxiliary Dependent Variable**, locate the **Auxiliary Dependent Variable** section.

3 In the **Field variable name** text field, type `noCollision`.

This auxiliary variable `noCollision` will be initialized to 1 for released particles and reinitialized to 0 if they hit the blades. It was used previously in the definition of `m12`.

Release molecules from one side of the pump stage. The gas in the adjoining domain is assumed to follow a Maxwellian distribution, so that the speeds of incoming molecules are randomly sampled based on the surrounding temperature.

Inlet 1

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

Define an **Inlet** boundary condition to release the molecules at $x = 0$.

2 Select Boundary 1 only.

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

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

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

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

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

8 Locate the **Initial Value of Auxiliary Dependent Variables** section. In the $\mathrm{noCollision}_0$ text field, type `1`.

The space between two adjacent blades is an inertial frame moving at constant velocity relative to the laboratory frame. Subtract the relative velocity between the two frames from the initial particle velocity.

9 Click to expand the **Advanced Settings** section. Select the **Subtract moving frame velocity from initial particle velocity** check box.

10 From the **Background velocity** list, choose **User defined**.

11 Specify the $\mathbf{v}_b$ vector as

0	x
-vb	y
0	z

Wall 1 (Symmetry Boundaries)

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

2 In the **Settings** window for **Wall**, type `Wall 1 (Symmetry Boundaries)` in the **Label** text field.

3 Locate the **Wall Condition** section. From the **Wall condition** list, choose **Bounce**.

The surfaces parallel to the xy-plane are treated as symmetry boundaries because the blade extends arbitrarily far in the z direction.

Use the **Thermal Re-Emission** boundary condition to resample the particle velocity from a distribution based on temperature at the blades.

Thermal Re-Emission 1 (Blade Surfaces)

1 In the **Physics** toolbar, click **Boundaries** and choose **Thermal Re-Emission**.

2 Select Boundaries 2 and 5 only.

3 In the **Settings** window for **Thermal Re-Emission**, locate the **Wall Properties** section.

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

5 In the **Label** text field, type `Thermal Re-Emission 1 (Blade Surfaces)`.

6 Click to expand the **New Value of Auxiliary Dependent Variables** section. Select the **Assign new value to auxiliary variable : noCollision** check box. Use the default value, `0`.

Outlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outlet**. The **Outlet** will stop particles when they either cross the pump stage completely or get deflected back to the **Inlet** boundary.

2 Select Boundaries 1 and 6 only.

Particle Counter 1

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

2 Select Boundary 6 only.

This **Particle Counter** does not affect particle trajectories in any way, but it defines some additional variables that are useful for postprocessing. In particular, this step resolves any unknown variable issues in the **Variables 1** node.

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 coarse**. The mesh quality is not important because all of the surfaces in the model are flat, and because no field variables are solved for in the domain. Hence a very coarse mesh can be used.

4 Click **Build All**.

SWEEP OVER SPEEDS

In the remaining steps, set up three separate parametric sweeps to analyze the effects of the velocity, angle, and spacing of blades on the transmission probability of the single-stage pump. Begin with a **Parametric Sweep** over the dimensionless blade velocity `C`.

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

2 In the **Settings** window for **Study**, type `Sweep Over Speeds` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

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 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
C (Velocity factor)	`range(-10,0.5,10)`	

Step 1: Time Dependent

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

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

3 From the **Time unit** list, choose **ms**.

4 In the **Output times** text field, type `0 0.2`.

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

RESULTS

Transmission Probability: Sweep Over Speeds

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

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

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

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

5 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Transmission Probability vs. Speed`.

7 Locate the **Plot Settings** section.

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

9 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Global 1

1 Right-click **Transmission Probability: Sweep Over Speeds** 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
M12	1	Transmission probability
m12	1	Direct transmission probability

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Outer solutions**.

5 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
M12
m12

7 In the **Transmission Probability: Sweep Over Speeds** toolbar, click **Plot**. Compare the resulting image to Figure 4.

ROOT

Repeat the previous steps with a new **Parametric Sweep** over the blade angle `alpha`.

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

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

SWEEP OVER ANGLES

1 In the **Model Builder** window, click **Study 2**.

2 In the **Settings** window for **Study**, type `Sweep Over Angles` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

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 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
alpha (Blade pitch angle)	`range(5,5,55)`	deg

Step 1: Time Dependent

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

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

3 From the **Time unit** list, choose **ms**.

4 In the **Output times** text field, type `0 0.2`.

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

RESULTS

Transmission Probability: Sweep Over Angles

1 In the **Model Builder** window, right-click **Transmission Probability: Sweep Over Speeds** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Sweep Over Angles/ Parametric Solutions 2 (sol45)**.

4 Locate the **Title** section. In the **Title** text area, type `Transmission Probability vs. Angle`.

5 In the **Transmission Probability: Sweep Over Angles** toolbar, click **Plot**. Compare the resulting image to Figure 5.

ROOT

Conclude with a third **Parametric Sweep** over the dimensionless aspect ratio `S0`, which is the ratio of the spacing between adjacent blades to the length of each blade.

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

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

SWEEP OVER ASPECT RATIOS

1 In the **Model Builder** window, click **Study 3**.

2 In the **Settings** window for **Study**, type `Sweep Over Aspect Ratios` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

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 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
S0 (Blade aspect ratio)	`range(0.5,0.1,1.5)`	

Step 1: Time Dependent

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

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

3 From the **Time unit** list, choose **ms**.

4 In the **Output times** text field, type `0 0.2`.

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

RESULTS

Transmission Probability: Sweep Over Aspect Ratios

1 In the **Model Builder** window, right-click **Transmission Probability: Sweep Over Speeds** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Sweep Over Aspect Ratios/ Parametric Solutions 3 (sol58)**.

4 Locate the **Title** section. In the **Title** text area, type `Transmission Probability vs. Aspect Ratio`.

5 In the **Transmission Probability: Sweep Over Aspect Ratios** toolbar, click **Plot**. Compare the resulting image to Figure 6.