

Quadrupole Mass Spectrometer

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.](#page-5-0) 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: F/m) and ε_r is the relative permittivity (taken as 1 in this model). The zero on the right-hand side of [Equation](#page-1-0) 1 indicates that the space charge density inside the quadrupole is negligible [\(Ref.](#page-5-0) 1). On the north and south rods, a positive potential of magnitude U_{dc} is applied:

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

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

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

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

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

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*:

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

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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:

$$
V = -V_{\text{ac}}
$$

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), **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 **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

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

and

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

where the tilde denotes that the AC electric potential is complex valued. The particle position, **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.](#page-5-0) 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 $0.25 \mu s$. 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](#page-4-0) 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](#page-4-1) 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.

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/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

- In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- In the **Settings** window for **Parameters**, locate the **Parameters** section.
- Click **Load from File**.
- Browse to the model's Application Libraries folder and double-click the file quadrupole mass spectrometer parameters.txt.

GEOMETRY 1

Work Plane 1 (wp1)

- In the **Geometry** toolbar, click **Work Plane**.
- In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.
- From the **Plane** list, choose **yz-plane**.
- Click **Show Work Plane**.

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

- In the **Work Plane** toolbar, click **Circle**.
- In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- In the **Radius** text field, type re.
- Locate the **Position** section. In the **xw** text field, type -(re+r0).

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

- In the **Work Plane** toolbar, click **Circle**.
- In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- In the **Radius** text field, type re.
- Locate the **Position** section. In the **xw** text field, type re+r0.

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

- In the **Work Plane** toolbar, click **Circle**.
- In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- In the **Radius** text field, type re.
- Locate the **Position** section. In the **yw** text field, type -(re+r0).

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

- In the **Work Plane** toolbar, click **Circle**.
- In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- In the **Radius** text field, type re.
- Locate the **Position** section. In the **yw** text field, type re+r0.
- In the **Work Plane** toolbar, click **Build All**.
- Click the **Zoom Extents** button in the **Graphics** toolbar.

Work Plane 1 (wp1)

In the **Model Builder** window, click **Work Plane 1 (wp1)**.

Extrude 1 (ext1)

- In the **Geometry** toolbar, click **Extrude**.
- In the **Settings** window for **Extrude**, locate the **Distances** section.
- In the table, enter the following settings:

Distances (m)

Lquad

- Click **Build All Objects**.
- Click the **Zoom Extents** button in the **Graphics** toolbar.

Work Plane 2 (wp2)

- In the **Geometry** toolbar, click **Work Plane**.
- In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.
- From the **Plane** list, choose **yz-plane**.
- In the **x-coordinate** text field, type -fd.
- Click **Show Work Plane**.

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

- In the **Work Plane** toolbar, click **Circle**.
- In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- In the **Radius** text field, type rcase.

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

- In the **Work Plane** toolbar, click **Circle**.
- In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- In the **Radius** text field, type rsrc.

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

- In the **Work Plane** toolbar, click **Circle**.
- In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- In the **Radius** text field, type 2*rsrc.
- In the **Work Plane** toolbar, click **Build All**.
- Click the **Zoom Extents** button in the **Graphics** toolbar.

Work Plane 2 (wp2)

In the **Model Builder** window, click **Work Plane 2 (wp2)**.

Extrude 2 (ext2)

- In the **Geometry** toolbar, click **Extrude**.
- In the **Settings** window for **Extrude**, locate the **Distances** section.
- In the table, enter the following settings:

Distances (m)

fd

Lquad

Click **Build All Objects**.

Difference 1 (dif1)

- In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.
- Select the object **ext2** only.
- In the **Settings** window for **Difference**, locate the **Difference** section.
- Find the **Objects to subtract** subsection. Select the **Activate selection** toggle button.
- Select the object **ext1** only.
- Click **Build All Objects**.
- Click the **Zoom Extents** button in the **Graphics** toolbar.

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

DEFINITIONS

Explicit 1

- In the **Definitions** toolbar, click **Explicit**.
- In the **Settings** window for **Explicit**, type Positive in the **Label** text field.
- Click the **Wireframe Rendering** button in the **Graphics** toolbar.
- Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- Select Boundaries 25, 26, 28, 29, 37, 38, 43, and 44 only.

Explicit 2

- **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.

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

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

Click **Replace**.

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

13 Specify the \mathbf{v}_0 vector as

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

Electric Force 1

- In the **Physics** toolbar, click **Domains** and choose **Electric Force**.
- In the **Settings** window for **Electric Force**, locate the **Electric Force** section.
- From the **E** list, choose **Electric field (es/ccn1)**.
- Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

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

Electric Force 2

- In the **Physics** toolbar, click **Domains** and choose **Electric Force**.
- In the **Settings** window for **Electric Force**, locate the **Electric Force** section.
- From the **E** list, choose **Electric field (ec/cucn1)**.
- Locate the **Advanced Settings** section. From the **Time dependence of field** list, choose **Time harmonic**.
- Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

MATERIALS

Material 1 (mat1)

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

3 In the table, enter the following settings:

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 **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **More Operations>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.
- **8** In the associated text field, type 0.15.
- **9** Click **Build All**.

Swept 1

- **1** In the **Model Builder** window, right-click **Mesh 1** and choose **Swept**.
- **2** In the **Settings** window for **Swept**, locate the **Domain Selection** section.
- From the **Geometric entity level** list, choose **Domain**.
- Select Domains 4–6 only.

Distribution 1

- Right-click **Swept 1** and choose **Distribution**.
- In the **Settings** window for **Distribution**, locate the **Distribution** section.
- From the **Distribution type** list, choose **Predefined**.
- In the **Number of elements** text field, type 35.
- In the **Element ratio** text field, type 15.
- Click **Build All**.
- Click the **Go to Default View** button in the **Graphics** toolbar.

Swept 2

- In the **Model Builder** window, right-click **Mesh 1** and choose **Swept**.
- In the **Settings** window for **Swept**, locate the **Domain Selection** section.
- From the **Geometric entity level** list, choose **Domain**.
- Select Domains 1–3 only.

Distribution 1

- Right-click **Swept 2** and choose **Distribution**.
- Click **Build All**.

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

ADD STUDY

- In the **Home** toolbar, click **Add Study** to open the **Add Study** window.
- Go to the **Add Study** window.
- Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Some Physics Interfaces>Stationary**.
- Click **Add Study** in the window toolbar.
- In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 1

Step 1: Stationary

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

- In the table, clear the **Solve for** check box for **Electric Currents** and **Charged Particle Tracing**.
- In the **Model Builder** window, right-click **Study 1** and choose **Rename**.
- In the **Rename Study** dialog box, type Electrostatic Study in the **New label** text field.
- Click **OK**.

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

ADD STUDY

- In the **Home** toolbar, click **Add Study** to open the **Add Study** window.
- Go to the **Add Study** window.
- Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Some Physics Interfaces>Frequency Domain**.
- Click **Add Study** in the window toolbar.
- In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Frequency Domain

- In the **Settings** window for **Frequency Domain**, locate the **Study Settings** section.
- In the **Frequencies** text field, type 4[MHz].
- Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Electrostatics** and **Charged Particle Tracing**.
- 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**.
- From the **Method** list, choose **Solution**.
- From the **Study** list, choose **Electrostatic Study, Stationary**.
- In the **Model Builder** window, right-click **Study 2** and choose **Rename**.
- In the **Rename Study** dialog box, type Electric currents Study in the **New label** text field.
- Click **OK**.

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

ADD STUDY

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 box for **Electrostatics** and **Electric Currents**.
- **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 **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](#page-4-0).

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

1D Plot Group 4

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

- In the **Settings** window for **1D Plot Group**, type Ion Energy Distribution Function in the **Label** text field.
- Locate the **Data** section. From the **Dataset** list, choose **Particle 1**.
- From the **Time selection** list, choose **Last**.

Histogram 1

- Right-click **Ion Energy Distribution Function** and choose **Histogram**.
- In the **Settings** window for **Histogram**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Charged Particle Tracing>Velocity and energy>cpt.Ep - Particle kinetic energy - J**.
- Locate the **Expression** section. From the **Unit** list, choose **eV**.
- Locate the **Bins** section. From the **Entry method** list, choose **Limits**.
- Click **Range**.
- In the **Range** dialog box, choose **Number of values** from the **Entry method** list.
- In the **Start** text field, type 0.
- In the **Stop** text field, type 10.
- In the **Number of values** text field, type 101.
- Click **Replace**.
- In the **Ion Energy Distribution Function** toolbar, click **Plot**. The resulting plot should look like [Figure 2](#page-4-1).