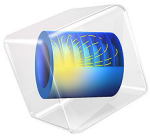

Quadrupole Mass Spectrometer

Introduction

The principal component of a quadrupole mass spectrometer is the mass filter which is used to filter ions with different charge-to-mass ratios. The quadrupole mass filter has been studied over many years (Ref. 1) and the physics and optimal design are well understood. In a real quadrupole mass spectrometer, fringe fields exist at both the entrance and exit of the mass filter. These fringe fields can play an important role in determining the transmission probability of a specific ion through the mass filter. This model computes the ion trajectories in a quadrupole mass spectrometer, including the effects of fringe fields.

Note: This application requires the Particle Tracing Module.

Model Definition

For the DC field, Poisson's equation is solved for the electric potential, U:

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

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

$$U = U_{\mathrm{dc}}$$

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

$$U = -U_{\mathrm{dc}}$$

A small DC bias is applied on the ion aperture to help accelerate the ions into the mass filter:

$$U = U_{\mathrm{bias}}$$

where U_{bias} is taken to be 3 V.

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 mass 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:

$$V = -V_{ac}$$

A small AC bias is applied on the ion aperture to help accelerate the ions into the mass filter:

$$V = V_{bias}$$

where V_{bias} is taken to be 3 V.

To construct the total electric field which the particles experience once they enter the modeling domain, the model uses superposition of the AC and DC fields. This is a valid assumption in this case because the equations solved for the AC and DC fields are linear.

Newton's second law governs the particle motion:

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

Here 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

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

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 are released from the ion aperture with a thermal velocity the equivalent of 2 electron volts, Ref. 1. The velocity only has an x-component:

$$v_x = \sqrt{\frac{2eA}{m}}$$

where A is 2 eV. 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 beginning at 0 s and ending at 0.25 µs. Because the frequency of the AC field is 4 MHz, this corresponds to one full RF cycle.

Results and Discussion

The particle trajectories are plotted in Figure 1. It is obvious from the plot that the ion transmission probability is very high, 100% actually. This is because a very stable operating point on the a-q curve has been chosen. The ions remain in the quadrupole mass filter for around 140 RF cycles.

Due to the presence of the biased plate surrounding the ion aperture, the ions gain energy as they move through the quadrupole. This can be seen in Figure 2; the ions have a mean energy of 5 eV over a range of around 3 eV. The spread in energy can be attributed to the fact that there is a small DC and AC bias. The AC bias can be positive or negative which accelerates or decelerates the ions depending on the phase of the RF cycle when they are released.

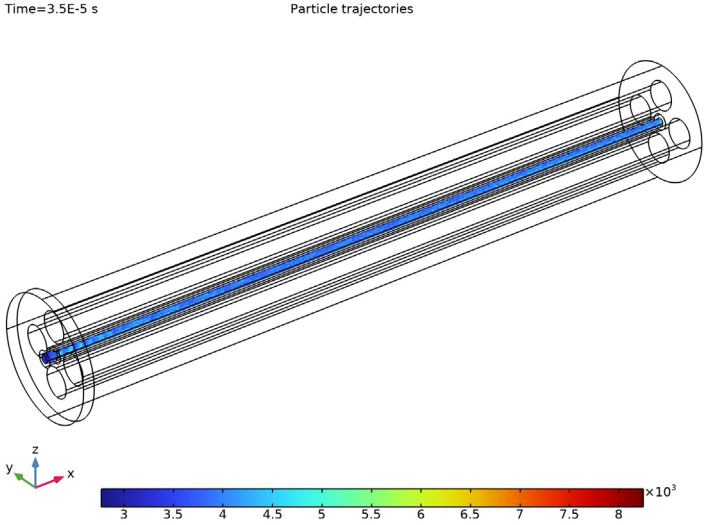

Figure 1: Plot of the particle trajectories inside the quadrupole. The color represents the particle velocity (m/s).

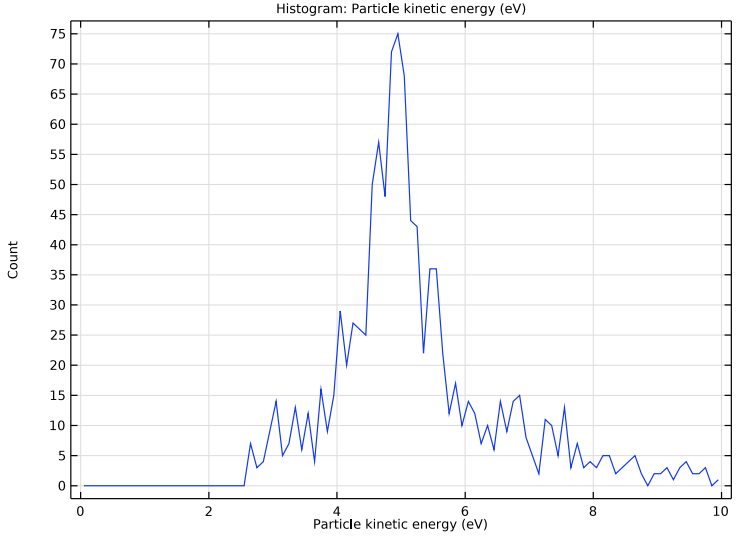

Figure 2: Plot of the energy distribution of the ions at the collector.

Notes About the COMSOL Implementation

The model is solved in two stages. First, the DC and AC fields are computed. Then the particle trajectories are computed and their motion is driven by the AC and DC electric fields.

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/Electromagnetics_and_Particle_Tracing/quadrupole_mass_spectrometer`

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 **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.

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_spectrometer_parameters.txt`.

GEOMETRY 1

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 **yz-plane**.

4 Click **Show Work Plane**.

Work Plane 1 (wp1)>Circle 1 (c1)

1 In the **Work Plane** 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 **xw** text field, type `-(re+r0)`.

Work Plane 1 (wp1)>Circle 2 (c2)

1 In the **Work Plane** 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 **xw** text field, type `re+r0`.

Work Plane 1 (wp1)>Circle 3 (c3)

1 In the **Work Plane** 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 **yw** text field, type `-(re+r0)`.

Work Plane 1 (wp1)>Circle 4 (c4)

1 In the **Work Plane** 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 **yw** text field, type `re+r0`.

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

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

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**, locate the **Distances** section.

3 In the table, enter the following settings:

Distances (m)
Lquad

4 Click **Build All Objects**.

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

Work Plane 2 (wp2)

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 **yz-plane**.

4 In the **x-coordinate** text field, type `-fd`.

5 Click **Show Work Plane**.

Work Plane 2 (wp2)>Circle 1 (c1)

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

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

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

Work Plane 2 (wp2)>Circle 2 (c2)

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

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

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

Work Plane 2 (wp2)>Circle 3 (c3)

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

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

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

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

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

Extrude 2 (ext2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** right-click **Work Plane 2 (wp2)** and choose **Extrude**.

2 In the **Settings** window for **Extrude**, locate the **Distances** section.

3 In the table, enter the following settings:

Distances (m)
fd
Lquad

4 Click **Build All Objects**.

Difference 1 (dif1)

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

2 Select the object **ext2** 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 **ext1** only.

6 Click **Build All Objects**.

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

Now define some selections for the positively and negatively charged rods.

DEFINITIONS

Positive

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

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

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

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

5 Select Boundaries 25, 26, 28, 29, 37, 38, 43, and 44 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 20–23 and 47–50 only.

ELECTROSTATICS (ES)

Define the boundary conditions for the electrostatics problem.

Electric Potential 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electrostatics (es)** 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 Potential 3

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

2 Select Boundaries 1, 4, and 7 only.

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

4 In the V_0 text field, type `3`.

ELECTRIC CURRENTS (EC)

Now define the boundary conditions for the AC part of the problem.

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

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`.

Electric Potential 3

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

2 Select Boundaries 1, 4, and 7 only.

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

4 In the V_0 text field, type `3`.

Specify the mass and charge number of the ions.

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 **Particle Mass** section.

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

4 Locate the **Charge Number** section. In the Z text field, type `1`.

The particles are released from a projected plane grid on the **Inlet** boundary. There are 100 particles per release and 11 releases in total. The particles all move in the x direction with initial energy 2 eV.

Inlet 1

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

2 Select Boundary 7 only.

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

4 From the **Initial position** list, choose **Projected plane grid**.

5 In the N text field, type `100`.

6 Locate the **Release Times** section. Click **Range**.

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

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

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

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

11 Click **Replace**.

I2 In the **Settings** window for **Inlet**, locate the **Initial Velocity** section.

I3 Specify the $\mathbf{v}_0$ vector as

vx0	x
0	y
0	z

Add an **Electric Force** feature for the DC field.

Electric Force 1

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

2 In the **Settings** window for **Electric Force**, locate the **Domain Selection** section.

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

4 Locate the **Electric Force** section. From the $\mathbf{E}$ list, choose **Electric field (es/ccn1)**.

Add another **Electric Force** feature for the AC field.

Electric Force 2

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

2 In the **Settings** window for **Electric Force**, locate the **Domain Selection** section.

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

4 Locate the **Electric Force** section. From the $\mathbf{E}$ list, choose **Electric field (ec/cucn1)**.

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

ADD MATERIAL

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

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

3 In the tree, select **Built-in>Perfect vacuum**.

4 Click **Add to Component** in the window toolbar.

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

Since the aspect ratio of the quadrupole is very high, it is more efficient to use a swept mesh. This is allowed in this case because the field does not change in the x direction once the particles have passed through the fringing fields.

MESH 1

Free Triangular 1

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

2 Select Boundaries 16, 19, 24, 27, 30, 33, and 46 only.

Size 1

1 Right-click **Free Triangular 1** and choose **Size**.

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

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

4 Click to expand the **Element Size Parameters** section. Locate the **Element Size** section. Click the **Custom** button.

5 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

6 Select the **Minimum element size** check box.

7 Select the **Curvature factor** check box. In the associated text field, type `0.15`.

8 Click  **Build All**.

Swept 1

1 In the **Mesh** toolbar, click  **Swept**.

2 In the **Settings** window for **Swept**, locate the **Domain Selection** section.

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

4 Select Domains 4–6 only.

Distribution 1

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

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

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type `35`.

5 In the **Element ratio** text field, type `15`.

6 Click  **Build All**.

7 Click the  **Go to Default View** button in the **Graphics** toolbar.

Swept 2

1 In the **Mesh** toolbar, click  **Swept**.

2 In the **Settings** window for **Swept**, locate the **Domain Selection** section.

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

4 Select Domains 1–3 only.

Distribution 1

1 Right-click **Swept 2** and choose **Distribution**.

2 Right-click **Distribution 1** and choose **Build All**.

Add a **Stationary** study to compute the electrostatic field.

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 **Preset Studies for Some Physics Interfaces>Stationary**.

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

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

STUDY 1

Step 1: Stationary

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

2 In the table, clear the **Solve for** check boxes for **Electric Currents (ec)** and **Charged Particle Tracing (cpt)**.

3 In the **Model Builder** window, right-click **Study 1** and choose **Rename**.

4 In the **Rename Study** dialog box, type `Electrostatic Study` in the **New label** text field.

5 Click **OK**.

Add a **Frequency Domain** study to compute the AC field.

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 **Preset Studies for Some Physics Interfaces>Frequency Domain**.

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

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

STUDY 2

Step 1: Frequency Domain

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

2 In the **Frequencies** text field, type `4[MHz]`.

3 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check boxes for **Electrostatics (es)** and **Charged Particle Tracing (cpt)**.

4 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**.

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

6 From the **Study** list, choose **Electrostatic Study, Stationary**.

7 In the **Model Builder** window, right-click **Study 2** and choose **Rename**.

8 In the **Rename Study** dialog box, type `Electric currents Study` in the **New label** text field.

9 Click **OK**.

Add a **Time Dependent** study to compute the particle trajectories.

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.

STUDY 3

Step 1: Time Dependent

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

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

3 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**.

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

5 From the **Study** list, choose **Electric currents Study, Frequency Domain**.

6 Locate the **Study Settings** section. In the **Output times** text field, type `range(0,1/4e6, 140/4e6)`.

7 Click **Range**.

8 In the **Range** dialog box, click **Replace**.

9 In the **Model Builder** window, right-click **Study 3** and choose **Rename**.

10 In the **Rename Study** dialog box, type `Particle tracing Study` in the **New label** text field.

11 Click **OK**.

ELECTROSTATIC STUDY

Compute the DC field.

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

ELECTRIC CURRENTS STUDY

Compute the AC field.

1 Click **Compute**.

PARTICLE TRACING STUDY

Now, compute the particle trajectories.

1 Click **Compute**.

RESULTS

Particle Trajectories (cpt)

1 In the **Settings** window for **3D Plot Group**, locate the **Color Legend** section.

2 From the **Position** list, choose **Bottom**.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Particle Trajectories (cpt)** node, then click **Particle Trajectories 1**.

2 In the **Settings** window for **Particle Trajectories**, locate the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Type** list, choose **Line**.

4 Find the **Point style** subsection. From the **Type** list, choose **None**.

5 Find the **Line style** subsection. From the **Interpolation** list, choose **Uniform**.

6 In the **Number of interpolated times** text field, type 1000.

DEFINITIONS

View 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **View 1**.

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

3 Clear the **Show grid** check box.

RESULTS

Particle Trajectories (cpt)

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

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

3 Click the **Zoom Extents** button in the **Graphics** toolbar. The resulting plot should look like Figure 1.

Finally, create a **Histogram** of the ion energy distribution function at the time all the ions have reached the current collector.

Ion Energy Distribution Function

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

2 In the **Settings** window for **1D Plot Group**, type `Ion Energy Distribution Function` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Particle 1**.

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

Histogram 1

1 Right-click **Ion Energy Distribution Function** and choose **Histogram**.

2 In the **Settings** window for **Histogram**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Charged Particle Tracing>Velocity and energy>cpt.Ep - Particle kinetic energy - J**.

3 Locate the **Expression** section. From the **Unit** list, choose **eV**.

4 Locate the **Bins** section. From the **Entry method** list, choose **Limits**.

5 Click **Range**.

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

7 In the **Start** text field, type 0.

8 In the **Stop** text field, type 10.

9 In the **Number of values** text field, type 101.

10 Click **Replace**.

11 In the **Ion Energy Distribution Function** toolbar, click  **Plot**. The resulting plot should look like Figure 2.