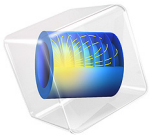

Ion Energy Distribution Function in a Capacitively Coupled Plasma Reactor

Introduction

Plasma processing techniques are widely used in the industry to modify the chemical and physical properties of surfaces. Some processes require energetic ion bombardment and a high degree of ion velocity anisotropy. Therefore, it is of great value to know the ion energy distribution function (IEDF) and the velocity dispersion at the surface.

In this example, the IEDF at the electrode surface is computed for a commercial capacitively coupled plasma reactor. The computed IEDF is compared with measurements from Ref. 1 and a reasonable agreement is found.

Note: This application requires the Plasma Module and the Particle Tracing Module.

Model Definition

The reactor that was used in Ref. 1 to measure the IEDF is simulated using the COMSOL Multiphysics Plasma Module. The reactor is the Plasmalab System 100 parallel plate, capacitively coupled, RIE plasma tool. It is an asymmetric capacitively coupled reactor with a 200 mm diameter powered electrode, and a gap between electrodes of 4.5 cm. The other dimensions of the reactor where inferred from diagrams and photos. Since the plasma volume and the area ratio between electrodes is not exactly known a direct comparison between simulations and measurements for absorbed power, applied voltage, and DC self–bias is only approximate.

Two physics interfaces are used in two consecutive steps. First, the **Plasma, Time Periodic (ptp)** interface is used to solve for the space and time-periodic evolution of the plasma. After, the **Charged Particle Tracing (cpt)** interface is used to obtained the IEDF collected at the powered electrode.

PLASMA SIMULATION

The simulations are for an Argon plasma sustained at a pressure of 20 mTorr with a periodic electric excitation of 13.56 MHz. The model is 2-dimensional and describes the space and time–periodic evolution of several macroscopic properties of the discharge.

The electron mobility and other electron transport properties are automatically computed from the electron impact reactions. For the ions, the mobility is given as a function of the reduced electric field using a lookup table. The ion diffusivity is obtained from the Einstein relation where the ion temperature comes from a local field approximation.

IEDF SIMULATION

To simulate the IEDF at the powered electrode particles representing ions are released from a point in the plasma and the ion trajectories are computed over several RF cycles until all the released particles reach the wall. The ions should be released from a point outside the plasma sheath in order to experience the full range of the sheath electric field. This point can be estimated by looking at the time averaged electric potential and identifying a region where the potential starts to have smaller variations in the axial direction. Also important is to release particles along the excitation period in order to sample the sheath motion.

The ions are released with a random Maxwellian distribution at 300 K. After the release, the ions are accelerated by a time varying electric field toward the surface. Eventually some ions experience collisions with the background gas. In this simulation two different types of collision events are used: elastic and resonant charge exchange collisions. The collisions are specified by energy dependent cross sections. For the charge exchange collision a scattering angle of 5 degrees is arbitrarily defined.

ELECTRIC EXCITATION

The driven electrode has a fixed power and computes the self DC bias. This corresponds to the following expression and set of constraints on the electric potential:

$$V_s = V_a \cos(2\pi f_p t + \alpha) + V_{\mathrm{dc,b}} \tag{1}$$

$$0 = f_p \int_{\partial t} \int_{\partial \Omega} (\mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e + \mathbf{n} \cdot \mathbf{J}_d) dS dt \tag{2}$$

$$P_{\mathrm{rf}} = f_p \int_{\partial t} \int_{\partial \Omega} (V_s - V_{\mathrm{dc,b}})(\mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e + \mathbf{n} \cdot \mathbf{J}_d) dS dt \,. \tag{3}$$

The constraint in Equation 2 is used to compute the self DC bias, $V_{\mathrm{dc,b}}$. The constraint in Equation 3 is used to compute the RF potential, V_a such that a fixed amount of power is deposited into the plasma.

PLASMA CHEMISTRY

Argon plasmas have one of the simplest reactions schemes. We use a simplified plasma chemistry that comprises 7 volume reactions involving electrons, atomic ion, and a lumped level representing the argon 4s states (electron impact cross-sections are obtained Ref. 3).

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

Reaction	Formula	Type	$\Delta\varepsilon$(eV)
1	e+Ar=>e+Ar	Elastic	0
2	e+Ar=>e+Ars	Excitation	11.5
3	e+Ars=>e+Ar	Superelastic	-11.5
4	e+Ar=>2e+Ar+	Ionization	15.8
5	e+Ars=>2e+Ar+	Ionization	4.24
6	Ars+Ars =>e+Ar+Ar+	Penning ionization	-
7	Ars+Ar => Ar+Ar	Metastable quenching	-

In addition to volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS.

Reaction	Formula	Sticking coefficient	Secondary emission coefficient	Mean energy of secondary electrons (V)
1	Ars=>Ar	1	0.07	5.8
2	Ar+=>Ar	0	0.07	5.8

When an excited states make contact with the wall, they revert to the ground state argon with some probability. At the metal electrodes, the ions and the excited state use their internal energy to extract one electron from the wall with a probability of 0.07 and a mean energy of 5.8 V. For the ions, the sticking coefficient is zero meaning that losses to the wall are assumed to be due to migration only.

Results and Discussion

Figure 1, Figure 2, and Figure 3 show the time averaged electron density, electron temperature and electric potential for a plasma sustained at 20 mTorr and 30 W. The period averaged electron density is largest in magnitude in the reactor center, decreasing considerable along the radial and axial directions as expected. The period averaged electron temperature is highest near the electrodes where intense electric fields exist. Since it is an asymmetric reactor the smaller electrode (the powered electrode in this model) has a sheath with more intense electric fields. This is reflected in higher electron temperature

at the power electrode. In Figure 3 it is possible to observe the DC self–bias potential developed in order to ensure that there is no period average conduction current through the electrode.

Figure 4 and Figure 5 presents the IEDF and the angular dispersion of the ion velocity at the power electrode. A double peak structure is observed at high energies meaning that the most energetic ions cross the sheath in a time comparable with the RF cycle. The midpoint energy between the two energetic peaks corresponds to the energy that the ions would gain while accelerating through the time–averaged electric potential. From Figure 3 it is possible to estimate that the midpoint energy should be around 350 V (potential difference from –200 V at the wall to 150 V in the discharge bulk), which is in agreement with the results of Figure 4.

The width between the two high energy peaks ΔE can be estimated from analytical models such as the model from Charles and others (from Ref. 1)

$$\Delta E = V_{pp}\left(1+\left(\frac{2\pi\tau_i}{3\tau_{rf}}\right)^2\right)^{-1/2} \tag{4}$$

and the model from Sobolewski and others (from Ref. 1)

$$\Delta E = V_{pp}\left(1+\pi^2\left(\frac{2T_e}{V_s}\right)^{1/2}\left(\frac{\tau_i}{\tau_{rf}}\right)^2\right)^{-1/2} \tag{5}$$

where V_{pp} is the peak-to-peak sheath voltage, V_s is the time-averaged sheath potential, τ_i is the ion transit time through the sheath, τ_{rf} is the RF period, and T_e is the electron temperature. The ΔE computed form Equation 4 and Equation 5 gives 42 V and 71 V, respectively, which is in good agreement with the 70 V from the simulated IEDF. The values used to compute ΔE are obtain from the simulations and are presented in Table 3.

TABLE 3: VALUES OBTAINED FROM SIMULATIONS AND USED TO COMPUTE ΔE.

T_c	4 V
V_s	340 V
V_{pp}	1070
τ_i	900 ns

The ions that cross the sheath without colliding (or with a collision in the beginning of the trajectory) contribute to the high-energy part of the IEDF. The low-energy part of the IEDF also has several well-defined peaks. These structures are created by ions that undergo resonant charge exchange collisions along their motion in direction to the wall. After such

collision events, a slow ion is created within the sheath, and consequently it experiences only part of the electric field range.

In Figure 5 it is possible to observe that the high energy ions have a –5 degree tilt relatively to their axial velocity. This is a consequence of the existence of important radial electric fields in this region. Also from Figure 5 you can see that there is a dispersion angle at the low-energy range. This is because it is used an arbitrary 5 degree scattering angle for the resonant charge exchange collision. To obtain realistic results for the ion dispersion velocity, a physical model for the scattering angle is needed.

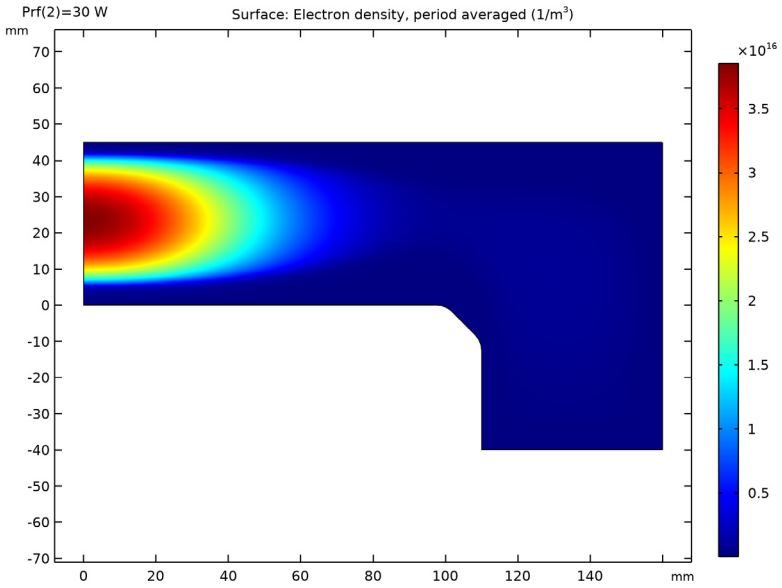

Figure 1: Plot of the period averaged electron density.

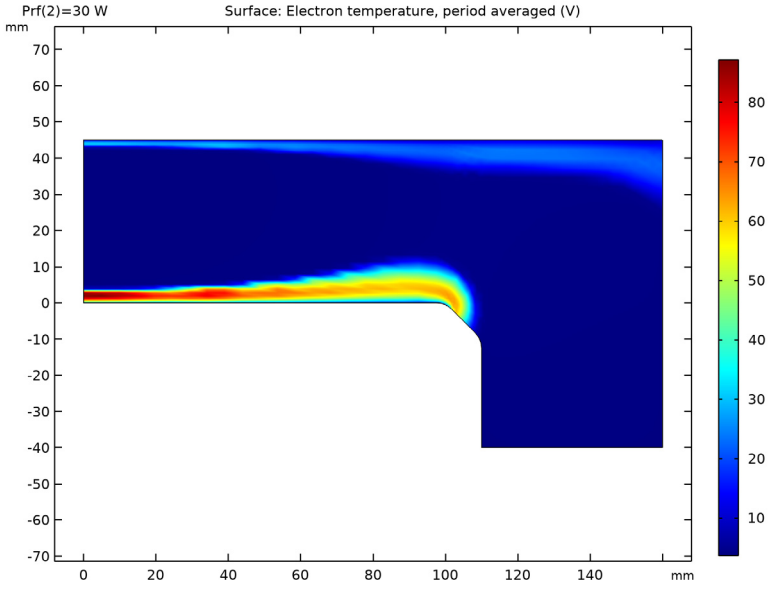

Figure 2: Plot of the period averaged electron temperature.

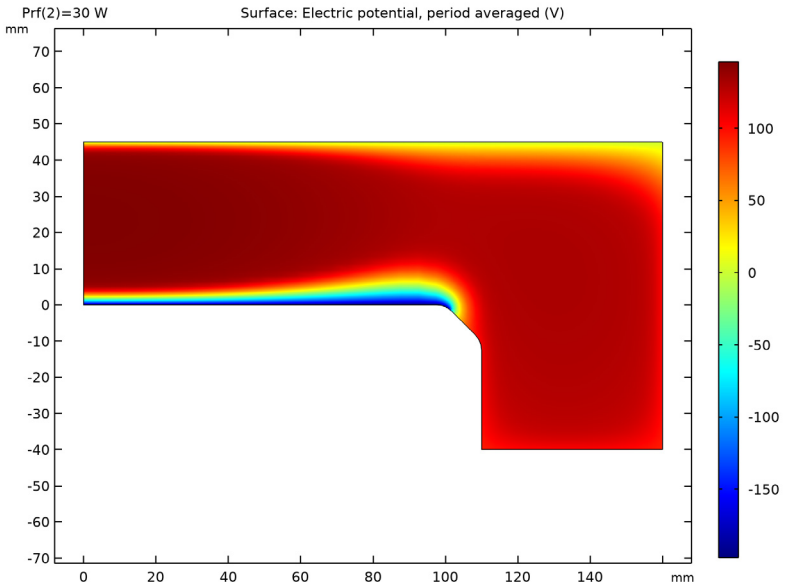

Figure 3: Plot of the period averaged electric potential.

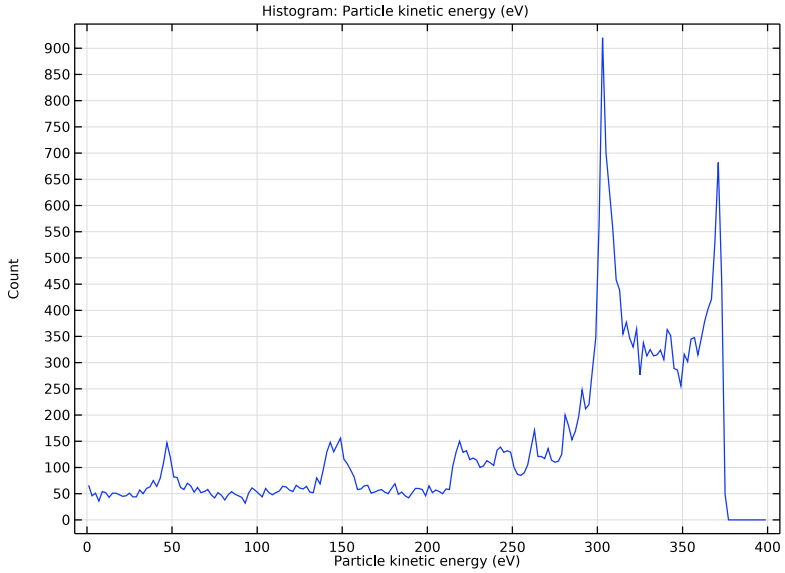

Figure 4: IEDF at the powered electrode.

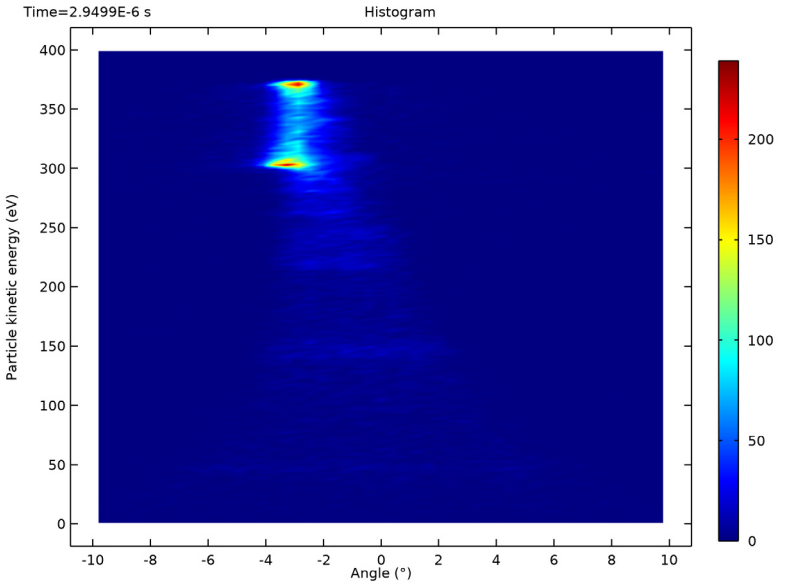

Figure 5: IEDF with velocity angular dispersion at the powered electrode.

References

1. D. Gahan, S. Daniels, C. Hayden, D. O'Sullivan, and M.B. Hopkins, "Characterization of an asymmetric parallel plate radio-frequency discharge using a retarding field energy analyzer," *Plasma Sources Sci. Technol.*, vol. 21, p. 015002 (12pp), 2012.

2. M.A. Lieberman and A.J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, John Wiley & Sons, 2005.

3. Phelps database, www.lxcat.net, retrieved 2017.

Application Library path: `Plasma_Module/Capacitively_Coupled_Plasmas/ccp_ion_energy_distribution_function`

Modeling Instructions

The following instructions show how to create a 2D model of a RF capacitively coupled plasma and how to obtain the IEDF at the electrode surface using the **Charge Particle Tracing (cpt)** interface. Three studies are needed:

- A **Time Periodic** study that computes the periodic steady-state solution of the plasma.
- A **Time Periodic to Time Dependent** study that converts the periodic steady-state solution to the time domain.
- A **Time Dependent** study that is used to compute the ion trajectories through the sheath.

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1. In the **Model Wizard** window, Select the **Plasma, Time Periodic (ptp)** interface and the **Time Periodic** study to compute the periodic steady state solution of the plasma.
2. click **2D Axisymmetric**.
3. In the **Select Physics** tree, select **Plasma>Plasma, Time Periodic (ptp)**.
4. Click **Add**.
5. Click **Study**.

6 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Periodic**.

7 Click **Done**.

GEOMETRY 1

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

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

Add some parameters for the reactor dimensions, power, pressure, and excitation frequency.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
r0	160[mm]	0.16 m	
h0	4.5[cm]	0.045 m	
r1	110[mm]	0.11 m	
h1	40[mm]	0.04 m	
Prf	1[W]	1 W	
f0	13.56[MHz]	1.356E7 Hz	
p0	0.02[torr]	2.6664 Pa	

GEOMETRY 1

Rectangle 1 (r1)

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

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

3 In the **Width** text field, type r0.

4 In the **Height** text field, type h0.

Rectangle 2 (r2)

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

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

3 In the **Width** text field, type `r0-r1`.

4 In the **Height** text field, type `h1`.

5 Locate the **Position** section. In the **r** text field, type `r1`.

6 In the **z** text field, type `-h1`.

Union 1 (uni1)

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

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

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

4 Clear the **Keep interior boundaries** check box.

5 Click **Build All Objects**.

Chamfer 1 (cha1)

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

2 On the object **uni1**, select Point 4 only.

3 In the **Settings** window for **Chamfer**, locate the **Distance** section.

4 In the **Distance from vertex** text field, type `10`.

Fillet 1 (fil1)

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

2 On the object **cha1**, select Points 3 and 5 only.

3 In the **Settings** window for **Fillet**, locate the **Radius** section.

4 In the **Radius** text field, type `6`.

Point 1 (pt1)

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

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

3 In the **r** text field, type `97.5`.

4 In the **z** text field, type `h0`.

Line Segment 1 (ls1)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 On the object **fil1**, select Point 3 only.

3 In the **Settings** window for **Line Segment**, locate the **Endpoint** section.

4 Find the **End vertex** subsection. Select the **Activate Selection** toggle button.

5 On the object **pt1**, select Point 1 only.

6 Click **Build Selected**.

Mesh Control Edges 1 (mce1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Edges**.

2 On the object **fin**, select Boundary 4 only.

3 In the **Geometry** toolbar, click **Build All**.

Set the period and the number of elements in the extra dimension.

PLASMA, TIME PERIODIC (PTP)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Plasma, Time Periodic (ptp)**.

2 In the **Settings** window for **Plasma, Time Periodic**, locate the **Extra Dimension Settings** section.

3 In the P_{xd} text field, type `1/f0`.

4 In the N text field, type `30`.

5 From the **Heavy species selection** list, choose **Base geometry**.

Import cross section data for Argon.

Cross Section Import 1

1 In the **Physics** toolbar, click **Global** and choose **Cross Section Import**.

2 In the **Settings** window for **Cross Section Import**, locate the **Cross Section Import** section.

3 Click **Browse**.

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

Add other reactions to complete the plasma chemistry.

Reaction 1

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

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `Ars+Ars=>e+Ar+Ar+`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `2.3E7`.

Reaction 2

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

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `Ars+Ar=>Ar+Ar`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1807`.

Species: Ar

1 In the **Model Builder** window, click **Species: Ar**.

2 In the **Settings** window for **Species**, locate the **Species Formula** section.

3 Select the **From mass constraint** check box.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **Ar**.

Species: Ars

1 In the **Model Builder** window, click **Species: Ars**.

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **Ar**.

The electric fields generated will be rather high in the sheath, so use the local field approximation for the ion temperature, and a lookup table for the ion mobility.

Species: Ar+

1 In the **Model Builder** window, click **Species: Ar+**.

2 In the **Settings** window for **Species**, locate the **Species Formula** section.

3 Select the **Initial value from electroneutrality constraint** check box.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **Ar**.

5 Click to expand the **Mobility and Diffusivity Expressions** section. From the **Specification** list, choose **Specify mobility, compute diffusivity**.

6 From the **Ion temperature** list, choose **Use local field approximation**.

7 Click to expand the **Mobility Specification** section. From the **Specify using** list, choose **Argon ion in argon**.

Define surface losses for ions and argon excited state. For the ions, set the **Forward sticking coefficient** to zero to assume that ion losses are due to migration only, and use the default **Secondary emission coefficient** of 0.07.

The argon excited state also uses the default **Secondary emission coefficient** of 0.07.

Electron secondary emission is made only possible on the electrodes.

Surface Reaction 1

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

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

3 In the **Formula** text field, type `Ar+=>Ar`.

4 Locate the **Reaction Parameters** section. In the γ_f text field, type `0`.

5 Select Boundaries 2 and 3 only.

2: Ar+=>Ar

1 Right-click **Surface Reaction 1** and choose **Duplicate**.

2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.

3 Click  **Clear Selection**.

4 Select Boundaries 4–9 only.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0`.

6 In the ε_i text field, type `0`.

3: Ar+=>Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)** right-click **1: Ar+=>Ar** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars=>Ar`.

4 Locate the **Reaction Parameters** section. In the γ_f text field, type `1`.

4: Ar+=>Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)** right-click **2: Ar+=>Ar** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars=>Ar`.

4 Locate the **Reaction Parameters** section. In the γ_f text field, type `1`.

Plasma Model 1

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

2 In the **Settings** window for **Plasma Model**, locate the **Model Inputs** section.

3 In the T text field, type `300[K]`.

4 In the p_A text field, type `p0`.

Wall 1

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

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

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

Define the electric excitation of the discharge. Set a ground electrode on the top and a RF power source on bottom.

At the other boundaries use dielectric contact to ensure that the period average conduction current is zero.

Ground 1

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

2 Select Boundary 3 only.

Dielectric Contact 1

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

2 Select Boundaries 4–9 only.

The most stable way of driving the electrode is to use a fixed power. Use the previously defined parameter Prf to set the **RF power**. The exact values for the power sweep are set later in the study.

Metal Contact 1

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

2 In the **Settings** window for **Metal Contact**, locate the **RF Source** section.

3 In the P_{rf} text field, type `Prf`.

4 In the f_p text field, type `f0`.

5 Locate the **DC Source** section. Select the **Compute DC self-bias** check box.

6 Select Boundary 2 only.

The mesh needs to be refined near the electrodes where the power is absorbed. A mapped mesh can be used across the main discharge area, and a free triangular mesh everywhere else.

MESH 1

Edge 1

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

2 Select Boundaries 1 and 12 only.

Distribution 1

1 Right-click **Edge 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 30.

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

6 Select the **Symmetric distribution** check box.

Edge 2

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

2 Select Boundaries 3 and 10 only.

Distribution 1

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

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

3 In the **Number of elements** text field, type 20.

Mapped 1

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

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

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

4 Select Domain 1 only.

5 Click  **Build Selected**.

Free Triangular 1

1 In the **Mesh** toolbar, click  **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click to expand the **Control Entities** section.

3 Clear the **Smooth across removed control entities** check box.

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**.

Boundary Layers 1

1 In the **Mesh** toolbar, click  **Boundary Layers**.

2 In the **Settings** window for **Boundary Layers**, click to expand the **Transition** section.

3 Clear the **Smooth transition to interior mesh** check box.

4 Click to expand the **Corner Settings** section. From the **Handling of sharp corners** list, choose **Trimming**.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.

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

4 Select Boundaries 2–11 only.

5 Locate the **Boundary Layer Properties** section. In the **Number of boundary layers** text field, type `2`.

6 In the **Boundary layer stretching factor** text field, type `1.4`.

7 Click **Build All**.

STUDY 1

In the **Study** toolbar, click **Get Initial Value**.

The objective is to obtain a solution at 30 W. To obtain a high power solution it is easier to start at a low power and then sweep over power until the desired power is reached.

In this study a solution of 1 W is used as initial condition. The power is then increased by 1 W until a value of 30 W is reached. Setting a maximum power increment for the parametric solver makes convergence smoother as the power is increased.

The maximum increase in the damping factor between nonlinear iterations is modified from its default value of 0.05 to 0.03. This makes it easier for the nonlinear solver to converge for the first power value. Lower values for the maximum increase makes convergence easier, although possibly at the expense of more nonlinear iterations and thus longer computation times.

Step 1: Time Periodic

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

2 In the **Settings** window for **Time Periodic**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Prf	1 30	W

Solver Configurations

In the **Model Builder** window, expand the **Study 1>Solver Configurations** node.

Solution 1 (sol1)

1 In the **Model Builder** window, expand the **Study 1>Solver Configurations> Solution 1 (sol1)>Stationary Solver 1** node, then click **Fully Coupled 1**.

2 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.

3 In the **Restriction for step-size increase** text field, type `0.03`.

4 Click to expand the **Results While Solving** section. Select the **Plot** check box.

5 In the **Model Builder** window, click **Parametric**.

6 In the **Settings** window for **Parametric**, click to expand the **Continuation** section.

7 Select the **Tuning of step size** check box.

8 In the **Initial step size** text field, type `0.25`.

9 In the **Maximum step size** text field, type `0.5`.

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

So far, we have computed the periodic steady-state solution only. In order to see the time-dependent behavior of the plasma, we need to convert the solution to the time domain. To do this, use the **Time Periodic to Time Dependent** study.

ADD STUDY

1 In the **Study** 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 Selected Physics Interfaces>Time Periodic to Time Dependent**.

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

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

STUDY 2

Step 1: Time Periodic to Time Dependent

The final output time should correspond to 1 RF cycle. The number of output times should typically be around 100. When computing the time-periodic solution, only 30 points were used in the (hidden) time axis. When converting to the time domain, COMSOL Multiphysics uses linear interpolation of the solution between these points.

1 In the **Settings** window for **Time Periodic to Time Dependent**, locate the **Study Settings** section.

2 Click **Range**.

3 In the **Range** dialog box, type `(1/f0)/101` in the **Step** text field.

4 In the **Stop** text field, type `1/f0`.

5 Click **Replace**.

6 In the **Settings** window for **Time Periodic to Time Dependent**, click to expand the **Values of Dependent Variables** section.

7 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

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

9 From the **Study** list, choose **Study 1, Time Periodic**.

10 From the **Parameter value (Prf (W))** list, choose **Last**.

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

Add the **Charged Particle Tracing (cpt)** interface to compute the IEDF.

ADD PHYSICS

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

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

3 In the tree, select **AC/DC>Particle Tracing>Charged Particle Tracing (cpt)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for **Study 1** and **Study 2**.

5 Click **Add to Component 1** in the window toolbar.

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

DEFINITIONS (COMP1)

Add analytic functions for the ion resonant charge exchange and elastic cross sections.

Analytic 1 (an1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, locate the **Definition** section.

3 In the **Expression** text field, type `(7*1e-10-0.6*1e-10*log(x))^2`.

4 Locate the **Units** section. In the **Arguments** text field, type `eV`.

5 In the **Function** text field, type `m^2`.

6 In the **Function name** text field, type `Qex`.

Analytic 2 (an2)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, locate the **Definition** section.

3 In the **Expression** text field, type `2e-19/(x^(0.5)*(1+x))+3e-19*x/(1+x/3)^(2.3)`.

4 Locate the **Units** section. In the **Arguments** text field, type `eV`.

5 In the **Function** text field, type `m^2`.

6 In the **Function name** text field, type `Qele`.

Variables 1

1 In the **Model Builder** window, 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
`Mion`	`0.04[kg/mol]/N_A_const`	kg	

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 `Mion`.

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

The electric force is computed with the time dependent potential from the previous study.

Electric Force 1

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

2 Select Domain 1 only.

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

4 From the **Specify force using** list, choose **Electric potential**.

5 From the V list, choose **Electric potential (ptp/pes1)**.

6 Locate the **Advanced Settings** section. From the **Time dependence of field** list, choose **Periodic**.

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

Allow for collision events that ions undergo along their trajectory. This is done by setting the background gas density and defining cross sections for resonant charge exchange and elastic collisions.

Collisions 1

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

2 In the **Settings** window for **Collisions**, locate the **Fluid Properties** section.

3 In the N_d text field, type `ptp.Nn`.

4 In the T text field, type `300[K]`.

5 Select Domain 1 only.

Resonant Charge Exchange 1

1 In the **Physics** toolbar, click **Attributes** and choose **Resonant Charge Exchange**.

2 In the **Settings** window for **Resonant Charge Exchange**, locate the **Collision Frequency** section.

3 In the σ text field, type `Qex(cpt.Ep)`.

4 In the χ text field, type `5[deg]`.

Collisions 1

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

Elastic 1

1 In the **Physics** toolbar, click **Attributes** and choose **Elastic**.

2 In the **Settings** window for **Elastic**, locate the **Collision Frequency** section.

3 In the σ text field, type `Qele(cpt.Ep)`.

Define where and when the ions are released. The ions should be released at different times along the period, and they should be released from a point outside the plasma sheath.

Release from Grid 1

1 In the **Physics** toolbar, click **Global** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Release Times** section.

3 Click **Range**.

4 In the **Range** dialog box, type `0` in the **Start** text field.

5 In the **Step** text field, type `(1/f0)/30`.

6 In the **Stop** text field, type `1/f0`.

7 Click **Replace**.

8 In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.

9 In the $q_{r,0}$ text field, type `40`.

10 In the $q_{z,0}$ text field, type `8`.

11 Locate the **Initial Velocity** section. From the **Initial velocity** list, choose **Maxwellian**.

12 From the **Sampling from distribution** list, choose **Random**.

13 In the $N_{\mathbf{v}}$ text field, type `30`.

14 In the T_0 text field, type `300[K]`.

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 **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Plasma, Time Periodic (ptp)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

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

6 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 **Study Settings** section.

2 Click **Range**.

3 In the **Range** dialog box, The study should run for a number of periods that allows for all released ions to reach the surface.

4 type `(1/f0)` in the **Step** text field.

5 In the **Stop** text field, type `(1/f0)*40`.

6 Click **Replace**.

7 In the **Settings** window for **Time Dependent**, click to expand the **Values of Dependent Variables** section.

8 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

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

10 From the **Study** list, choose **Study 2, Time Periodic to Time Dependent**.

Solution 3 (sol3)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 3 (sol3)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

4 From the **Maximum step constraint** list, choose **Constant**.

5 In the **Maximum step** text field, type `1E-9`.

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

Create a plot to show the IEDF at the electrode surface.

RESULTS

Ion Energy Distribution Function (IEDF)

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 (IEDF)` 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 (IEDF)** and choose **Histogram**.

2 In the **Settings** window for **Histogram**, locate the **Expression** section.

3 In the **Expression** text field, type `cpt.Ep`.

4 From the **Unit** list, choose **eV**.

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

6 Click **Range**.

7 In the **Range** dialog box, type `0` in the **Start** text field.

8 In the **Step** text field, type `2`.

9 In the **Stop** text field, type `400`.

10 Click **Replace**.

11 In the **Ion Energy Distribution Function (IEDF)** toolbar, click **Plot**.

Create a plot to show the IEDF and the angular distribution at the electrode surface.

Ion Angular Energy Distribution Function (IAEDF)

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

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

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

4 Click **Plot Last**.

Histogram 1

1 In the **Ion Angular Energy Distribution Function (IAEDF)** toolbar, click **More Plots** and choose **Histogram**.

2 In the **Settings** window for **Histogram**, locate the **x-Expression** section.

3 In the **Expression** text field, type `atan(cpt.vr/cpt.vz)`.

4 From the **Unit** list, choose **°**.

5 Select the **Description** check box.

6 In the associated text field, type `Angle`.

7 Locate the **y-Expression** section. In the **Expression** text field, type `cpt.Ep`.

8 From the **Unit** list, choose **eV**.

9 Locate the **Bins** section. Find the **x bins** subsection. From the **Entry method** list, choose **Limits**.

10 Click **Range**.

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

12 In the **Start** text field, type `-10`.

13 In the **Stop** text field, type `10`.

14 In the **Number of values** text field, type `50`.

15 Click **Replace**.

16 In the **Settings** window for **Histogram**, locate the **Bins** section.

17 Find the **y bins** subsection. From the **Entry method** list, choose **Limits**.

18 Click **Range**.

19 In the **Range** dialog box, type `0` in the **Start** text field.

20 In the **Step** text field, type `2`.

21 In the **Stop** text field, type `400`.

22 Click **Replace**.

23 In the **Ion Angular Energy Distribution Function (IAEDF)** toolbar, click **Plot**.

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

Obtain the voltage amplitude and the DC bias.

Global Evaluation 1

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

2 In the **Settings** window for **Global Evaluation**, click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)> Plasma, Time Periodic>Metal Contact 1>ptp.mct1.Va_per - Voltage amplitude - V**.

3 Click **Add Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Plasma, Time Periodic>Metal Contact 1> ptp.mct1.Vdcb_per - DC bias voltage - V**.

4 Click  **Evaluate**.