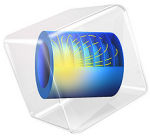

Quadrupole Mass Filter

Introduction

A quadrupole mass filter (QMF) is a key component of a modern mass spectrometer. A QMF uses direct current (DC) and alternating current (AC) electric fields to analyze positive or negative ions by mass-to-charge ratio. A QMF consists of four parallel rods spaced equidistantly. The ratio of the rod radius to the radius of the inscribed circle is 1.148 (Ref. 1). Opposite pairs of rods are electrically connected. Adjacent rods have opposite DC potentials and their AC potentials are out of phase. Typical rod diameters are between 5 and 12 mm with rod lengths between 100 and 200 mm. The frequency of the AC component of the electric field is typically in the range 1 to 10 MHz.

Ions are created using a number of different techniques depending on the application. They are injected along the axis of the QMF. Typical ion energies at the QMF entrance aperture are 3 to 5 electron volts. The ions experience forces due to the AC and DC fields near the quadrupole axis. For certain AC and DC field values only an ion of a specific mass to charge ratio is transmitted. Ions are detected by measuring the ion current at the exit of the quadrupole.

Note: This application requires the Particle Tracing Module.

Model Definition

The cross section of a typical QMF is shown in Figure 1. The ions are injected in such a way that their initial velocity is directed only in the out-of-plane direction. As long as the ions remain in the QMF they experience forces in the x and y direction due to the DC and AC fields. The rod radius is 2.78 mm and the radius of the inscribed circle is about 2.42 mm. Since this is a 2D model, there is no rod length. However, since the ion velocity is assumed constant in the out-of-plane direction, the effective rod length can be computed by multiplying the out-of-plane ion velocity by the total simulation time. The total simulation time is 40 μs, which, for an RF frequency of 4 MHz, corresponds to 160 RF cycles. For an initial ion energy of 3 eV and an ion mass of 40 amu, this corresponds to an effective rod length of 152 mm.

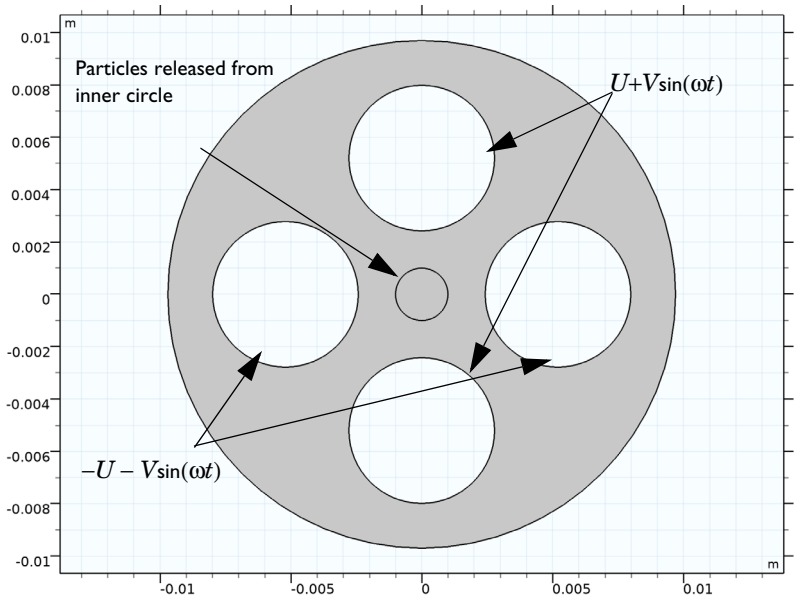

Figure 1: Plot of the model geometry. The geometry length unit is meters.

This application is designed to find the transmission probability of ions in the QMF for different values of two dimensionless parameters, a and q. These are coefficients in the Mathieu equation, which can be used to solve the same problem as this application. However, this application can be generalized to 3D and the effects of fringing fields may also be included. The parameters a and q are scaled values for the DC and AC voltages respectively. It is important to note that in order to gain an accurate statistical measure of the transmission probability, it may be necessary to solve for a much larger number of particles (Ref. 1). The parameter, a, is related to the applied DC voltage by:

$$a = \frac{8eZU_{\mathrm{dc}}}{mr_0^2\omega^2}$$

where

- Z (dimensionless) is the charge number,
- $e = 1.602176565 \times 10^{-19}$ C is the elementary charge,
- U_{dc} (SI unit: V) is the applied DC voltage,
- m (SI unit: kg) is the particle mass,

- r_0 (SI unit: m) is the inscribed radius, and
- ω (SI unit: Hz) is the angular frequency.

The parameter q is related to the applied AC voltage by:

$$q = \frac{4eZV_{ac}}{mr_0^2\omega^2}$$

By solving the Mathieu equation it is possible to construct a stability diagram that shows whether the particles undergo stable or unstable oscillatory motion down the QMF. The stability diagram is plotted in Figure 2.

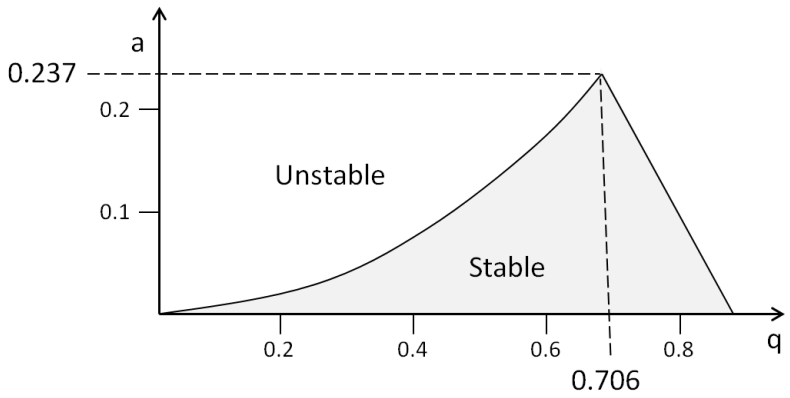

Figure 2: Stability diagram for a quadrupole mass filter.

So long as the values of a and q (and thus U_{dc} and V_{ac}) remain within the gray region, the particles do not make contact with the rods. The operating principle of a QMF is to sweep through a range of values for q whilst keeping the ratio of a/q constant. The idea is illustrated in Figure 3. The values of a and q are both increased simultaneously such that they follow the red line. The ion trajectories are initially unstable, which results in a transmission probability of zero. Once the value of q reaches about 0.6, the ions enter the stable operating region and some particles are transmitted to the detector. As the value of q increases further, the ions end up back in the unstable region and the transmission probability is reduced to zero.

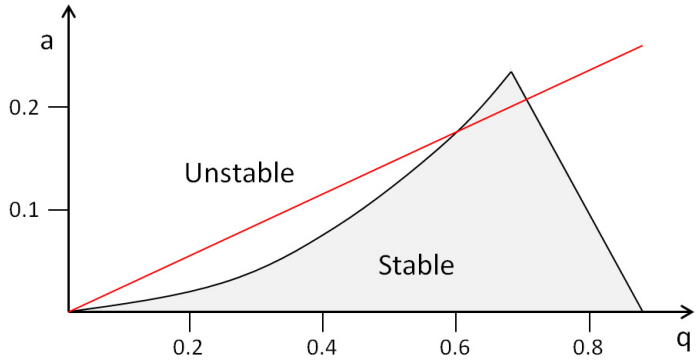

Figure 3: Operating principle of a quadrupole mass filter.

For the DC field, the application solves Poisson's equation for the electric potential, U:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla U = 0 \tag{1}$$

Here ε_0 is the permittivity of free space (SI unit: $\mathrm{F/m}$) and ε_r is the relative permittivity of the medium (taken as 1 in this application). The zero on the right-hand side of Equation 1 indicates that the space charge density inside the quadrupole is negligible. On the north and south rods, a positive potential of magnitude U_{dc} is applied:

$$U = U_{dc}$$

and on the east and west rods, a negative potential is applied:

$$U = -U_{dc}$$

For the AC fields, the conservation of electric currents is used to compute the AC potential, V:

$$-\nabla \cdot (\sigma + j\omega\varepsilon_0\varepsilon_r)\nabla V = 0$$

where σ is the electrical conductivity in the filter (taken as zero here) and ω is the angular frequency (SI unit: Hz).

On the north and south rods, a positive potential of magnitude V_{ac} is applied:

$$V = V_{ac}$$

and on the east and west rods, a negative potential is applied:

$$V = -V_{ac}$$

In order to construct the total electric field which the particles experience once they enter the modeling domain, superposition of the AC and DC fields is used. This is a valid assumption in this case since the equations solved for the AC and DC fields are linear.

Particle motion is governed by Newton's second law:

$$\frac{d}{dt}(m\mathbf{v}) = Ze\mathbf{E}$$

where m is the particle mass (SI unit: kg), $\mathbf{v}$ is the particle velocity (SI unit: m/s), Z is the dimensionless charge number, e is the elementary charge (SI unit: s A), and $\mathbf{E}$ is the electric field (SI unit: V/m). The electric field contains two contributions, a stationary electric field and one which is changing over time:

$$\mathbf{E} = \mathbf{E}_{dc} + \mathbf{E}_{ac}$$

where:

$$\mathbf{E}_{dc} = -\nabla U$$

and

$$\mathbf{E}_{ac} = -\mathrm{real}(\nabla \tilde{V} \exp(j\omega t))$$

where the tilde denotes that the AC electric potential is complex-valued. The particle position, $\mathbf{q}$, is simply computed from the definition of the velocity:

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

The particles have no initial velocity in the modeling plane. Particles are not only released at the simulation start time, they must be released at uniformly spaced times over the first RF cycle of the AC field. Particles are released at 11 times from 0 s to 0.25 μs; since the frequency of the AC field is 4 MHz, this corresponds to one full RF cycle.

The location of the ions for different values of the parameter q after 140 RF cycles are plotted in Figure 4. As expected, all the injected ions make contact with the rods up to a value of $q = 0.6$. For $q = 0.7$, however, there are ions that have clearly not made contact with the rods. These ions are detected by a current collector at the end of the QMF.

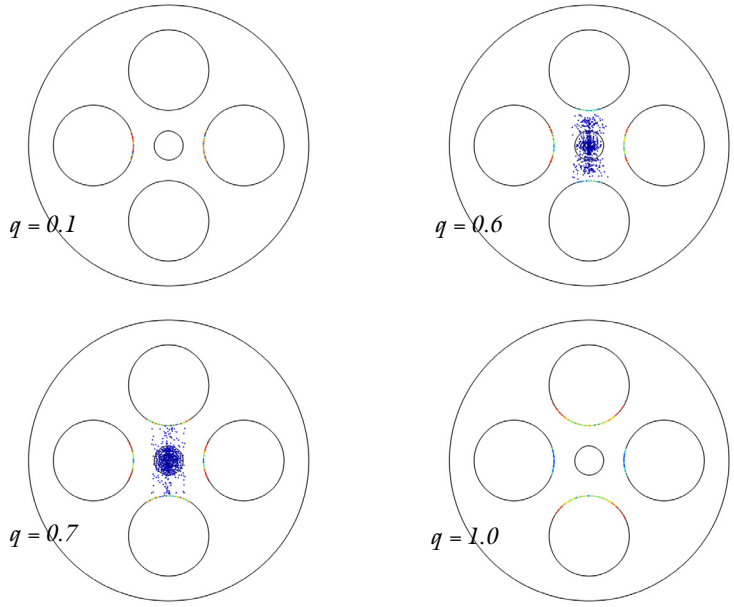

Figure 4: Plot of the ion location after 140 RF cycles inside the QMF.

The transmission probability is plotted in Figure 5. There is a clear stable window of operation between the values $q = 0.6$ and $q = 0.75$. This result agrees well with the theory outlined in the Model Definition section. In this example the slope of a/q was fixed to be $0.2/0.7$, meaning the width of the transmission peak spans over a q range of 0.15. If the slope of a/q were to be increased, the width of the peak where stable operation occurs would be reduced. If the slope of the curve is greater than $0.237/0.706$ then there are no regions of stable operation for any value of q.

As the slope of a/q decreases, the range of q values for which the ion trajectories are stable increases.

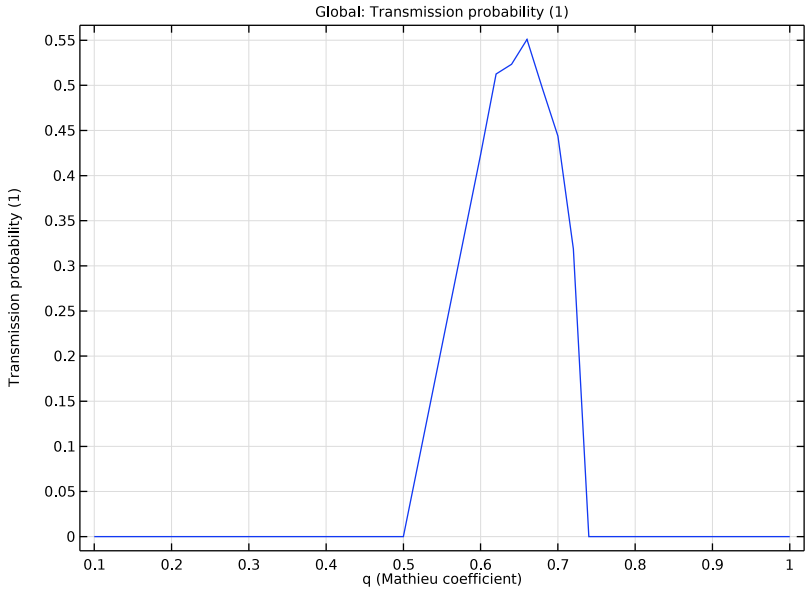

Figure 5: Plot of the transmission probability through the QMF for different values of q.

Notes About the COMSOL Implementation

Use the **Parametric Sweep** feature on the parameter q while keeping the ratio a/q constant. For each value of q, separate study steps are called to solve for the fields and particle trajectories.

Reference

1. J.R. Gibson, S. Taylor, and J.H. Leck, "Detailed simulation of mass spectra for quadrupole mass spectrometer systems," *J. Vac. Sci. Technol. A*, vol. 18, no. 1, p. 237, 2000.

Application Library path: `ACDC_Module/Particle_Tracing/quadrupole_mass_filter`

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 **AC/DC>Electric Fields and Currents>Electrostatics (es)**.
3. Click **Add**.
4. In the **Select Physics** tree, select **AC/DC>Electric Fields and Currents>Electric Currents (ec)**.
5. Click **Add**.
6. In the **Select Physics** tree, select **AC/DC>Particle Tracing>Charged Particle Tracing (cpt)**.
7. Click **Add**.
8. Click **Done**.

GLOBAL DEFINITIONS

Add some parameters for the quadrupole geometry and physics settings. To save time, the parameters can be loaded from a file. The optimum inscribed radius is the rod radius divided by 1.147.

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 `quadrupole_mass_filter_parameters.txt`.

   The parameter `q` will be varied during a **Parametric Sweep** but the ratio of the DC and AC applied voltages will stay the same. The ionic mass is that of argon.

GEOMETRY 1

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 **Radius** text field, type `rcase`.

Circle 2 (c2)

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

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

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

4 Locate the **Position** section. In the **x** text field, type `re+r0`.

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 **Radius** text field, type `re`.

4 Locate the **Position** section. In the **y** text field, type `re+r0`.

Circle 4 (c4)

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

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

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

4 Locate the **Position** section. In the **x** text field, type `-(re+r0)`.

Circle 5 (c5)

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

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

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

4 Locate the **Position** section. In the **y** text field, type `-(re+r0)`.

Circle 6 (c6)

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

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

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

Difference 1 (dif1)

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

2 Select the object **c1** only.

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

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

5 Select the objects **c2**, **c3**, **c4**, and **c5** only.

6 Click **Build All Objects**. The geometry should look like Figure 1.

MATERIALS

The ion trap is at near vacuum conditions. The relative permittivity is hence 1 and the conductivity 0.

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	1	1	Basic
Electrical conductivity	sigma_iso ; sigmaii = sigma_iso, sigmaij = 0	0	S/m	Basic

DEFINITIONS

It is convenient to define some selections for the positive and negative electrodes.

Positive

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundaries 7–10, 14, 15, 18, and 19 only.

Negative

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundaries 3–6 and 21–24 only.

Set the **Equation form** to **Stationary** so that the correct equation contribution is generated. This is necessary because the **Frequency Domain** study step will be used to compute both the AC and DC fields later on.

ELECTROSTATICS (ES)

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

2 In the **Settings** window for **Electrostatics**, click to expand the **Equation** section.

3 From the **Equation form** list, choose **Stationary**.

Change the name of the dependent variable for the DC field to `U`.

4 Click to expand the **Dependent Variables** section. In the **Electric potential** text field, type `U`.

Now define the boundary conditions for the DC field.

Electric Potential 1

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

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

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

4 Locate the **Electric Potential** section. In the V_0 text field, type `Udc`.

Electric Potential 2

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

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

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

4 Locate the **Electric Potential** section. In the V_0 text field, type `-Udc`.

ELECTRIC CURRENTS (EC)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electric Currents (ec)**.

2 In the **Settings** window for **Electric Currents**, click to expand the **Dependent Variables** section.

3 In the **Electric potential** text field, type `V`.

Now define the boundary conditions for the AC field.

Electric Potential 1

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

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

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

4 Locate the **Electric Potential** section. In the V_0 text field, type `Vac`.

Electric Potential 2

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

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

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

4 Locate the **Electric Potential** section. In the V_0 text field, type `-Vac`.

Specify the properties of the ions. The charge number remains at 1 and the ion mass is set by a parameter which was defined eariler.

CHARGED PARTICLE TRACING (CPT)

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Particle Properties 1**.

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

3 In the Z text field, type `1`.

4 Locate the **Particle Mass** section. In the m_p text field, type `mi`.

5 In the **Model Builder** window, click **Charged Particle Tracing (cpt)**.

6 In the **Settings** window for **Charged Particle Tracing**, locate the **Particle Release and Propagation** section.

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

The particles are released based on the mesh elements in the aperture. Furthermore, the particles are released at different phases of the first RF cycle.

Release 1

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

2 Select Domain 2 only.

3 In the **Settings** window for **Release**, locate the **Release Times** section.

4 Click **Range**.

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

6 In the **Start** text field, type `0`.

7 In the **Stop** text field, type `1/4E6`.

8 In the **Number of values** text field, type `11`.

9 Click **Replace**.

There are two forces acting on the particles. One is due to the DC electric field and one is due to the AC electric field. To add these, simply add two **Electric Force** features. The **Use**

piecewise polynomial recovery check box is selected so that the electric field is as accurate as possible.

Electric Force 1

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

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

3 In the **Settings** window for **Electric Force**, locate the **Electric Force** section.

4 From the **E** list, choose **Electric field (es/ccn1)**.

5 Locate the **Advanced Settings** section. Select the **Use piecewise polynomial recovery on field** check box.

For the AC force, the **Multiply force by phase angle** check box must be selected. This ensures that the magnitude of the electric field is multiplied by $e^{j\omega t}$ as the particles are traveling down the trap.

Electric Force 2

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

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

3 In the **Settings** window for **Electric Force**, locate the **Electric Force** section.

4 From the **E** list, choose **Electric field (ec/cucn1)**.

5 Locate the **Advanced Settings** section. From the **Time dependence of field** list, choose **Time harmonic**.

6 Select the **Use piecewise polynomial recovery on field** check box.

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 **Extra fine**.

4 Click **Build All**.

Now add the study to compute the fields and the particle trajectories. Solve the problem using two study steps. First, compute the AC and DC electric fields. Then, using the computed fields to define the electric force, solve for the particle trajectories. These steps are wrapped with a parametric sweep over the parameter q. The number of parameters in the sweep is increased between the limits of 0.6 and 0.8 since this is where the transmission probability will be highest.

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 **Empty Study**.

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

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

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 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
q (Mathieu coefficient)	`0.1 0.5 range(0.6,0.2/10,0.8) 1`	

Frequency Domain

1 In the **Study** toolbar, click **Study Steps** and choose **Frequency Domain> Frequency Domain**.

2 In the **Settings** window for **Frequency Domain**, locate the **Study Settings** section.

3 In the **Frequencies** text field, type `4E6`.

4 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Charged Particle Tracing (cpt)**.

Time Dependent

1 In the **Study** toolbar, click **Study Steps** and choose **Time Dependent> Time Dependent**.

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

3 Click **Range**.

4 In the **Range** dialog box, type `160/4e6` in the **Stop** text field.

5 In the **Step** text field, type `1/4e6`.

6 Click **Replace**.

7 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

8 In the table, clear the **Solve for** check boxes for **Electrostatics (es)** and **Electric Currents (ec)**.

9 Click to expand the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

10 From the **Method** list, choose **Solution**.

11 From the **Study** list, choose **Study 1, Frequency Domain**.

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

RESULTS

Three plots are created by default. The first two show the electric potential distributions for the AC and DC fields.

Particle Trajectories (cpt)

1 In the **Model Builder** window, under **Results** click **Particle Trajectories (cpt)**.

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

3 From the **Parameter value (q)** list, choose **0.1**.

4 In the **Particle Trajectories (cpt)** toolbar, click **Plot**.

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

The particle positions at the final time are plotted for $q = 0.1$. To reproduce the remaining plots in Figure 4, select the values **0.6**, **0.7**, and **1.0** from the **Parameter value (q) list**, then click **Plot**.

Particle 1

In order to compute the transmission probability, it is necessary to add a second **Particle** dataset, and then add a **Selection** to it. The number of particles counted on this selection divided by the total number of particles is the transmission probability for the selection. This value is stored in a variable called `alpha`. The fraction of particles that do not strike the rods, `1-alpha`, is the transmission probability for the QMF.

Particle 2

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

2 Right-click **Results>Datasets>Particle 1** 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 **All boundaries**.

5 Select Boundaries 1–10, 13–15, and 18–24 only.

Now plot the transmission probability of the QMF as a function of `q`.

Transmission Probability

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Particle 2**.

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

Global 1

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
`1-cpt.alpha`	`1`	`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. Clear the **Show legends** check box.

6 In the **Transmission Probability** toolbar, click **Plot**. Compare the resulting plot to Figure 5.