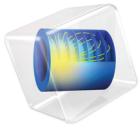

Plasma Module

Application Library Manual

5.3

COMSOL

Plasma Module Application Library Manual

Version: COMSOL 5.3

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Part number: CM021404

Dielectric Barrier Discharge

Introduction

This model simulates electrical breakdown in an atmospheric pressure gas. Because electrical breakdown is a complicated process, a 1D model is considered. To highlight the physics of the breakdown process, this example uses a simple argon chemistry which keeps the number of species and reactions to a minimum.

Model Definition

The operating principle for a dielectric barrier discharge is as follows: there is a small gap filled with a gas in between two dielectric plates. The gap between the two dielectric plates is typically less than one millimeter. On one of the dielectric plates, a sinusoidal voltage is applied. The other plate is electrically grounded. As the voltage applied to the top plate increases, a stronger electric field forms in the gap between the plates. Any free electrons in the gap[1] are accelerated and if the electric field is strong enough they may acquire enough energy to cause ionization. This can lead to a cascade effect where the number of electrons in the gap increases exponentially on a nanosecond timescale. Electrons created via electron impact ionization rush towards one of the dielectric plates, in the opposite direction to the electric field. An equal number of ions are also generated during electron impact ionization (electrons and ions must be created in equal pairs to preserve the overall charge balance). The ions rush toward the opposite dielectric plate in the same direction as the electric field. As a result, surface charge with opposite sign accumulates on both dielectric plates. This causes the electric field to become shielded from the gas filled gap. In fact, the electric field across the gap cannot exceed the breakdown electric field, which is highly dependent on the gas. The breakdown electric field is also a function of the surface properties of the dielectric material. Surface charge accumulation temporarily terminates the discharge until the field reverses direction and the process repeats in the opposing direction.

Modeling dielectric barrier discharges in more than one dimension is, of course possible, but the results can be difficult to interpret due to the amount of competing physics in the problem. In this simple model the problem is reduced to 1D by assuming the dielectric gap is much smaller than the diameter of the plates. It also allows us to quickly gain some insight into the characteristics of the discharge without excessive computation time.

1. There are typically around 1,000,000 m^{-3} free electrons in air at sea level.

The geometry for a typical dielectric barrier discharge is shown in Figure 1. The dielectric plates may be up to 15cm in diameter, the dielectric and gap thickness are typically less than 1 millimeter.

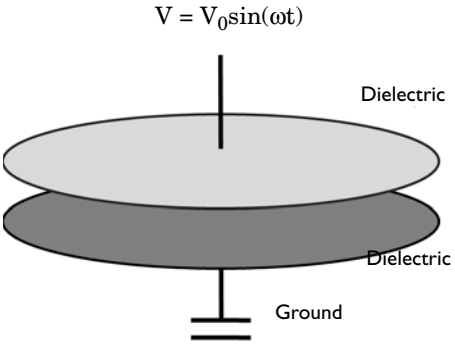

Figure 1: Graphic illustration of a typical dielectric barrier discharge.

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\mathrm{C}^{1/2}/\mathrm{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

BOUNDARY CONDITIONS

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the following boundary condition for the electron flux:

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} v_{e,\,\mathrm{th}} n_e\right) - \sum_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{1}$$

and the electron energy flux:

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6} v_{e,\,\mathrm{th}} n_\varepsilon\right) - \sum_p \varepsilon_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{2}$$

The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed toward the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n}) [Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

Surface charge accumulation is added to the dielectric surfaces that are adjacent to the gap where the plasma forms by way of the following boundary condition:

$$\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

where ρ_s is the surface charge density, which is computed by solving the following distributed ODE on the surfaces:

$$\frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e$$

where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density at the wall, and $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density at the wall.

The discharge is driven by a sinusoidal electric potential applied to the exterior boundary of one of the dielectric plates:

$$V = V_0 \sin(\omega t)$$

where the applied peak voltage, V_0 is 750 V and the angular frequency, the RF frequency being 50 kHz. The exterior boundary of the other dielectric plate is grounded.

PLASMA CHEMISTRY

Argon is an attractive gas to use in a benchmark problem since only a handful of reactions and a few species need to be considered. The list of chemical reactions considered is as follows:

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	-

Initially a small number of seed electrons are present. These are necessary in order to initiate the discharge on the first RF cycle. In addition to the volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When the ions reach the wall they are assumed to change back to neutral argon atoms and donate their charge to the wall.

Results and Discussion

It is more convenient to analyze the results of this one dimensional problem by extruding the solution into two dimensions. The extra dimension represents time. In COMSOL Multiphysics this is accomplished by adding a *Parametric Extrusion 1D* data set. The surface plot is convenient because you can immediately see how the variables of interest evolve over time.

The mass fraction of excited argon atoms is plotted in Figure 2. The excited species have a much longer lifetime in the gap than the electrons or ions. This is because the primary mechanism for destruction of excited argon species is de-excitation upon contact with the wall. The excited argon atoms can only reach the wall via diffusion whereas the electrons and ions reach the wall very rapidly due to migration. It is also apparent from Figure 2 that

the discharge reaches a periodic steady state solution after only two RF cycles.

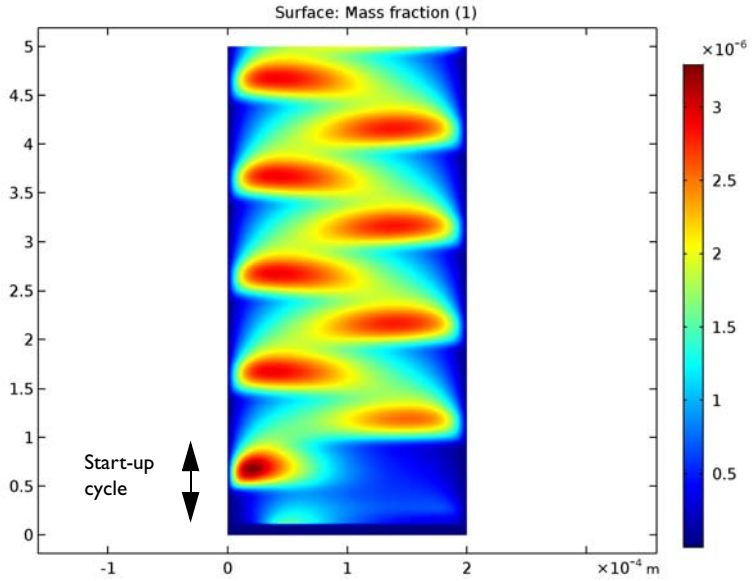

Figure 2: Mass fraction of excited argon.

The electric potential is plotted in Figure 3. The voltage is relatively uniform across the discharge gap. This can be seen more clearly by examining the electric field in Figure 4. There is a much stronger electric field in the dielectric materials than in the gap. This is because the surface charge which accumulates on the dielectric surfaces tends to shield out the electric field.

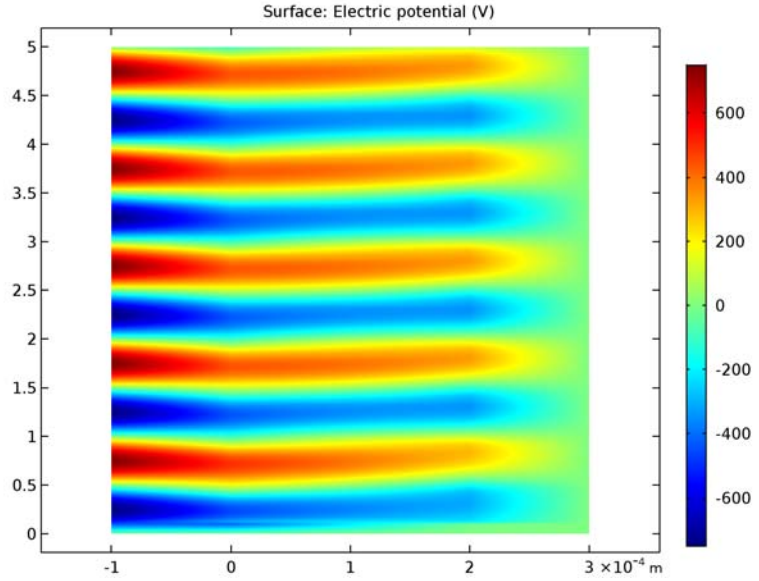

Figure 3: Electric potential (x-axis) vs. time (y-axis).

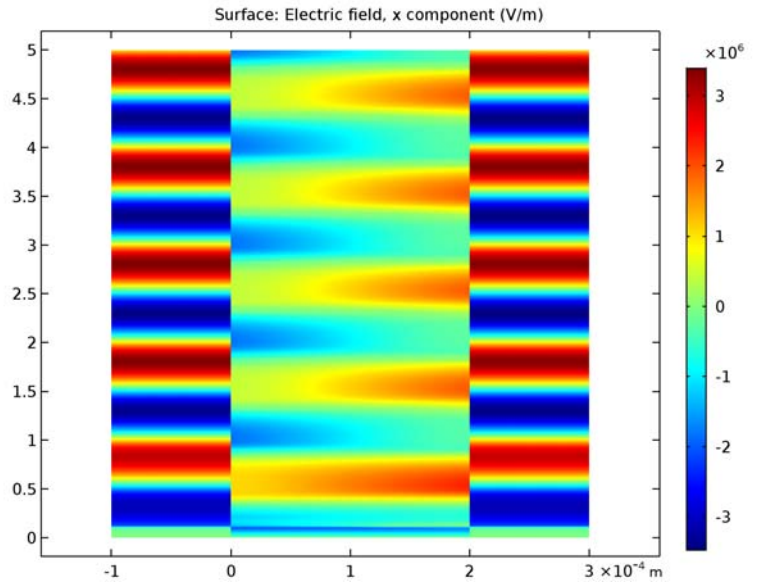

Figure 4: Electric field across the gap (x-axis) vs. time (y-axis).

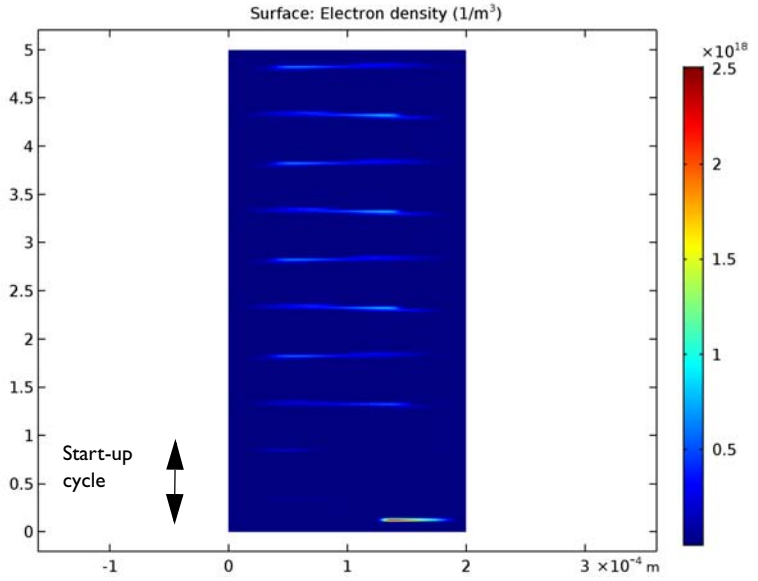

Figure 5: Extruded plot of the electron density.

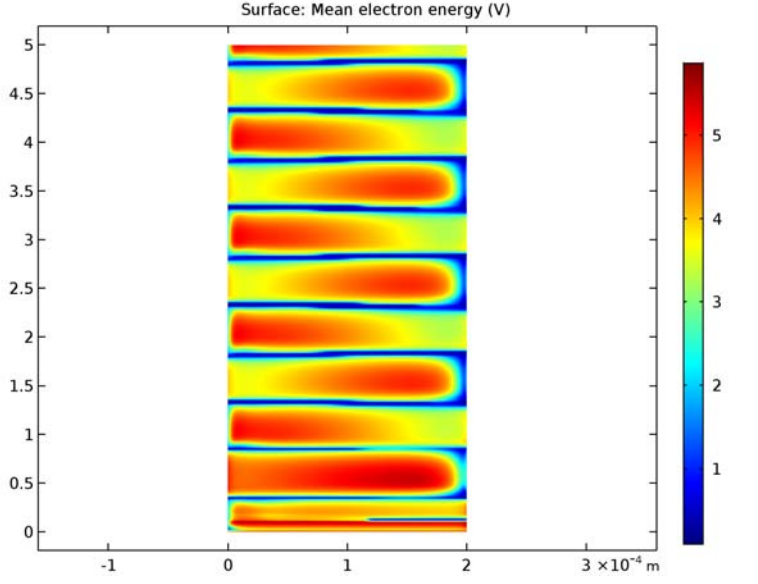

Figure 6: Extruded plot of the mean electron energy.

Implicit in the equations solved for the number of charged particles and electrostatic potential is that the total electrical current is conserved. Mathematically, this means that:

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t} \approx 0$$

where $\mathbf{J}$ is the total plasma current density (SI unit: A/m^2), and ρ is the space charge density (SI unit: C/m^3). Since electrons and ions are created in equal pairs the time derivative of the space charge density should be approximately zero. For this 1D model, this means the total current density must be constant across the gap at any snapshot in time. In Figure 7, the current density due to electrons (left) and ions (right) is plotted. The current density is not symmetric because of the different secondary emission coefficients used on the dielectric surfaces.

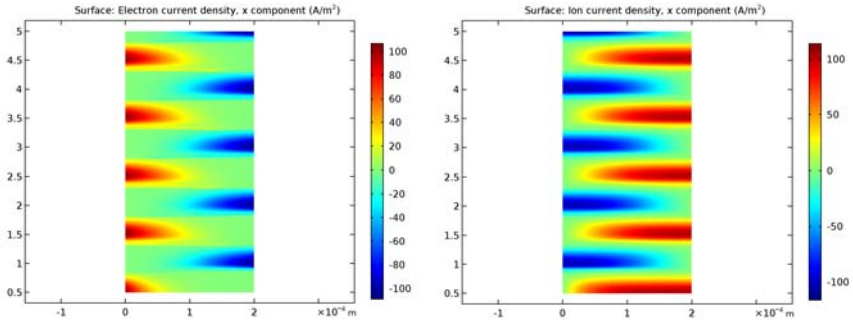

Figure 7: Plot of the electron current density (left) and the ion current density (right) in the discharge, excluding the first RF cycle.

The total plasma current density is plotted in Figure 8. As expected, the total current density is constant across the gap at any point in time.

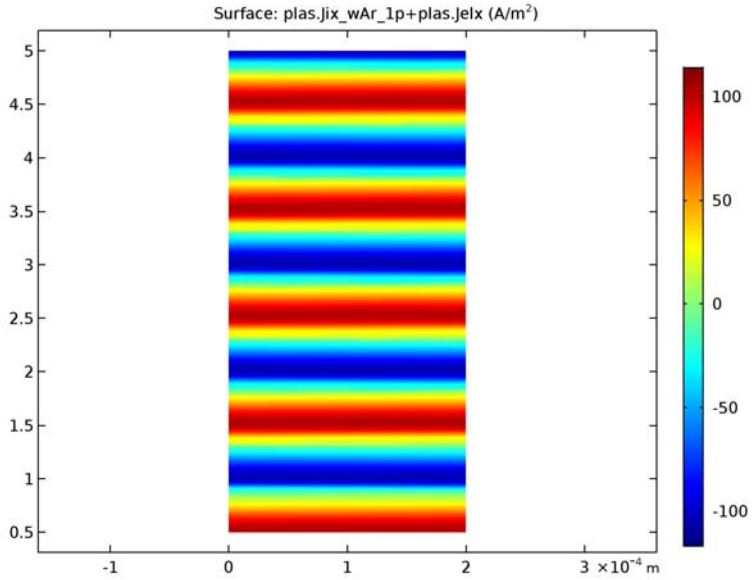

Figure 8: Plot of the total plasma current density (sum of the electron and ion current density), excluding the first RF cycle. Conservation of charge requires that the total current density be constant across the gap at any point in time.

The total current at the grounded electrode is plotted in Figure 9. In the absence of the plasma, the current would be a perfect cosine wave. However, the presence of the plasma and flow of charged particles leads to a non-sinusoidal current waveform. The instantaneously absorbed power in the plasma is plotted in Figure 10. Time averaging this over 1 RF cycle yields the power absorbed by the plasma. The power is around 16.7 W on one half cycle and 17.7 W on the other half cycle. The difference is because the secondary emission coefficients are different on the upper and lower plates.

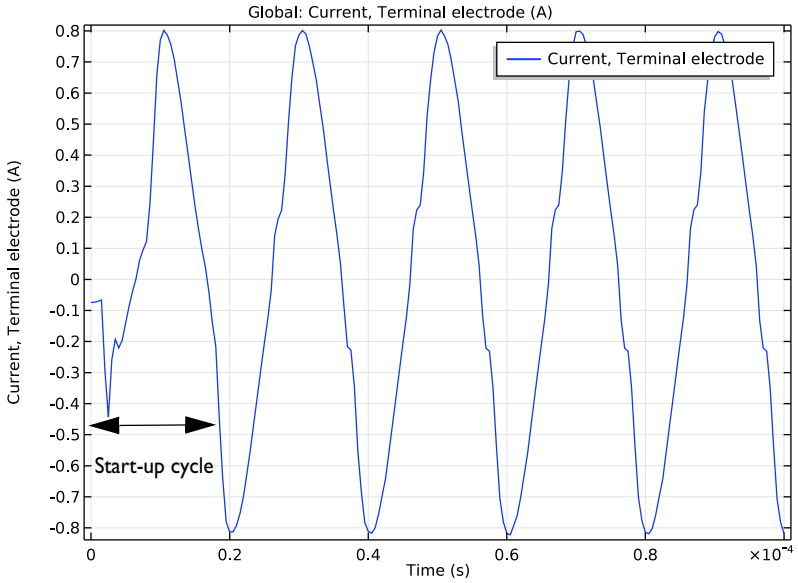

Figure 9: Plot of the total discharge current vs. time.

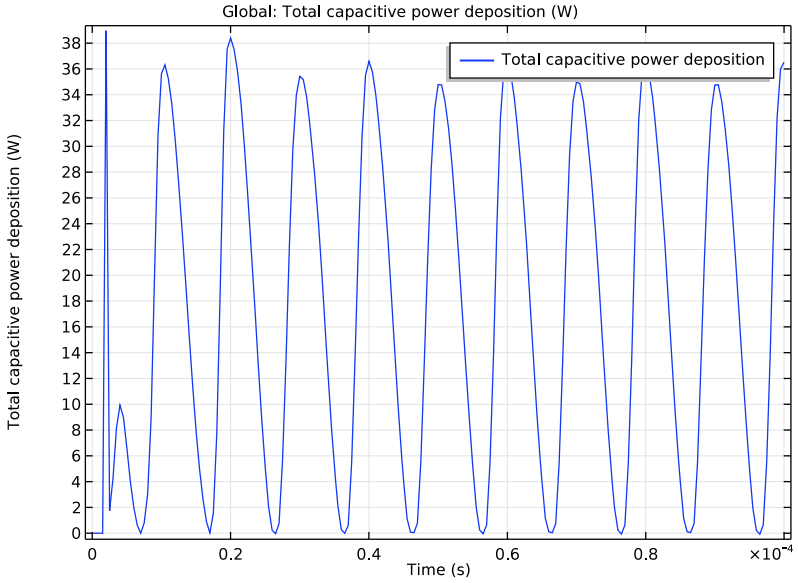

Figure 10: Plot of power vs. time for the dielectric barrier discharge.

Application Library path: `Plasma_Module/Direct_Current_Discharges/argon_dbd_1d`

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 **1D**.

2 In the **Select Physics** tree, select **Plasma>Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GEOMETRY 1

You start by defining the geometry for the problem. This model has a simple 1D geometry consisting of 3 domains. Two dielectric domains and a gap where the plasma forms.

Interval 1 (i1)

1 On the **Geometry** toolbar, click **Interval**.

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

3 From the **Number of intervals** list, choose **Many**.

4 In the **Points** text field, type `-1e-4, 0, 2e-4, 3e-4`.

5 Click **Build All Objects**.

DEFINITIONS

Variables 1

1 On the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
freq	50e3[Hz]	Hz	RF Frequency
omega	2*pi*freq	Hz	Angular frequency
Vrf	-750[V]*sin(omega*t)	V	Applied voltage
dplate	0.1[m]	m	Plate diameter
As	0.25*pi*dplate^2	m^2	Plate area

Now add the charge conservation to the dielectric materials. This means that only a charge conservation equation is solved in the dielectric material and all the plasma components are solved for in the gap between the dielectrics.

PLASMA (PLAS)

Charge Conservation 1

1 On the **Physics** toolbar, click **Domains** and choose **Charge Conservation**.

2 Select Domains 1 and 3 only.

Load in the argon cross sections from file. They form the basis of the plasma chemistry under investigation.

Cross Section Import 1

1 On 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`.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Out-of-Plane Thickness** section.

7 In the *A* text field, type `As`.

8 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** check box.

Reaction 1

1 On 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 `3.3734e8`.

Reaction 2

1 On 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, under **Component 1 (comp1)>Plasma (plas)** 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, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ars**.

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

3 In the x_0 text field, type `1e-11`.

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

Now let the initial number density of Argon ions be the same as the initial number of electrons. This forces the plasma to be initially charge neutral.

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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**.

Plasma Model 1

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

2 In the **Settings** window for **Plasma Model**, locate the **Electron Density and Energy** section.

3 From the **Electron transport properties** list, choose **From electron impact reactions**.

4 Locate the **Model Inputs** section. In the T text field, type `400[K]`.

The initial number density of seed electrons is very small, only one million free electrons per cubic meter. This corresponds to a near zero conductivity. So, the gap is truly acting as an insulator initially.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1e6`.

4 In the ε_0 text field, type `5`.

Secondary emission of electrons is important when studying discharge curves from DBDs. In this example you add a higher secondary emission coefficient on the left wall.

Surface Reaction 1

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

2 Select Boundary 2 only.

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

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

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0.01`.

6 In the ε_i text field, type `2.5`.

Surface Reaction 2

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

2 Select Boundary 3 only.

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

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

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `1E-6`.

6 In the ε_i text field, type `2.5`.

Surface Reaction 3

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

2 Select Boundaries 2 and 3 only.

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

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

Wall 1

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

2 Select Boundaries 2 and 3 only.

Surface charge will begin to accumulate when the gas begins to break down. This will cause the electric field to be shielded in the gap. This is the phenomena responsible for terminating the discharge and also the reason why the breakdown voltage cannot be exceeded across the gap. COMSOL automatically computes the amount of surface charge accumulation when the feature is added to the model. The surface charge accumulation is computed by integration the electron and ion fluxes to the wall.

Surface Charge Accumulation 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Surface Charge Accumulation**.

2 Select Boundaries 2 and 3 only.

Ground 1

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

2 Select Boundary 4 only.

Terminal 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Terminal**.

2 Select Boundary 1 only.

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

4 In the **Terminal name** text field, type `electrode`.

5 In the V_0 text field, type `Vrf`.

Now assign the relative permittivity to the dielectric material and the air gap where the plasma forms.

MATERIALS

Material 1 (mat1)

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

2 Right-click **Material 1 (mat1)** and choose **Rename**.

3 In the **Rename Material** dialog box, type `Dielectric 1` in the **New label** text field.

4 Click **OK**.

5 Select Domains 1 and 3 only.

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

7 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permittivity	epsilonr	10	1	Basic

MESH 1

There must be sufficient mesh density to resolve the sharp gradients in the electron and ion density in the gap. Therefore you specify that there are 200 elements across the width of the gap.

1 In the **Settings** window for **Mesh**, locate the **Mesh Settings** section.

2 From the **Element size** list, choose **Extremely fine**.

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1** and choose **Edge**.

2 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** right-click **Edge 1** and choose **Distribution**.

3 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

4 Click **Clear Selection**.

5 Select Domain 2 only.

6 Locate the **Distribution** section. From the **Distribution properties** list, choose **Predefined distribution type**.

7 In the **Number of elements** text field, type 200.

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

9 From the **Distribution method** list, choose **Geometric sequence**.

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

11 Click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

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

3 Click **Range**.

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

5 In the **Stop** text field, type `1e-4`.

6 In the **Number of values** text field, type `201`.

7 Click **Replace**.

8 On the **Home** toolbar, click **Compute**.

RESULTS

Parametric Extrusion 1D 1

1 On the **Results** toolbar, click **More Data Sets** and choose **Parametric Extrusion 1D**.

2 In the **Settings** window for **Parametric Extrusion 1D**, locate the **Settings** section.

3 Clear the **Separate levels** check box.

4 In the **Level scale factor** text field, type `50e3`.

Now create a new parametric dataset which ignores the first startup RF cycle so the current density can be visualized later

Parametric Extrusion 1D 2

1 Right-click **Parametric Extrusion 1D 1** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Extrusion 1D**, locate the **Data** section.

3 From the **Time selection** list, choose **From list**. In the **Times (s)** list, choose **1E-5** through **1E-4**.

4 Locate the **Settings** section. In the **Level scale factor** text field, type `50e3`.

2D Plot Group 4

1 On the **Results** toolbar, click **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Excited Argon Mass Fraction` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, under **Results** right-click **Excited Argon Mass Fraction** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Plasma (Heavy Species Transport)>Mass fractions>plas.wArs - Mass fraction**.

3 On the **Excited Argon Mass Fraction** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Excited Argon Mass Fraction 1

1 Right-click **Excited Argon Mass Fraction** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electric Potential` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electric Potential** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Plasma (Electrostatics)>Electric>V - Electric potential**.

3 On the **Electric Potential** toolbar, click **Plot**.

4 Click **Plot**.

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

Electric Potential 1

1 In the **Model Builder** window, under **Results** right-click **Electric Potential** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electric Field` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electric Field** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Plasma (Electrostatics)>Electric>Electric field>plas.Ex - Electric field, x component**.

3 On the **Electric Field** toolbar, click **Plot**.

4 Click **Plot**.

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

Electric Field 1

1 In the **Model Builder** window, under **Results** right-click **Electric Field** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electron Density` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electron Density** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Plasma (Drift Diffusion)>Electron density>plas.ne - Electron density**.

3 On the **Electron Density** toolbar, click **Plot**.

4 Click **Plot**.

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

Electron Density 1

1 In the **Model Builder** window, under **Results** right-click **Electron Density** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Mean Electron Energy` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Mean Electron Energy** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Plasma (Drift Diffusion)>Electron energy density>plas.ebar - Mean electron energy**.

3 On the **Mean Electron Energy** toolbar, click **Plot**.

4 Click **Plot**.

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

Mean Electron Energy 1

1 In the **Model Builder** window, under **Results** right-click **Mean Electron Energy** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electron Current Density` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Parametric Extrusion 1D 2**.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electron Current Density** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Plasma (Drift Diffusion)>Current>Electron current density>plas.Jelx - Electron current density, x component**.

3 On the **Electron Current Density** toolbar, click **Plot**.

4 Click **Plot**.

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

Electron Current Density 1

1 In the **Model Builder** window, under **Results** right-click **Electron Current Density** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Argon Ion Current Density` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Argon Ion Current Density** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Model>Component 1> Plasma (Heavy Species Transport)>Species>Species wAr_1p>Ion current density> plas.Jix_wAr_1p - Ion current density, x component**.

3 On the **Argon Ion Current Density** toolbar, click **Plot**.

4 Click **Plot**.

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

Argon Ion Current Density 1

1 In the **Model Builder** window, under **Results** right-click **Argon Ion Current Density** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Total Conduction Current Density` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Total Conduction Current Density** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `plas.Jix_wAr_1p+plas.Jelx`.

4 On the **Total Conduction Current Density** toolbar, click **Plot**.

5 Click **Plot**.

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

1D Plot Group 12

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

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

Global 1

1 Right-click **Terminal Current** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1> Plasma (Electrostatics)>plas.I_electrode - Current, Terminal electrode**.

3 On the **Terminal Current** toolbar, click **Plot**.

1D Plot Group 13

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

2 In the **Settings** window for **1D Plot Group**, type `Total Power Deposition` in the **Label** text field.

Global 1

1 Right-click **Total Power Deposition** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1>Plasma> Power and collisions>plas.Pcap_tot - Total capacitive power deposition**.

3 On the **Total Power Deposition** toolbar, click **Plot**.

Global Evaluation 1

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

Use the `timeavg` operator to compute the time averaged power deposition for cycles 2-10.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

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

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`timeavg(1e-5,2e-5,plas.Pcap_tot,'nointerp')`	`W`	`Cycle 2`
`timeavg(2e-5,3e-5,plas.Pcap_tot,'nointerp')`	`W`	`Cycle 3`
`timeavg(3e-5,4e-5,plas.Pcap_tot,'nointerp')`	`W`	`Cycle 4`
`timeavg(4e-5,5e-5,plas.Pcap_tot,'nointerp')`	`W`	`Cycle 5`
`timeavg(5e-5,6e-5,plas.Pcap_tot,'nointerp')`	`W`	`Cycle 6`
`timeavg(6e-5,7e-5,plas.Pcap_tot,'nointerp')`	`W`	`Cycle 7`
`timeavg(7e-5,8e-5,plas.Pcap_tot,'nointerp')`	`W`	`Cycle 8`

Expression	Unit	Description
`timeavg(8e-5,9e-5,plas.Pcap_tot,'nointerp')`	W	Cycle 9
`timeavg(9e-5,10e-5,plas.Pcap_tot,'nointerp')`	W	Cycle 10

5 Click **Evaluate**.

As you can see, the average power deposited to the plasma remains the same for each cycle after only 3 RF cycles. The power is around 16.7 W on one half cycle and 17.7 W on the other half cycle. The difference is due to the fact that the secondary emission coefficients are different on the upper and lower plates.

GEC CCP Reactor, Argon Chemistry, 1D

Introduction

The NIST (National Institute of Standards and Technology) GEC CCP reactor provides a platform for studying capacitively coupled plasmas (CCP). Even the simplest plasma models are quite involved, so a 1D example helps in understanding the physics without excessive CPU time. The problem has no steady-state solution, although a periodic steady-state solution is reached after a suitable number of RF cycles (usually >1000).

Model Definition

The operating principle of a capacitively coupled plasma is different to the inductive case. In a CCP reactor, there are no induction currents. Instead, the plasma is sustained by applying a sinusoidal electrostatic potential across a small gap (2.54 cm in this case) filled with a low pressure (1 Torr in this case) gas. This case uses argon because the plasma chemistry is very simple. The mechanism of power deposition into a CCP reactor is highly nonlinear and occurs at multiple different frequencies. Therefore, the electrostatic potential cannot be solved for in the frequency domain. The model must be transient, with the system allowed to reach a periodic steady state solution. This condition is reached after a suitable number of RF cycles.

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth

or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\mathrm{C}^{1/2}/\mathrm{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

BOUNDARY CONDITIONS

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the following boundary condition for the electron flux:

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} v_{e,\,\mathrm{th}} n_e\right) - \sum_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{1}$$

and the electron energy flux:

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6} v_{e,\,\mathrm{th}} n_\varepsilon\right) - \sum_p \varepsilon_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{2}$$

The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

Surface charge accumulation is added to the dielectric surface by way of the following boundary condition:

$$\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_\mathrm{s}$$

where ρ_s is the surface charge density, which is computed by solving the following distributed ODE on the surfaces:

$$\frac{d\rho_\mathrm{s}}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e$$

where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density at the wall, and $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density at the wall.

The discharge is driven by a sinusoidal electric potential applied to the exterior boundary of the dielectric plate:

$$V = V_0 \sin(\omega t)$$

where the applied peak voltage, V_0 is 300 V and the angular frequency, the RF frequency being 13.56 MHz. The exterior boundary of the other dielectric plate is grounded. The left boundary is grounded.

PLASMA CHEMISTRY

Argon is one of the simplest mechanisms to implement at low pressures. The electronically excited states can be lumped into a single species which results in a chemical mechanism consisting of only 3 species and 7 reactions:

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 a CCP reactor the electron density and density of excited species is relatively low so stepwise ionization is not as important as in high density discharges. In addition to volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When a metastable argon atom makes contact with the wall, it will revert to the ground state argon atom with some probability (the sticking coefficient).

Results and Discussion

Due to the fact that capacitively coupled discharges never reach steady state, you have to run the problem long enough to obtain a quasi steady state, that is, until the time-averaged properties do not change from cycle to cycle. Once reached, quantities of interest can be plotted at different phases of the RF cycle.

The electric potential, electric field, electron density, and ion density are all quantities of interest. Figure 1 plots the electron density at different phases of the RF cycle.

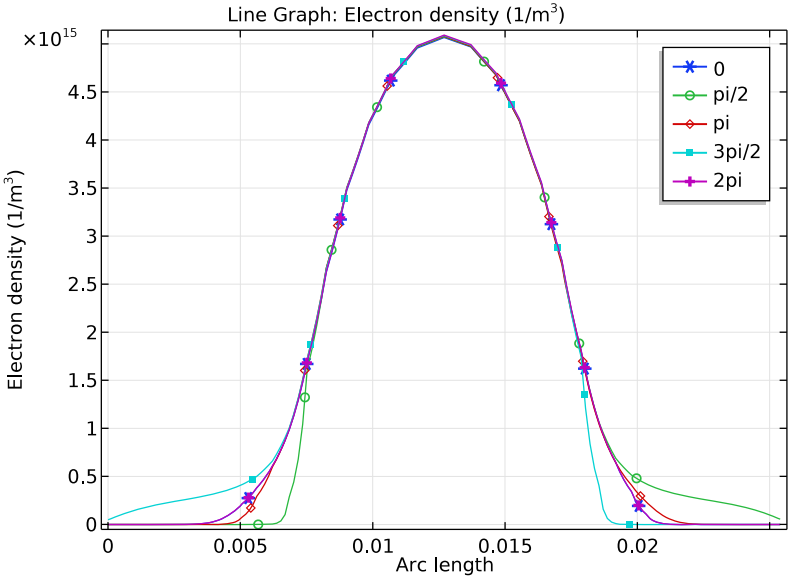

Figure 1: Plot of the electron density at different phases of the RF cycle.

The electrons, with their low mass can respond to the electric field very rapidly. This means that the electrons can move back and forth in the x-direction as the electric field changes sign. The electrostatic potential is the same at t=0 and t=2π. At these times the electrostatic potential is positive in the bulk plasma. The electrons are more mobile than the heavier ions, so they respond to the applied electric field over the course of one RF cycle. The pushing and pulling of electrons back and forth, coupled with the fact that the ions essentially remain stationary leads to a separation of space charge in the plasma sheath.

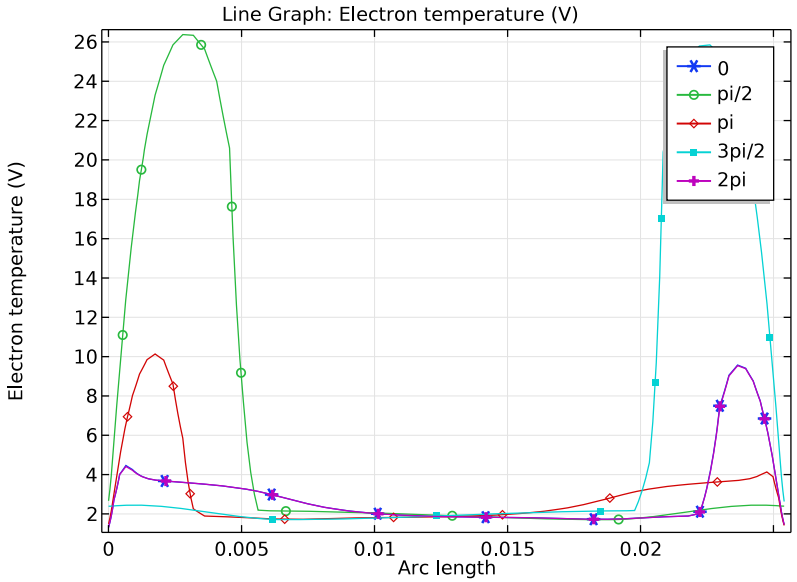

Figure 2: Plot of electron temperature at different phases of the RF cycle.

The space charge separation produces an electric field as well as a flux of electrons. This is how power is deposited into the plasma. Figure 2 plots the electron temperature in the plasma and Figure 3 and Figure 4 plot the electric potential and electric field respectively. Figure 5 plots the ion density at different phases of the RF cycle. Over 1RF cycle, there is a net positive power deposition. At quasi steady state, the power deposition is balanced by the power lost due to chemical reactions and energy loss to the wall.

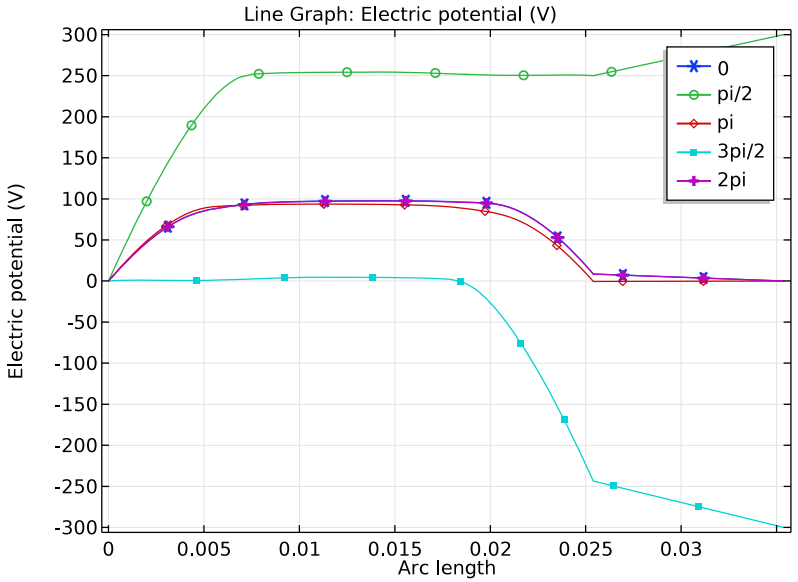

Figure 3: Plot of the electric potential at different phases of the RF cycle.

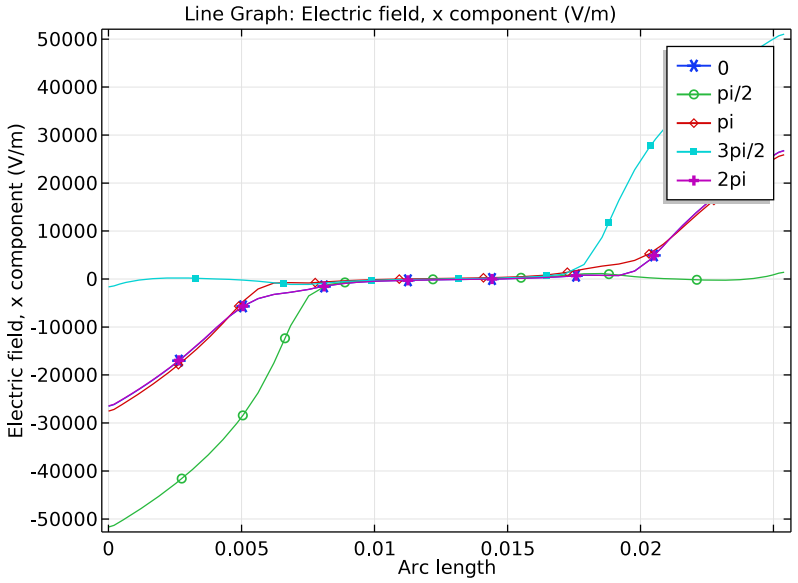

Figure 4: Plot of the electric field at different phases of the RF cycle.

Figure 6 plots the power deposition at different phases of the RF cycle. The maximum power deposition occurs when the applied voltage is 0. Power deposition is at a minimum when the applied voltage is at a maximum (300V) or minimum (-300V).

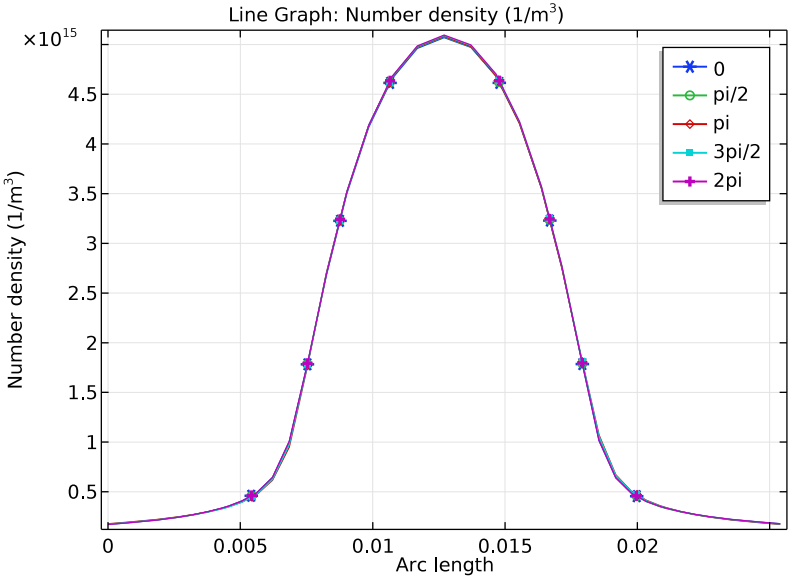

Figure 5: Plot of the ion density at different phases of the RF cycle.

This model also demonstrates two of the shielding mechanisms that occur in a capacitively coupled plasma. The electric field is shielded from the plasma bulk over several Debye lengths. The Debye length is defined as:

$$\lambda_D = \sqrt{\frac{\varepsilon_0 T_e}{n_e q}}$$

where T_e is in electron volts, ε_0 is the permittivity of free space, n_e is the electron density and q is the electron charge. This is the distance over which the electric field is shielded from the plasma. One can see from Figure 4 that the electric field in the plasma bulk does not change over 1 RF cycle.

The other shielding mechanism is caused by the difference in transport time scales between electrons and ions. Since the electrons are more mobile than the ions, they can accumulate a substantial drift velocity directed toward the walls, even at the high operating frequencies. This results in an accumulation of surface charge on the dielectric surface.

This accumulation of surface charge tends to further shield the electric field from the plasma.

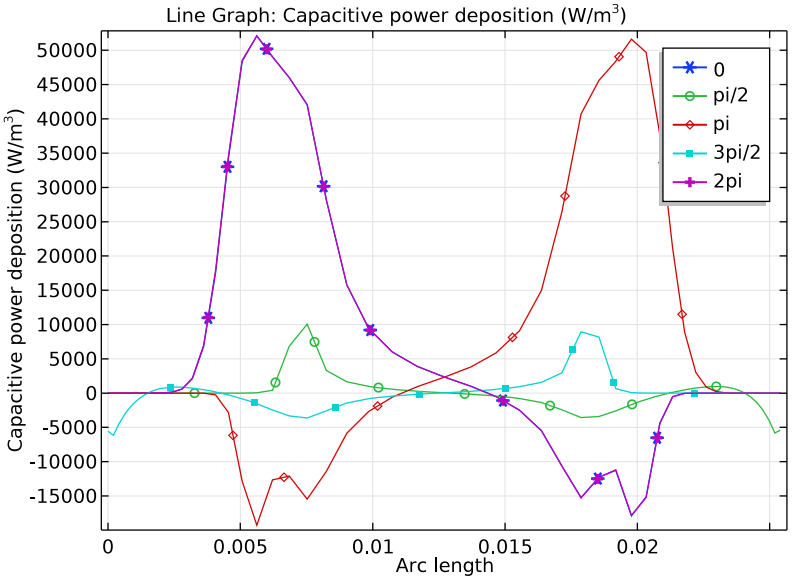

Figure 6: Plot of the power deposition into the plasma at different phases of the RF cycle.

Reference

1. G.J.M. Hagelaar and L.C. Pitchford, "Solving the Boltzmann Equation to Obtain Electron Transport Coefficients and Rate Coefficients for Fluid Models," *Plasma Sources Sci. Technol*, vol. 14, 722–733, 2005.

Application Library path: `Plasma_Module/Capacitively_Coupled_Plasmas/argon_gec_ccp_1d`

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 **1D**.

2 In the **Select Physics** tree, select **Plasma>Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
V0	300[V]	300 V	Applied voltage
freq	13.56[MHz]	1.356E7 Hz	RF Frequency
omega	2*pi*freq	8.52E7 Hz	Angular frequency
p0	1[torr]	133.3 Pa	Gas pressure
T0	400[K]	400 K	Gas temperature
mueN	4E24[1/(V*m*s)]	4E24 1/(V·m·s)	Reduced electron mobility

GEOMETRY 1

Interval 1 (i1)

1 On the **Geometry** toolbar, click **Interval**.

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

3 In the **Right endpoint** text field, type 0.0254.

Interval 2 (i2)

1 On the **Geometry** toolbar, click **Interval**.

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

3 In the **Left endpoint** text field, type 0.0254.

4 In the **Right endpoint** text field, type 0.0354.

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

PLASMA (PLAS)

In the **Model Builder** window, expand the **Component 1 (comp1)>Plasma (plas)** node.

Cross Section Import 1

1 Right-click **Plasma (plas)** 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`.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Plasma Properties** section.

7 Select the **Use reduced electron transport properties** check box.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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 `3.734E8`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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`.

Surface Reaction 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> 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 Select Boundaries 1 and 2 only.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

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

4 Select Boundaries 1 and 2 only.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar**.

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

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

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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.

Plasma Model 1

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

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

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

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

5 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `mueN`.

Charge Conservation 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the domain setting **Electrostatics>Charge Conservation**.

2 Select Domain 2 only.

Wall 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

2 Select Boundaries 1 and 2 only.

The surface charge accumulation models the effect of charged particle build up on dielectric surfaces. This shields the electric field from the plasma.

Surface Charge Accumulation 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics> Surface Charge Accumulation**.

2 Select Boundary 2 only.

Ground 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

2 Select Boundary 1 only.

The terminal feature is used to drive the CCP with a sinusoidal voltage. In this case the voltage is 300 volts and the pressure is 1 torr. If the ratio of the voltage to the pressure is higher, numerical instabilities may occur. In these cases the mesh refinement may be necessary.

Terminal 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>More> Terminal**.

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

3 In the **Terminal name** text field, type `plate`.

4 Select Boundary 3 only.

5 From the **Terminal type** list, choose **Voltage**.

6 In the V_0 text field, type `V0*sin(omega*t)`.

MATERIALS

Material 1 (mat1)

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

2 Select Domain 2 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permittivity	epsilonr	4.7	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 1 (mat1)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Dielectric` in the **New label** text field.

7 Click **OK**.

MESH 1

Edge 1

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

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

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

4 Select Domain 1 only.

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Distribution**.

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

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

4 In the **Number of elements** text field, type `50`.

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

6 From the **Distribution method** list, choose **Geometric sequence**.

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

Edge 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Edge**.

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

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

4 Select Domain 2 only.

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 2** and choose **Distribution**.

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

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

4 In the **Number of elements** text field, type `50`.

5 From the **Distribution method** list, choose **Geometric sequence**.

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

7 Click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: 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 `100/freq` in the **Stop** text field.

5 In the **Step** text field, type `2/freq`.

6 Click **Replace**.

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

8 Click **Range**.

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

10 In the **Start** text field, type `101/13.56E6`.

11 In the **Stop** text field, type `102/13.56E6`.

12 In the **Number of values** text field, type `5`.

13 Click **Add**.

The model can solve faster by deactivating the convergence plots. Also, the default plots are unnecessary since custom plots will be used during results processing.

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

15 In the **Settings** window for **Study**, locate the **Study Settings** section.

16 Clear the **Generate default plots** check box.

17 Clear the **Generate convergence plots** check box.

18 On the **Home** toolbar, click **Compute**.

RESULTS

1D Plot Group 1

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

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Time selection** list, choose **From list**.

4 In the **Times (s)** list, choose **7.448E-6**, **7.467E-6**, **7.485E-6**, **7.504E-6**, and **7.522E-6**.

Line Graph 1

1 Right-click **1D Plot Group 1** and choose **Line Graph**.

2 Select Domain 1 only.

3 On the **1D Plot Group 1** toolbar, click **Plot**.

4 In the **Settings** window for **Line Graph**, click to expand the **Legends** section.

5 Select the **Show legends** check box.

6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
0
pi/2
pi
3pi/2
2pi

8 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

9 On the **1D Plot Group 1** toolbar, click **Plot**.

10 Click the **Zoom Extents** button on the **Graphics** toolbar.

1D Plot Group 1

1 In the **Model Builder** window, under **Results** click **1D Plot Group 1**.

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

Electron Density 1

1 Right-click **Results>Electron Density** and choose **Duplicate**.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electron Density 1** node, then click **Results> Electron Temperature>Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Drift Diffusion)>Electron energy density>plas.Te - Electron temperature**.

3 On the **Electron Temperature** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Electron Temperature 1

1 In the **Model Builder** window, under **Results** right-click **Electron Temperature** and choose **Duplicate**.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electron Temperature 1** node, then click **Results>Electric Potential>Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

4 Click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Plasma (Electrostatics)>Electric>V - Electric potential**.

5 On the **Electric Potential** toolbar, click **Plot**.

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

Electric Potential 1

1 In the **Model Builder** window, under **Results** right-click **Electric Potential** and choose **Duplicate**.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electric Potential 1** node, then click **Results> Electric Field>Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Plasma (Electrostatics)> Electric>Electric field>plas.Ex - Electric field, x component**.

3 Locate the **Selection** section. In the list, select **2**.

4 Select the **Active** toggle button.

5 Click **Remove from Selection**.

6 Select Domain 1 only.

7 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

8 On the **Electric Field** toolbar, click **Plot**.

9 Click the **Zoom Extents** button on the **Graphics** toolbar.

Electric Field 1

1 In the **Model Builder** window, under **Results** right-click **Electric Field** and choose **Duplicate**.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electric Field 1** node, then click **Results> Ion Density>Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Number densities>plas.n_wAr_1p - Number density**.

3 On the **Ion Density** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Ion Density 1

1 In the **Model Builder** window, under **Results** right-click **Ion Density** and choose **Duplicate**.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Ion Density 1** node, then click **Results> Power Deposition>Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Drift Diffusion)>Power and collisions>plas.Pcap - Capacitive power deposition**.

3 On the **Power Deposition** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

GEC ICP Reactor, Argon Chemistry

Introduction

The GEC cell was introduced by NIST (National Institute of Standards and Technology) in order to provide a standardized platform for experimental and modeling studies of discharges in different laboratories. The plasma is sustained via inductive heating. The Reference Cell operates as an inductively-coupled plasma in this model.

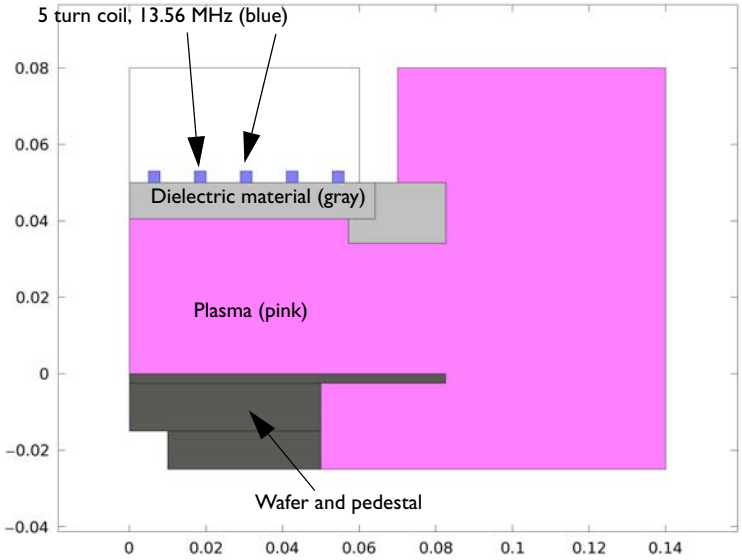

Figure 1: GEC ICP reactor geometry consisting of a 5 turn copper coil, plasma volume, dielectrics, and wafer with pedestal.

Note: This application requires the Plasma Module and the AC/DC Module.

Model Definition

Inductively coupled discharges typically operate at low pressures (<10 Pa) and high charge density (>10^{17} m^{-3}). High density plasma sources are popular because low pressure ion bombardment can provide a greater degree of anisotropy on the surface of the wafer.

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of

electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\mathrm{C}^{1/2}/\mathrm{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho\frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u}\cdot\nabla)w_k = \nabla\cdot\mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla\cdot\varepsilon_0\varepsilon_r\nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

For a nonmagnetized, nonpolarized plasma, the induction currents are computed in the frequency domain using the following equation:

$$(j\omega\sigma - \omega^2\varepsilon_0)\mathbf{A} + \nabla\times(\mu_0^{-1}\nabla\times\mathbf{A}) = \mathbf{J}^e$$

The plasma conductivity needs to be specified as a material property, usually from the cold plasma approximation:

$$\sigma = \frac{n_e q^2}{m_e(\nu_e + j\omega)}$$

where n_e is the electron density, q is the electron charge, m_e is the electron mass, ν_e is the collision frequency, and ω is the angular frequency.

BOUNDARY CONDITIONS

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the following boundary condition for the electron flux:

$$\mathbf{n}\cdot\Gamma_e = \left(\frac{1}{2}\nu_{e,\,\mathrm{th}} n_e\right) \tag{1}$$

and the electron energy flux:

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6} \nu_{e,\,\mathrm{th}} n_\varepsilon\right) \tag{2}$$

The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

The walls of the reactor are grounded.

PLASMA CHEMISTRY

Because the physics occurring in an inductively coupled plasma is rather complex, it is always best to start a modeling project with a simple chemical mechanism. Argon is one of the simplest mechanisms to implement at low pressures. The electronically excited states can be lumped into a single species, which results in a chemical mechanism consisting of only 3 species and 7 reactions:

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	-

Stepwise ionization (reaction 5) can play an important role in sustaining low pressure argon discharges. Excited argon atoms are consumed via superelastic collisions with electrons, quenching with neutral argon atoms, ionization or Penning ionization where two metastable argon atoms react to form a neutral argon atom, an argon ion and an

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

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When a metastable argon atom makes contact with the wall, it reverts to the ground state argon atom with some probability (the sticking coefficient).

ELECTRICAL EXCITATION

From an electrical point of view, the GEC reactor behaves as a transformer. A current is applied to the driving coil (the primary) and this induces a current in the plasma (the secondary). The plasma then induces an opposing current back in the coil, increasing its resistance. The current flowing in the plasma depends on the current applied to the coil and the reaction kinetics. The total plasma current can vary from no current (plasma not sustained) to the same current as the primary which corresponds to perfect coupling between the coil and the plasma.

In this example a fixed power of 1500 W is applied to the coil. Some of this power is dissipated in the coil, some is deposited into the plasma.

The peak electron density occurs at the center of the reactor, underneath the RF coil. The electron density in this case is high enough to cause some shielding of the azimuthal electric field.

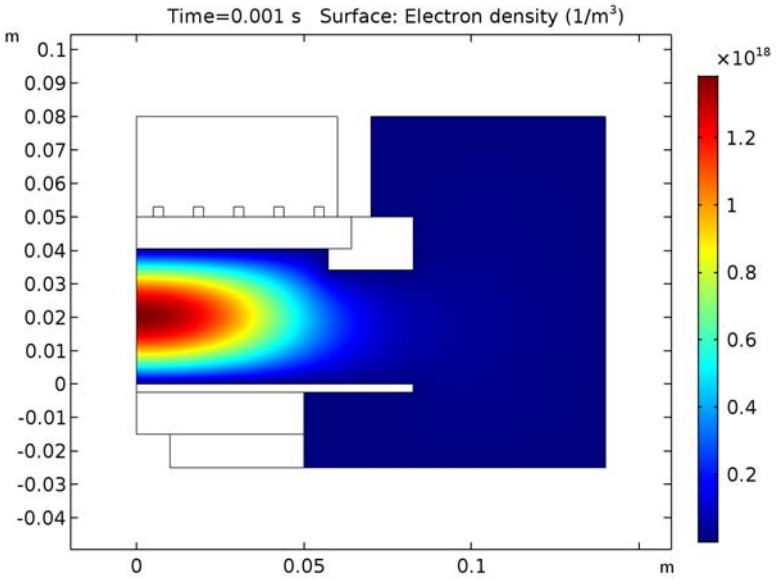

Figure 2: Plot of the electron density inside the GEC ICP reactor.

The electron "temperature" is highest directly underneath the coil, which is where the bulk of the power deposition occurs.

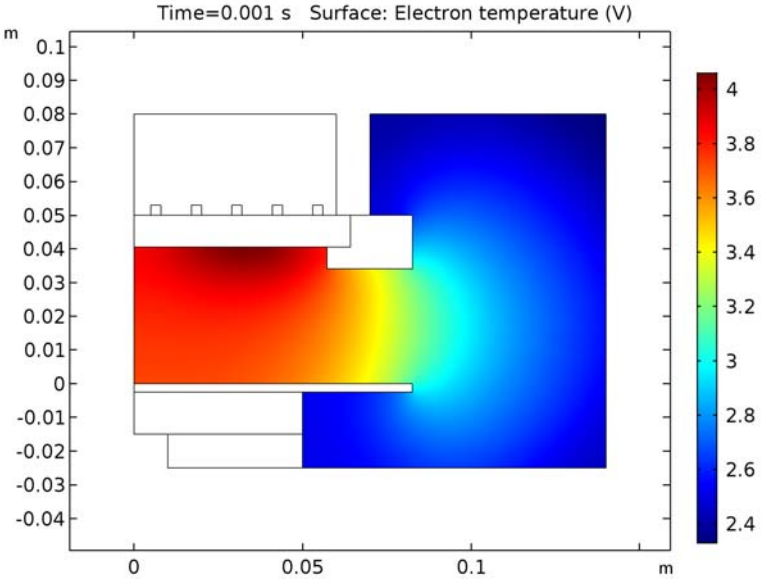

Figure 3: Plot of the electron "temperature" inside the GEC ICP reactor.

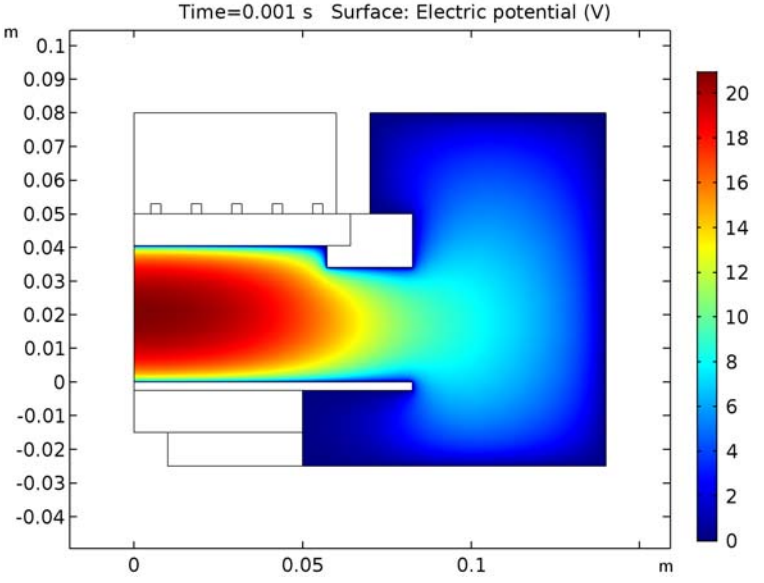

Figure 4: Plot of the electric potential inside the GEC ICP reactor.

From an electrical standpoint, the quantities of interest are total power deposition, coil resistance and inductance, and reactor efficiency. These "global" parameters are relatively easy to measure when the plasma is on or off, so such quantities provide an easy route for comparison with experimental data, without the need for expensive optical emission spectroscopy equipment or Langmuir probes.

The resistance of the coil increases by a little less than a factor of 4 when the plasma is on. When the plasma is on, there is a substantial opposing current induced back into the coil from the plasma. The electric potential applied across the coil needs to increase in order to maintain the same total current.

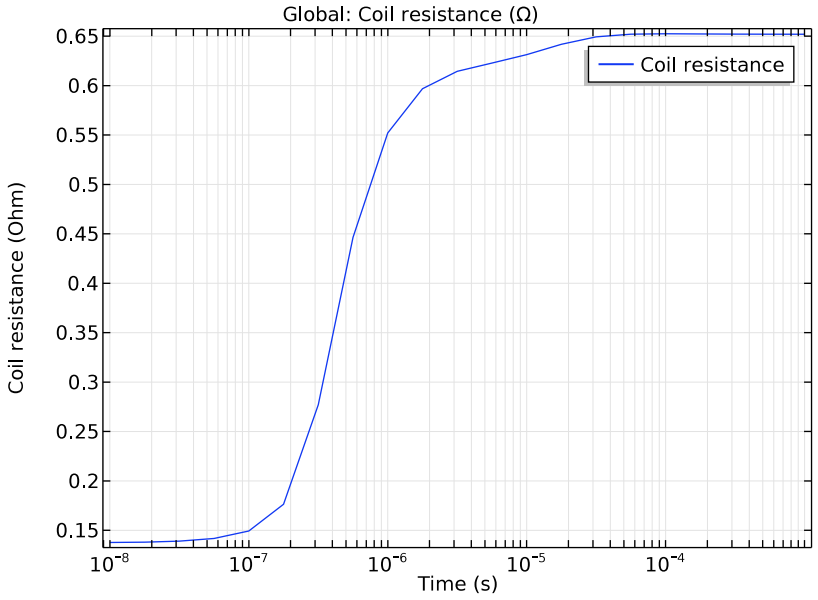

Figure 5: Plot of coil resistance v.s. time in GEC ICP reactor.

Initially the power dissipated is all dissipated in the coil (~500 W). After about 1 microsecond, the plasma ignition begins and as the neutral gas atoms split into electrons and ions, the electrons begin to absorb more and more power. Over a period of 2 microseconds, the plasma goes from absorbing no power to absorbing around 1600 W.

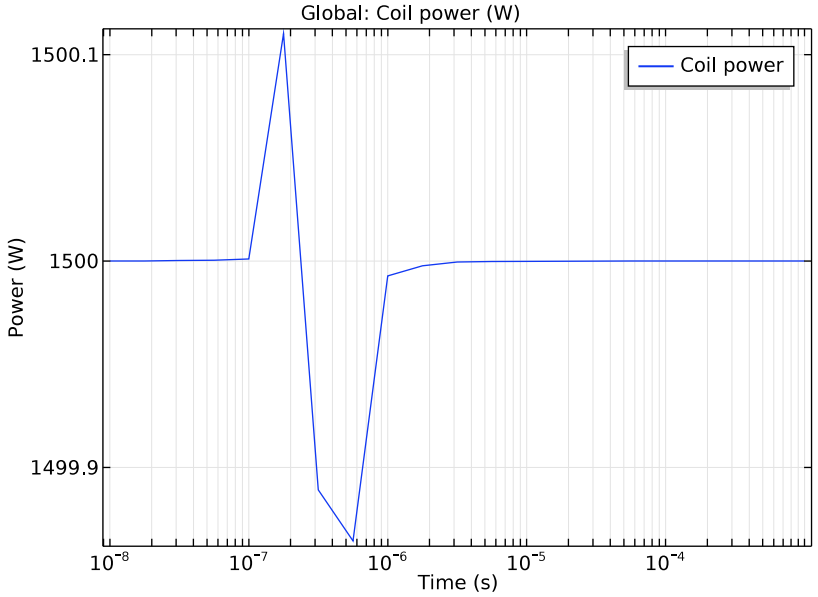

Figure 6: Plot of total power versus time in GEC ICP reactor.

The ion density is exactly the same except from in a thin region close to the walls. In this region, the ion density dominates the electron density which leads to a positive potential in the plasma bulk with respect to the walls. The positive potential increases the flux of ions and reduces the flux of electrons to the wall.

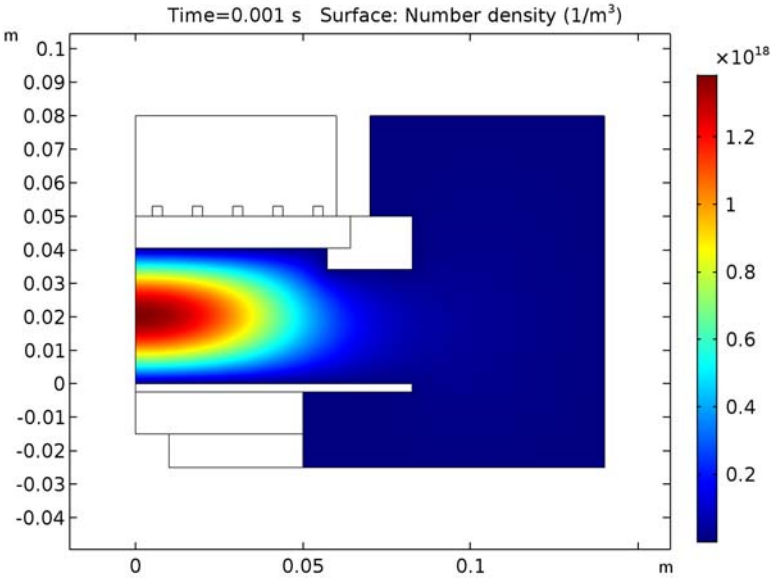

Figure 7: Plot of number density of argon ions in the GEC ICP reactor.

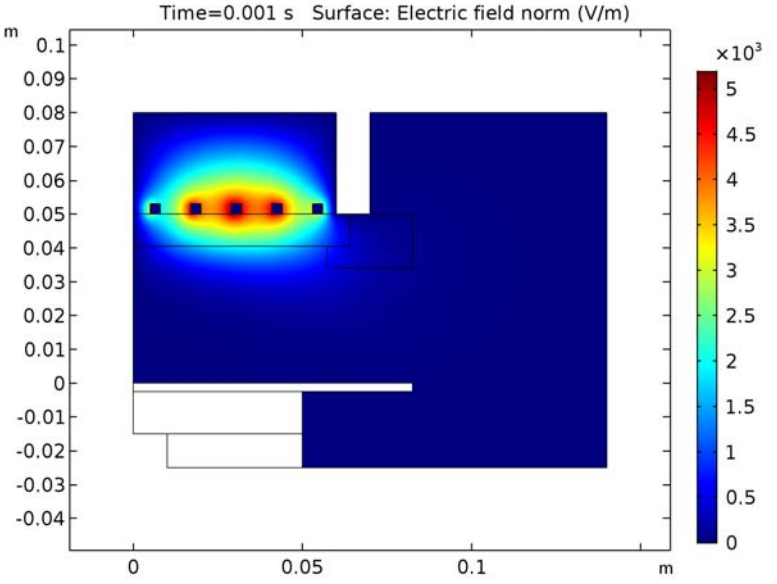

Figure 8: Plot of the norm of the electric field due to the induction currents.

The number density of excited species is also greatest in the center of the reactor. Unlike the charged species, there is no rapid drop off in number density close to the walls. The physics of the excited species is relatively simple: they are formed in the center of the reactor by high energy electrons and are lost to the via either stepwise ionization or diffusion to the wall. Because the excited argon atoms are not susceptible to migration due to the electric field, they can exist in much higher quantities than ions. The peak number density of excited argon atoms represents a mass fraction of around 0.02.

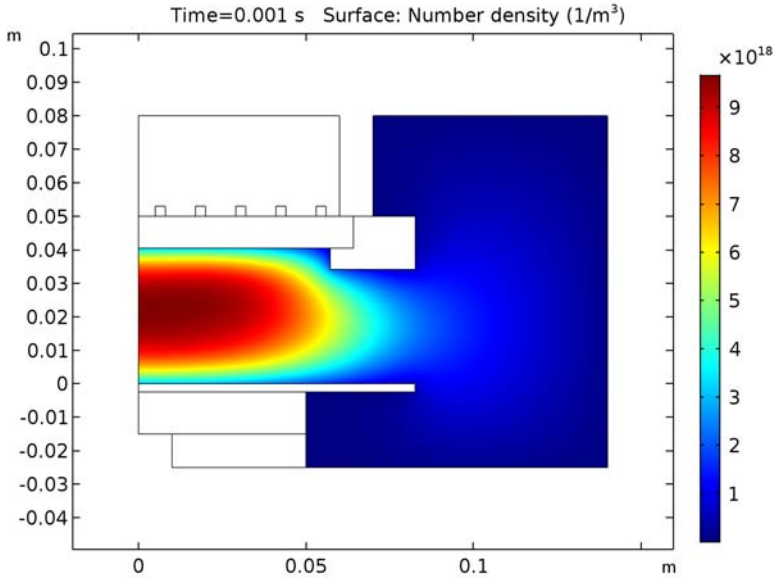

Figure 9: Plot of the number density of excited argon atoms in the GEC ICP reactor.

The skin depth of the plasma is on the order of 1cm which prevents the electric field from penetrating into the core of the plasma. The skin depth is defined as:

$$\delta = \sqrt{\frac{2}{\mu\omega\sigma}}$$

where μ is the permeability, σ is the plasma conductivity, and ω is the angular frequency. This tells us that increasing the driving frequency does not necessarily couple more power into the plasma. As the frequency increases, the plasma tends to shield the region over which power is deposited into a thin layer close to the upper wall.

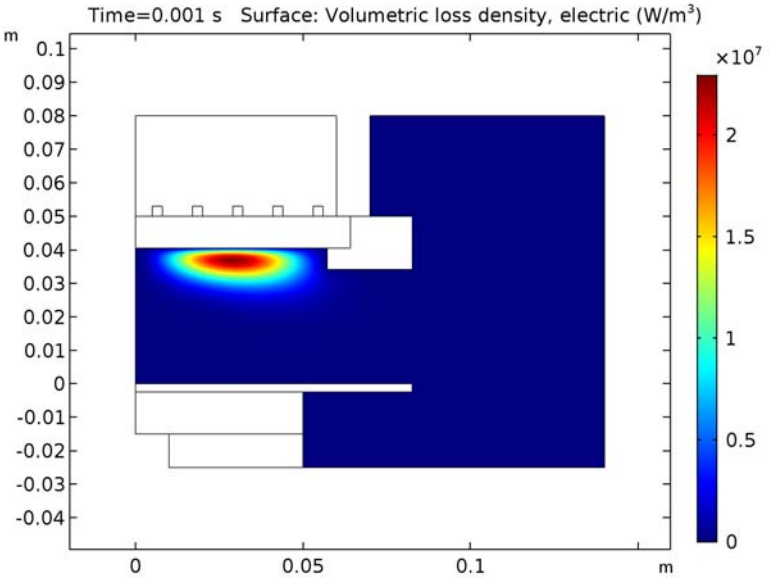

Figure 10: Plot of the power deposition into the plasma in the GEC ICP reactor. The region over which power is deposited to the plasma is governed by the plasma skin depth.

References

1. G.J.M. Hagelaar and L.C. Pitchford, "Solving the Boltzmann Equation to Obtain Electron Transport Coefficients and Rate Coefficients for Fluid Models," *Plasma Sources Sci. Technol,* vol. 14, pp. 722–733, 2005.

2. D.P. Lymberopolous and D.J. Economou, "Two-Dimensional Self-Consistent Radio Frequency Plasma Simulations Relevant to the Gaseous Electronics Conference RF Reference Cell," *J. Res. Natl. Inst. Stand. Technol.*, vol. 100, p. 473, 1995.

Application Library path: `Plasma_Module/Inductively_Coupled_Plasmas/argon_gec_icp`

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 **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Plasma>Inductively Coupled Plasma**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Frequency-Transient**.

6 Click **Done**.

Start by importing the geometry of the GEC reference cell.

GEOMETRY 1

Import 1 (imp1)

1 On the **Home** toolbar, click **Import**.

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

3 Click **Browse**.

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

5 Click **Import**.

Add some predefined selections for the geometric entities which will be referenced later on.

DEFINITIONS

Explicit 1

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

2 In the **Model Builder** window, right-click **Explicit 1** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Walls` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundaries 6, 8, 35–38, 44, 45, and 51–56 only.

Explicit 2

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

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

3 In the **Rename Explicit** dialog box, type `Coils` in the **New label** text field.

4 Click **OK**.

5 Select Domains 6 and 8–11 only.

Explicit 3

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

2 In the **Model Builder** window, right-click **Explicit 3** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Coil Boundaries` in the **New label** text field.

4 Click **OK**.

5 Select Domains 6 and 8–11 only.

6 In the **Settings** window for **Explicit**, locate the **Output Entities** section.

7 From the **Output entities** list, choose **Adjacent boundaries**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Psp	1500[W]	1500 W	Power input
mueN	4E24[1/(m*V*s)]	4E24 1/(V·m·s)	Reduced electron mobility
T0	300[K]	300 K	Gas temperature
p0	0.02[torr]	2.666 Pa	Gas pressure

PLASMA (PLAS)

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

2 Select Domain 3 only.

Cross Section Import 1

1 Right-click **Component 1 (comp1)>Plasma (plas)** 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`.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Plasma Properties** section.

7 Select the **Use reduced electron transport properties** check box.

Now you add two more regular reactions which describe how electronically excited Argon atoms are consumed on the volumetric level. The rate coefficients for these reactions are taken from the literature.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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 `3.734E8`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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`.

When solving any type of reacting flow problem there always needs to be one species which is selected to fulfill the mass constraint. This should be taken as the species with the largest mass fraction.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar**.

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

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

When solving a plasma problem the plasma must be initially charge neutral. COMSOL automatically computes the initial concentration of a selected ionic species such that the

initial electroneutrality constraint is satisfied. Once the simulation begins to timestep, the plasma need not be charge neutral. In fact, the separation of space charge between the ions and electrons close to the wall is a critical component in sustaining the discharge.

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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.

Initial conditions for the electron number density and mean electron energy are critical for any plasma model. If the initial electron density is too low then the plasma may not be able to sustain itself and may self extinguish. If the initial electron density is too high then convergence problems may occur during initial timesteps.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E15`.

4 In the ε_0 text field, type `5`.

The **Magnetic Fields** are computed everywhere except the wafer and the wafer pedestal.

MAGNETIC FIELDS (MF)

On the **Physics** toolbar, click **Plasma (plas)** and choose **Magnetic Fields (mf)**.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Magnetic Fields (mf)**.

2 Select Domains 3–6 and 8–12 only.

The **Coil** feature is used to electrically excite the system. The coil operates with a fixed total power of 1500 watts.

Coil 1

1 In the **Model Builder** window, right-click **Magnetic Fields (mf)** and choose the domain setting **Coil**.

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

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

4 Locate the **Coil** section. From the **Coil excitation** list, choose **Power**.

5 Select the **Coil group** check box.

6 In the P_{coil} text field, type `Psp`.

PLASMA (PLAS)

Plasma Model 1

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

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

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

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

5 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `mueN`.

Next, define the material properties. There is no need to define the material properties in the plasma domain, as these are defined by the **Plasma Conductivity Coupling** feature.

MATERIALS

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 **Geometric Entity Selection** section.

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

4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Electrical conductivity	sigma	6e7	S/m	Basic
Relative permittivity	epsilonr	1	1	Basic
Relative permeability	mur	1	1	Basic

Material 2 (mat2)

1 Right-click **Materials** and choose **Blank Material**.

2 Select Domain 5 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	I	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	1	I	Basic

Material 3 (mat3)

1 Right-click **Materials** and choose **Blank Material**.

2 Select Domains 4 and 12 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	I	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	4.2	I	Basic

PLASMA (PLAS)

Surface reactions must always be included in a plasma model since they describe how ionic, excited and radical species interact with the wall.

Surface Reaction 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

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 **Boundary Selection** section. From the **Selection** list, choose **Walls**.

Surface Reaction 2

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>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 **Boundary Selection** section. From the **Selection** list, choose **Walls**.

Now, add boundary conditions to describe how the electrons interact with the wall.

Wall 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

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

3 In the r_e text field, type `0.2`.

4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

Ground 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

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

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

MESH 1

Meshing is a critical step in any plasma model. Boundary layer meshing on the reactor walls is nearly always necessary. This is needed to capture the separation of space charge between the electrons and ions close to the wall. You also add a fine mesh in the coil domains since the skin depth needs to be resolved.

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

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

3 From the **Element size** list, choose **Finer**.

Edge 1

1 Right-click **Component 1 (comp1)>Mesh 1** and choose **More Operations>Edge**.

2 Select Boundaries 6, 8, 44, 45, and 54 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Entire geometry**.

4 Locate the **Element Size** section. Click the **Custom** button.

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

6 In the associated text field, type `1E-3`.

Free Triangular 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

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

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

4 Select Domain 3 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>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 **Model Builder** window, right-click **Mesh 1** and choose **Boundary Layers**.

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

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

4 Select Domain 3 only.

Boundary Layer Properties

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Boundary Layers 1** click **Boundary Layer Properties**.

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

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

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

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

Mapped 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Mapped**.

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

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

4 From the **Selection** list, choose **Coils**.

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1>Mapped 1** and choose **Distribution**.

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

3 From the **Selection** list, choose **Coil Boundaries**.

4 Locate the **Distribution** section. From the **Distribution properties** list, choose **Predefined distribution type**.

5 In the **Number of elements** text field, type `25`.

6 In the **Element ratio** text field, type `20`.

7 From the **Distribution method** list, choose **Geometric sequence**.

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

9 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

10 In the **Settings** window for **Mesh**, click **Build All**.

STUDY 1

Step 1: Frequency-Transient

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

2 In the **Times** text field, type `0 10^{range(-8,5/20,-3)}`.

3 In the **Frequency** text field, type `13.56E6`.

4 On the **Home** toolbar, click **Compute**.

RESULTS

Electron Density (plas)

Click the **Zoom Extents** button on the **Graphics** toolbar.

Electron Temperature (plas)

Click the **Zoom Extents** button on the **Graphics** toolbar.

Electric Potential (plas)

1 Click the **Zoom Extents** button on the **Graphics** toolbar.

Now add a global plot for the coil resistance. This is defined as the real part of the total voltage drop over the coil divided by the applied current. The **Coil** feature creates predefined expressions for the resistance.

1D Plot Group 6

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

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

3 Locate the **Plot Settings** section. Select the **x-axis label** check box.

4 In the associated text field, type `Time (s)`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `Coil resistance (Ohm)`.

Global 1

1 Right-click **Coil Resistance** 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
`mf.RCoil_1`	Ω	`Coil resistance`

4 Click the **x-Axis Log Scale** button on the **Graphics** toolbar.

5 On the **Coil Resistance** toolbar, click **Plot**.

Now verify that 1500 watts is being applied to the system.

1D Plot Group 7

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

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

3 Locate the **Plot Settings** section. Select the **x-axis label** check box.

4 In the associated text field, type `Time (s)`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `Power (W)`.

Global 1

1 Right-click **Coil Power** 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
`mf.PCoil_1`	`W`	`Coil power`

4 Click the **x-Axis Log Scale** button on the **Graphics** toolbar.

5 On the **Coil Power** toolbar, click **Plot**.

2D Plot Group 8

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

2 In the **Settings** window for **2D Plot Group**, type `Ion Number Density` in the **Label** text field.

Surface 1

1 Right-click **Ion Number Density** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Number densities>plas.n_wAr_1p - Number density**.

3 On the **Ion Number Density** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Ion Number Density 1

1 In the **Model Builder** window, under **Results** right-click **Ion Number Density** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `High Frequency Electric Field` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>High Frequency Electric Field** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Magnetic Fields>Electric> mf.normE - Electric field norm**.

3 On the **High Frequency Electric Field** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Observe that the electric field is slightly shielded by the plasma. This is due to the skin effect in the plasma. As the electron number density increases, the plasma tends to shield itself from the electric field.

High Frequency Electric Field 1

1 In the **Model Builder** window, under **Results** right-click **High Frequency Electric Field** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Excited Argon Number Density` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Excited Argon Number Density** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Number densities>plas.n_wArs - Number density**.

3 On the **Excited Argon Number Density** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

2D Plot Group 11

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

2 In the **Settings** window for **2D Plot Group**, type `Power Deposition` in the **Label** text field.

Surface 1

1 Right-click **Power Deposition** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Magnetic Fields> Heating and losses>mf.Qrh - Volumetric loss density, electric**.

Selection 1

1 In the **Model Builder** window, right-click **Surface 1** and choose **Selection**.

2 Select Domain 3 only.

3 On the **Power Deposition** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

The effect of the shielding of the electric field due to the skin depth of the plasma is also apparent when plotting the power deposition.

Argon Boltzmann Analysis

Introduction

The electron energy distribution function (EEDF) plays an important role in the overall behavior of discharges. Analytic forms of the EEDF exist such as Maxwellian or Druyvesteyn, but in some cases they fail to fit the discharge physics. Factors such as ionization degree (n_e/N), mole fraction of excited species, and reduced angular frequency of the electromagnetic field can all influence the shape of the EEDF. This can lead to differences in the magnitude of electron impact rate coefficients which are in turn used in a fluid model for the electron density and mean electron energy. This tutorial example shows how these factors influence the EEDF and the rate coefficients for argon.

Model Definition

This model is based on the results obtained in Ref 1. In this model, the x-coordinate represents electron energy, ε (eV), rather than physical space. First a set of electron impact collision cross sections are read from a file. The first time the model is solved, the EEDF is assumed to be Maxwellian:

$$f(\varepsilon) = \varphi^{-3/2}\beta_1 \exp(-(\varepsilon\beta_2/\varphi))$$

where

$$\beta_1 = \Gamma(5/2)^{3/2}\Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2)\Gamma(3/2)^{-1}$$

Subsequently, the Two-term Boltzmann equation is solved which computes the EEDF rather than assuming a specific form. The Two-term Boltzmann equation is:

$$\frac{\partial}{\partial\varepsilon}\left(Wf - D\frac{\partial f}{\partial\varepsilon}\right) = S$$

where f is the EEDF ($\mathrm{eV}^{-3/2}$) and

$$W = -\gamma\varepsilon^2\sigma_\varepsilon - 3a\left(\frac{n_e}{N_n}\right)A_1 \tag{1}$$

and

$$D = \frac{\gamma}{3}\left(\frac{E}{N_n}\right)^2\left(\frac{\varepsilon}{\sigma_m}\right) + \frac{\gamma k_b T}{q}\varepsilon^2\sigma_\varepsilon + 2a\left(\frac{n_e}{N_n}\right)(A_2 + \varepsilon^{3/2}A_3) \tag{2}$$

For definitions of the quantities in the equations Equation 1 and Equation 2, see the chapter The Boltzmann Equation, Two-Term Approximation Interface in the *Plasma Module User's Guide*.

At zero energy, the condition that energy flux is zero must hold:

$$\mathbf{n} \cdot \left(Wf - D\frac{\partial f}{\partial \varepsilon} \right) = 0$$

and as $\varepsilon \to \infty, f \to 0$. In practice, this boundary condition is applied by setting f to zero for a suitably large ε. The default maximum ε is 100 eV by default.

Results and Discussion

Solving the Boltzmann equation allows various conditions for ionization degree, mole fraction of excited species and reduced angular frequencies to be tested.

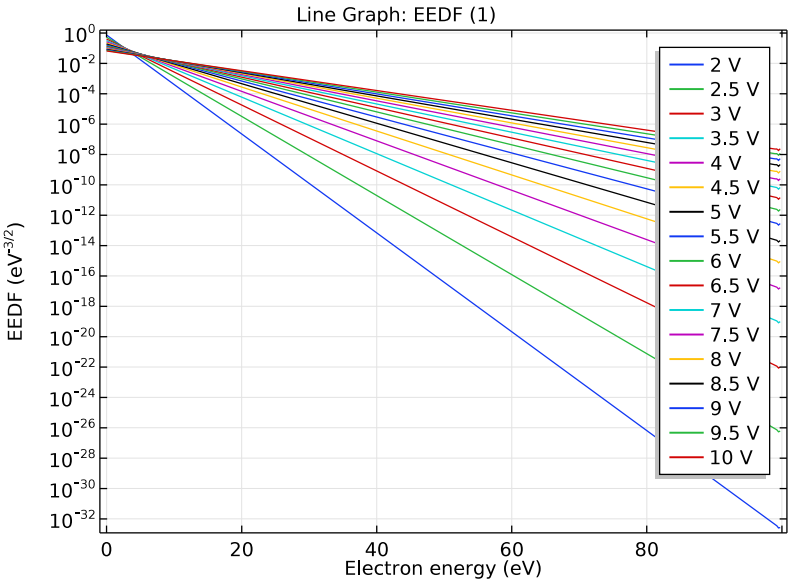

Figure 1: Maxwellian EEDF for a range of different mean electron energies.

Figure 1 shows the distribution function assuming Maxwellian. Electron-electron collisions tend to make the shape of the EEDF closer to a Maxwellian distribution. The

influence of different degrees of ionization is shown in Figure 2.

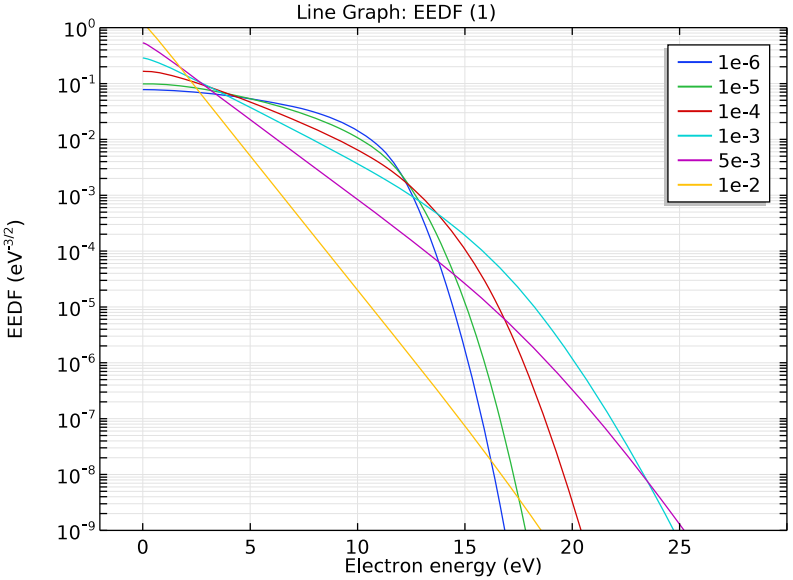

Figure 2: EEDF in argon for an applied reduced electric field of 10 Td for different degrees of ionization.

As the ionization degree increases, the EEDF tends to become more Maxwellian (which would be represented by a linear line on a log scale). The electron-electron collisions tend to push the electrons at the tail to higher energies, which has an effect on the rate coefficients for electron impact reactions with a high activation energy.

The effect on the rate coefficients can be seen in Figure 3. The ionization rate coefficient is substantially higher at a given mean electron energy when the ionization degree is higher.

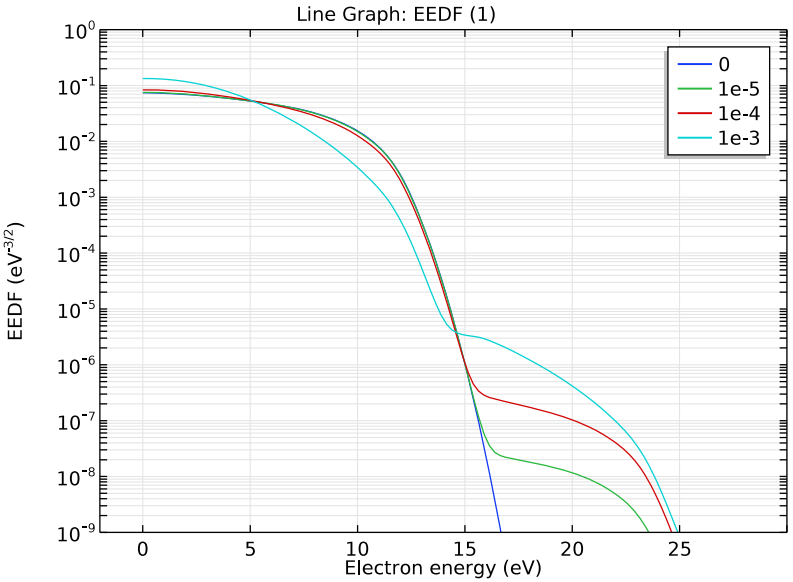

Figure 3: Plot of ionization rate coefficient versus mean electron energy for different ionization degrees.

If the mole fraction of electronically excited species is non zero then superelastic collisions can influence the shape of the EEDF. Figure 4 plots the EEDF for different mole fractions of electronically excited argon. The superelastic collisions leads to a high energy tail in the distribution function. This results in an increase in the magnitude of the ionization rate coefficients.

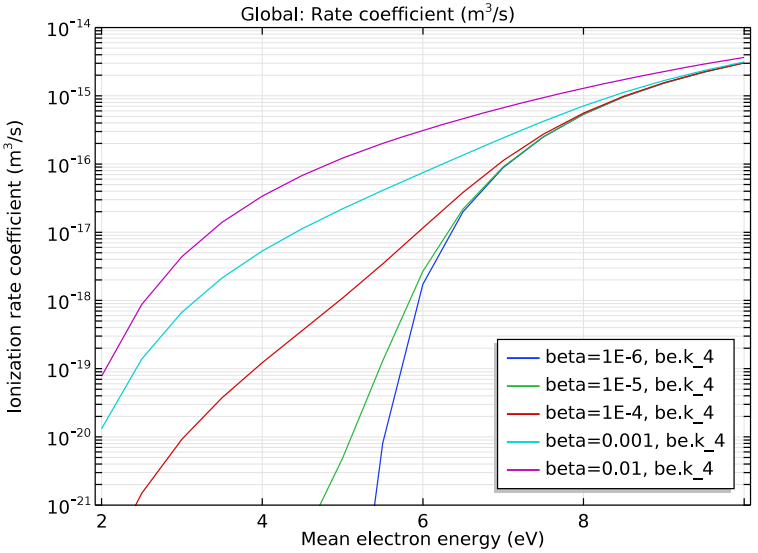

Figure 4: EEDF for argon at a reduced electric field of 10 Td for different mole fractions of electronically excited argon.

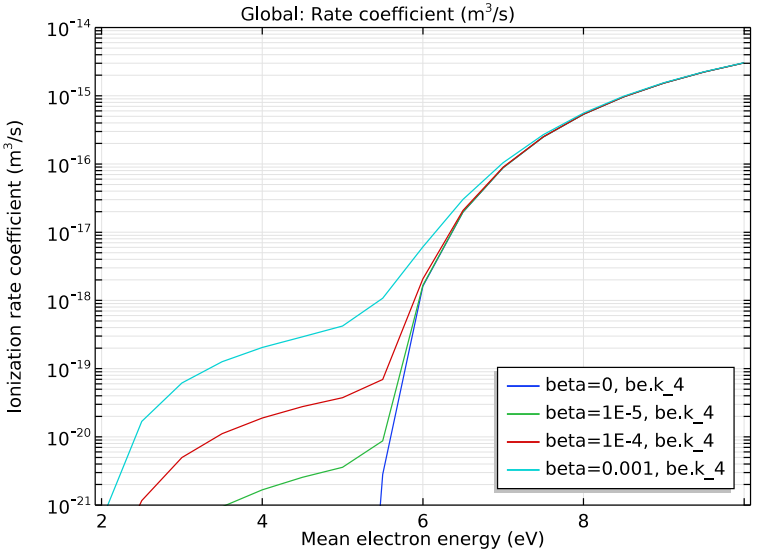

Figure 5: Ionization rate coefficient for different mole fractions of electronically excited argon.

Finally, the influence of a high frequency oscillating field on the EEDF is studied by applying different reduced angular frequencies. The EEDF is plotted in Figure 6.

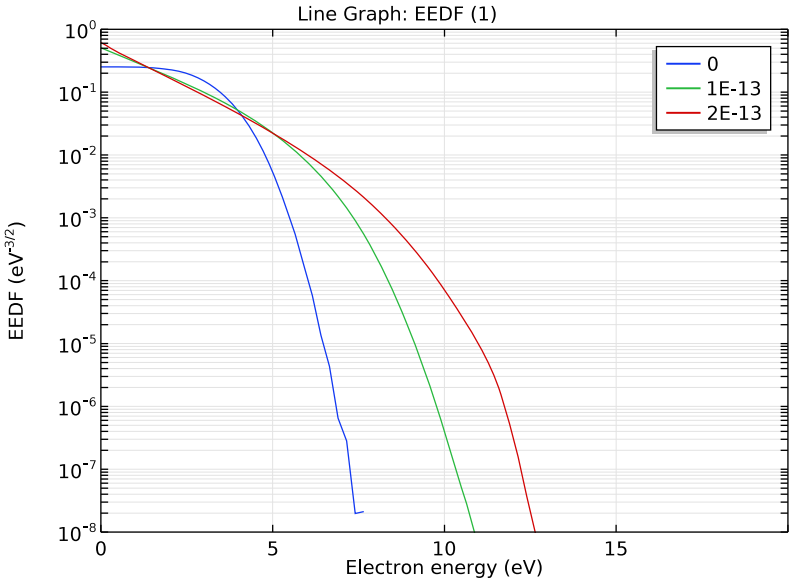

Figure 6: Plot of EEDF for different reduced angular frequencies for the same mean electron energy.

Reference

1. G.J.M. Hagelaar and L.C. Pitchford, "Solving the Boltzmann Equation to Obtain Electron Transport Coefficients and Rate Coefficients for Fluid Models," *Plasma Sources Science and Technology*, vol. 14, pp. 722–733, 2005.

Application Library path: `Plasma_Module/Two-Term_Boltzmann_Equation/boltzmann_argon`

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 **1D**.

2 In the **Select Physics** tree, select **Plasma>Boltzmann Equation, Two-Term Approximation (be)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Mean Energies**.

6 Click **Done**.

GLOBAL DEFINITIONS

Begin by defining beta, the ionization degree, as a global parameter. This makes it available for selection as a parameter in a parametric sweep.

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
beta	1e-6	1E-6	Ionization degree

GEOMETRY 1

Notice that the geometry and mesh are automatically generated for this physics interface and they very rarely need to be changed.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Boltzmann Equation, Two-Term Approximation (be)**.

2 In the **Settings** window for **Boltzmann Equation, Two-Term Approximation**, 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`.

Zero Probability 1

1 Right-click **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** and choose **Zero Probability**.

2 Select Boundary 2 only.

Zero Energy Flux 1

1 In the **Model Builder** window, right-click **Boltzmann Equation, Two-Term Approximation (be)** and choose **Zero Energy Flux**.

2 Select Boundary 1 only.

STUDY 1

Step 1: Mean Energies

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Mean Energies**.

2 In the **Settings** window for **Mean Energies**, locate the **Study Settings** section.

3 In the **Mean energies** text field, type `range(2,0.5,10)`.

4 On the **Home** toolbar, click **Compute**.

RESULTS

EEDF (be)

1 In the **Model Builder** window, click **EEDF (be)**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Axis** section.

3 Click the **Zoom Extents** button on the **Graphics** toolbar.

4 On the **EEDF (be)** toolbar, click **Plot**.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Boltzmann Equation, Two-Term Approximation (be)**.

2 In the **Settings** window for **Boltzmann Equation, Two-Term Approximation**, locate the **Electron Energy Distribution Function Settings** section.

3 From the **Electron energy distribution function** list, choose **Boltzmann**.

4 Locate the **Boltzmann Properties** section. From the **Electron-electron collisions** list, choose **On**.

Now parameterize the ionization degree of the argon.

Boltzmann Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** click **Boltzmann Model 1**.

2 In the **Settings** window for **Boltzmann Model**, locate the **Mole Fraction Settings** section.

3 In the x_{Ar} text field, type `1`.

4 In the x_{Ars} text field, type `0`.

5 Locate the **Boltzmann Settings** section. In the β text field, type `beta`.

6 In the n_e text field, type `1E18`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the E/N_0 text field, type `10[Td]`.

ADD STUDY

1 On 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> Reduced Electric Fields**.

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

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

STUDY 2

Step 1: Reduced Electric Fields

1 In the **Model Builder** window, under **Study 2** click **Step 1: Reduced Electric Fields**.

2 In the **Settings** window for **Reduced Electric Fields**, locate the **Study Settings** section.

3 In the **Reduced electric fields** text field, type `10[Td]`.

4 Click to expand the **Study extensions** section. Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
beta	`1e-6 1e-5 1e-4 1e-3 5e-3 1e-2`	

7 On the **Home** toolbar, click **Compute**.

RESULTS

EEDF (be) 1

1 In the **Model Builder** window, under **Results** click **EEDF (be) 1**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Axis** section.

3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `-2`.

5 In the **x maximum** text field, type `30`.

6 In the **y minimum** text field, type `10^(-9)`.

7 In the **y maximum** text field, type `1`.

Line Graph 1

1 In the **Model Builder** window, expand the **EEDF (be) 1** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click to expand the **Legends** section.

3 From the **Legends** list, choose **Manual**.

4 In the table, enter the following settings:

Legends
1e-6
1e-5
1e-4
1e-3
5e-3
1e-2

5 On the **EEDF (be) 1** toolbar, click **Plot**.

Now parameterize the mole fraction of excited argon atoms.

ADD STUDY

1 On 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> Reduced Electric Fields**.

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

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

STUDY 3

Step 1: Reduced Electric Fields

1 In the **Model Builder** window, under **Study 3** click **Step 1: Reduced Electric Fields**.

2 In the **Settings** window for **Reduced Electric Fields**, locate the **Study Settings** section.

3 In the **Reduced electric fields** text field, type `10[Td]`.

4 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
beta	`0 1e-5 1e-4 1e-3`	

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

Boltzmann Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** click **Boltzmann Model 1**.

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

3 In the β text field, type `0`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} text field, type `1-beta`.

5 In the x_{Ars} text field, type `beta`.

STUDY 3

On the **Home** toolbar, click **Compute**.

RESULTS

EEDF (be) 2

1 In the **Model Builder** window, click **EEDF (be) 2**.

2 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `-2`.

5 In the **x maximum** text field, type `30`.

6 In the **y minimum** text field, type `10^(-9)`.

7 In the **y maximum** text field, type 1.

Line Graph 1

1 In the **Model Builder** window, expand the **EEDF (be) 2** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **Legends** section.

3 From the **Legends** list, choose **Manual**.

4 In the table, enter the following settings:

Legends
0
1e-5
1e-4
1e-3

5 On the **EEDF (be) 2** toolbar, click **Plot**.

Now use the parametric sweep feature to compute the rate coefficients over a wide range of mean electron energies for different degrees of ionization.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

Boltzmann Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** click **Boltzmann Model 1**.

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

3 In the β text field, type `beta`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} text field, type 1.

5 In the x_{Ars} text field, type 0.

ADD STUDY

1 On 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>Mean Energies**.

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

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

STUDY 4

Step 1: Mean Energies

1 In the **Model Builder** window, under **Study 4** click **Step 1: Mean Energies**.

2 In the **Settings** window for **Mean Energies**, locate the **Study Settings** section.

3 In the **Mean energies** text field, type `range(2,0.5,10)`.

Parametric Sweep

1 On 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
beta	`1e-6 1e-5 1e-4 1e-3 1e-2`	

5 In the **Model Builder** window, click **Study 4**.

6 In the **Settings** window for **Study**, locate the **Study Settings** section.

7 Clear the **Generate default plots** check box.

8 On the **Study** toolbar, click **Compute**.

RESULTS

1D Plot Group 10

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

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Data set** list, choose **Study 4/Parametric Solutions 1 (sol5)**.

Global 1

1 Right-click **1D Plot Group 10** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Boltzmann Equation, Two-Term Approximation>Rate coefficients>be.k_4 - Rate coefficient**.

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

4 Click to expand the **Legends** section. Find the **Include** subsection. Select the **Expression** check box.

5 Clear the **Description** check box.

6 On the **1D Plot Group 10** toolbar, click **Plot**.

1D Plot Group 10

1 In the **Model Builder** window, under **Results** click **1D Plot Group 10**.

2 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

3 Select the **y-axis log scale** check box.

4 Click to expand the **Legend** section. From the **Position** list, choose **Lower right**.

5 On the **1D Plot Group 10** toolbar, click **Plot**.

6 Locate the **Plot Settings** section. Select the **x-axis label** check box.

7 In the associated text field, type `Mean electron energy (eV)`.

8 Select the **y-axis label** check box.

9 In the associated text field, type `Ionization rate coefficient (m<sup>3</sup>/s)`.

10 Locate the **Axis** section. Select the **Manual axis limits** check box.

11 In the **y minimum** text field, type `10^(-21)`.

12 In the **y maximum** text field, type `10^(-14)`.

13 On the **1D Plot Group 10** toolbar, click **Plot**.

Next, use the parametric sweep feature to compute the rate coefficients over a wide range of mean electron energies for different mole fractions of excited argon

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

Boltzmann Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** click **Boltzmann Model 1**.

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

3 In the β text field, type `0`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} text field, type `1-beta`.

5 In the x_{Ars} text field, type `beta`.

ADD STUDY

1 On 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>Mean Energies**.

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

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

STUDY 5

Step 1: Mean Energies

1 In the **Model Builder** window, under **Study 5** click **Step 1: Mean Energies**.

2 In the **Settings** window for **Mean Energies**, locate the **Study Settings** section.

3 In the **Mean energies** text field, type `range(2,0.5,10)`.

4 Click to expand the **Study extensions** section.

Parametric Sweep

1 On 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
beta	`0 1e-5 1e-4 1e-3`	

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

6 In the **Settings** window for **Study**, locate the **Study Settings** section.

7 Clear the **Generate default plots** check box.

8 On the **Study** toolbar, click **Compute**.

RESULTS

1D Plot Group 11

1 In the **Model Builder** window, under **Results** right-click **1D Plot Group 10** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Data set** list, choose **Study 5/Parametric Solutions 2 (sol12)**.

4 On the **1D Plot Group 11** toolbar, click **Plot**.

Finally, compute the EEDF for a mean electron energy of 2.15 eV for different reduced angular frequencies.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Boltzmann Equation, Two-Term Approximation (be)**.

2 In the **Settings** window for **Boltzmann Equation, Two-Term Approximation**, locate the **Boltzmann Properties** section.

3 From the **Oscillating field** list, choose **On**.

Boltzmann Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** click **Boltzmann Model 1**.

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

3 In the ω/N text field, type `beta`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} text field, type `1`.

5 In the x_{Ars} text field, type `0`.

ADD STUDY

1 On 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>Mean Energies**.

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

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

STUDY 6

Step 1: Mean Energies

1 In the **Model Builder** window, under **Study 6** click **Step 1: Mean Energies**.

2 In the **Settings** window for **Mean Energies**, locate the **Study Settings** section.

3 In the **Mean energies** text field, type `2.15`.

Parametric Sweep

1 On 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
beta	`0 1e-13 2e-13`	

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

RESULTS

EEDF (be) 3

1. Click the **Zoom Extents** button on the **Graphics** toolbar.
2. In the **Model Builder** window, click **EEDF (be) 3**.
3. In the **Settings** window for **1D Plot Group**, locate the **Axis** section.
4. Select the **Manual axis limits** check box.
5. In the **x minimum** text field, type `0`.
6. In the **x maximum** text field, type `20`.
7. In the **y minimum** text field, type `10^(-8)`.
8. In the **y maximum** text field, type `1`.
9. On the **EEDF (be) 3** toolbar, click **Plot**.

Oxygen Boltzmann Analysis

Introduction

The Boltzmann equation can be solved to validate sets of electron impact collision cross sections. In fact, sets of collision cross sections are traditionally inferred by solving a two-term approximation to the Boltzmann equation and comparing the results to swarm experiments. This model solves a two-term approximation to the Boltzmann equation and compares the computed drift velocity and electron temperature to experimental data.

Model Definition

The model uses molecular oxygen as the gas. For molecular oxygen, the model considers the following set of electron impact collisions:

TABLE 1: TABLE OF COLLISIONS

REACTION	FORMULA	TYPE	$\Delta\varepsilon$ (eV)
1	e+O2=>e+O2	Momentum	0
2	e+O2=>O+O	Attachment	0
3	e+O2=>e+O2(rot)	Excitation	0.02
4	e+O2=>e+O2(v=1)	Excitation	0.19
5	e+O2=>e+O2(v=1)	Excitation	0.19
6	e+O2=>e+O2(v=2)	Excitation	0.38
7	e+O2=>e+O2(v=2)	Excitation	0.38
8	e+O2=>e+O2(v=3)	Excitation	0.75
9	e+O2=>e+O2(v=3)	Excitation	0.75
10	e+O2=>e+O2(a1d)	Excitation	0.977
11	e+O2(a1d)=>e+O2	Superelastic	-0.977
12	e+O2=>e+O2(b1s)	Excitation	1.627
13	e+O2(b1s)=>e+O2	Superelastic	-1.627
14	e+O2=>e+O2(45)	Excitation	4.5
15	e+O2(45)=>e+O2	Superelastic	-4.5
16	e+O2=>e+O+O	Dissociation	6.0
17	e+O2=>e+O+O(1D)	Dissociation	8.4
18	e+O2=>e+O+O(1S)	Dissociation	9.97
19	e+O2=>e+O2+	Ionization	12.06

In a superelastic collision, the electrons gain energy from excited species. The mole fraction of each species is given in the table below and is estimated from typical discharge conditions that occur in a drift tube. The degree of ionization is 10^{-6}.

TABLE 2: TABLE OF MOLE FRACTIONS OF EACH SPECIES

SPECIES	MOLE FRACTION
O2	0.99997
O2(a1d)	1.5E-5
O2(b1s)	1E-5
O2(45)	5E-6

The Two-term Boltzmann equation is solved which computes the EEDF rather than assuming a specific form. The two-term approximation of the Boltzmann equation is:

$$\frac{\partial}{\partial \varepsilon}\left(Wf - D\frac{\partial f}{\partial \varepsilon}\right) = S$$

where f is the EEDF ($\mathrm{eV}^{-3/2}$) and

$$W = -\gamma\varepsilon^2\sigma_\varepsilon - 3a\left(\frac{n_e}{N_n}\right)A_1 \tag{1}$$

and

$$D = \frac{\gamma}{3}\left(\frac{E}{N_n}\right)^2\left(\frac{\varepsilon}{\sigma_m}\right) + \frac{\gamma k_b T}{q}\varepsilon^2\sigma_\varepsilon + 2a\left(\frac{n_e}{N_n}\right)(A_2 + \varepsilon^{3/2}A_3) \tag{2}$$

For definitions of the quantities in the equations Equation 1 and Equation 2, see the chapter The Boltzmann Equation, Two-Term Approximation Interface in the *Plasma Module User's Guide*.

At zero energy, the condition that energy flux is zero must hold:

$$\mathbf{n}\cdot\left(Wf - D\frac{\partial f}{\partial \varepsilon}\right) = 0$$

and as $\varepsilon \to \infty, f \to 0$. In practice, this boundary condition is applied by setting f to zero for a suitably large ε. The default maximum ε is 100 eV by default.

When the Boltzmann equation has been the drift velocity and electron "temperature" for a given reduced electric field can be compared to experimental results. The drift velocity is defined as:

$$w = -\left(\frac{\gamma}{3}\right)\left|\left(\frac{E}{N_n}\right)\right|\int_0^\infty \frac{\varepsilon}{\sigma_m}\left(\frac{\partial f}{\partial \varepsilon}\right)d\varepsilon$$

which is linear in the reduced electric field by has a rather complicated integral dependence on the EEDF. The electron "temperature" is simply two thirds of the mean electron energy which is defined as:

$$\bar{\varepsilon} = \int_0^\infty f\varepsilon^{3/2}d\varepsilon$$

The experimental data comes from Ref. 2.

Results and Discussion

The two-term approximation to the Boltzmann equation is solved by parametrically varying the mean electron energy. This parametric analysis allows the EEDF to be plotted for different mean electron energies. Figure 1 plots the EEDF for different values of the mean electron energy. The mean electron energy has its lowest value indicated by the blue line on the left of the plot, corresponding to a mean electron energy of 2 electron volts. At such a low energy the population of electrons with energy above the ionization threshold is very low. As the mean electron energy increases, the population of electrons with higher energy increases. This makes ionization processes more likely. Ionization is important as it is usually the primary mechanism for sustaining plasmas. Notice also that

the EEDF is not linear on the log scale. This indicates that the EEDF is non-Maxwellian under these conditions.

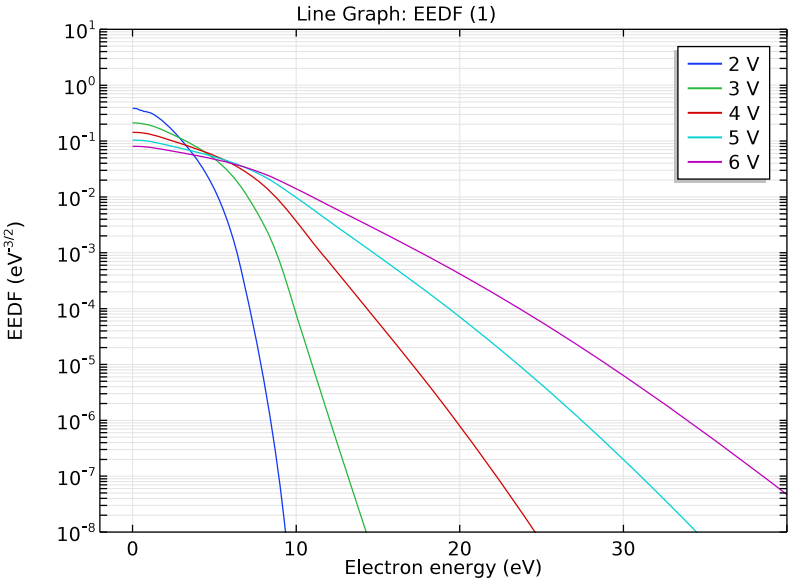

Figure 1: Plot of the EEDF for different values of the mean electron energy.

The reduced electron transport properties are plotted in Figure 2. The transport properties have a much weak dependence on the EEDF compared to rate or Townsend coefficients. The electron mobility and electron energy mobility decrease as the mean electron energy increases. The electron diffusivity and electron energy diffusivity increase as the mean electron energy increases. If the EEDF was Maxwellian then the following relations would hold:

$$D_e = \mu_e T_e, \mu_\varepsilon = \left(\frac{5}{3}\right)\mu_e, D_\varepsilon = \mu_\varepsilon T_e$$

In the case that the EEDF is non-Maxwellian, this relation does not necessarily hold true. The drift velocity of the electrons at a given mean electron energy or reduced electric field is an important parameter because it is easy to measure experimentally in drift tubes. Traditionally, the electron drift velocity is tabulated v.s. the reduced electric field (E/N). The simulated and experimental drift velocity is plotted in Figure 3 for a range of reduced electric fields. The agreement between the two is good over a wide range of reduced electric field, indicating that the cross section data is consistent with experimental measurements.

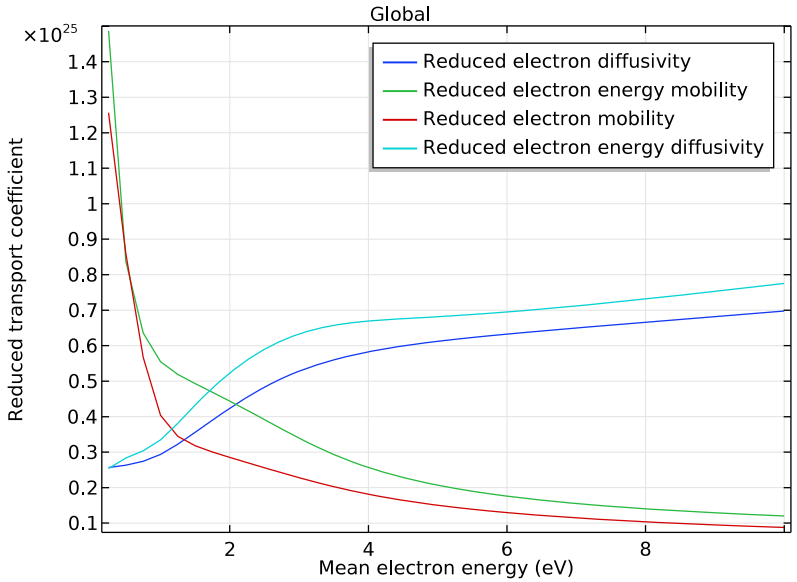

Figure 2: Reduced transport properties v.s. mean electron energy.

Another quantity which is relatively easy to measure experimentally is the ratio of the electron diffusivity and the mobility. The simulated and experimental ratio of the diffusivity and mobility is plotted in Figure 4. Einstein's relation dictates that this ratio is equal to the electron temperature when the EEDF is Maxwellian.

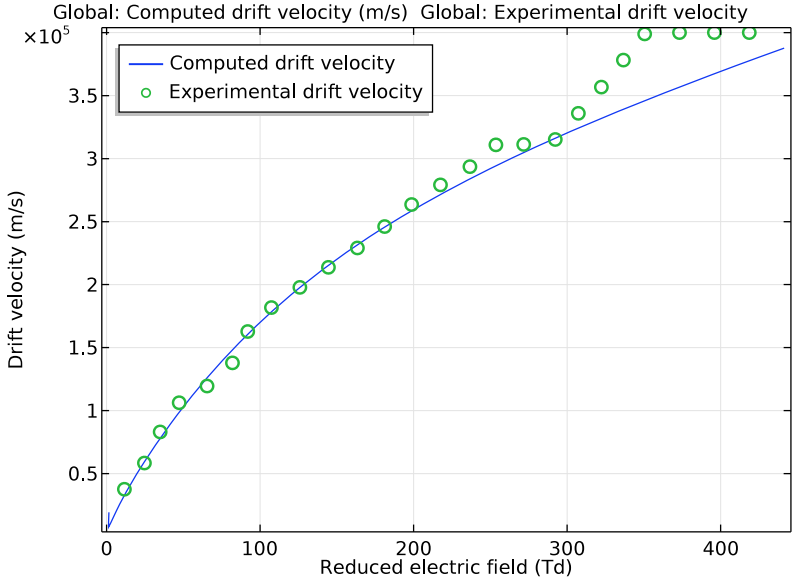

Figure 3: Computed and experimental drift velocity for oxygen.

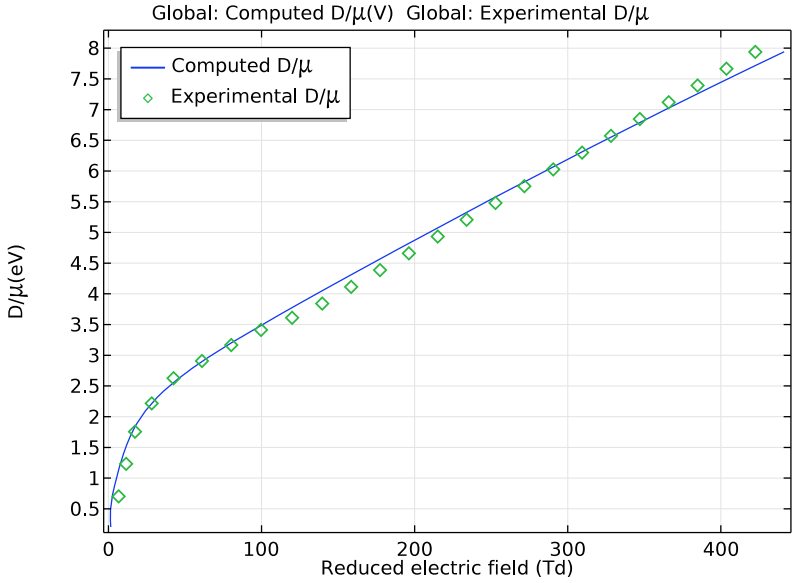

Figure 4: Computed and experimental D/μ for different reduced electric fields.

The fraction of power channeled into various reactions is shown in Figure 5. This is important in design of plasma sources because often the desired reactive species is known in advance. The plot gives an indication of what the target mean electron energy should be in order to channel as much of the available power into a specific reaction. Of course, the power channeled into ionization must be high enough to sustain the plasma.

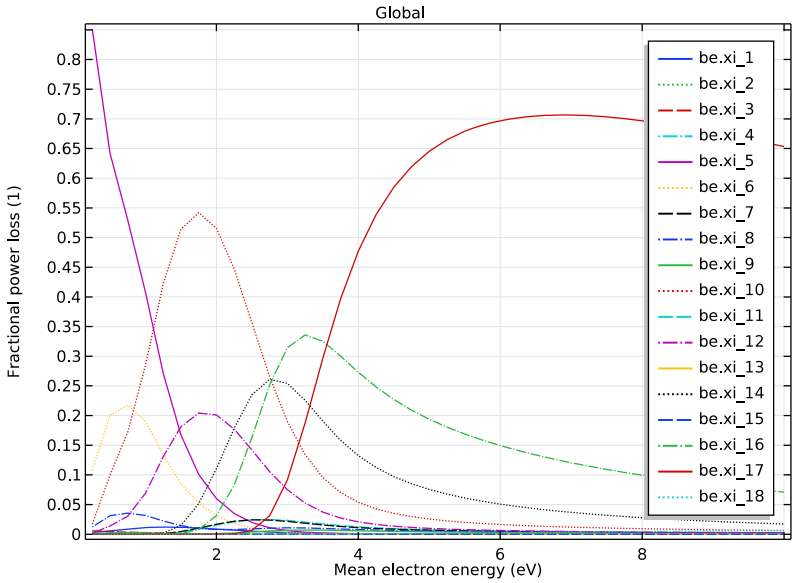

Figure 5: Plot of the fraction of the total power channeled into each reaction v.s. mean electron energy.

The Townsend coefficients are plotted in Figure 6. The Townsend coefficients offer an alternative way of defining reaction rates. The reaction rate depends on the electron flux rather than the electron density. Townsend coefficients should be used when modeling DC discharges.

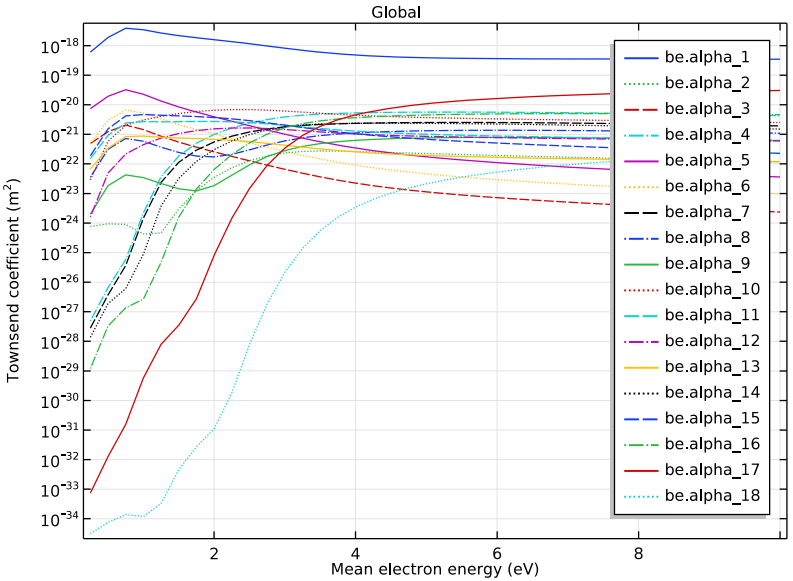

Figure 6: Townsend coefficients v.s. mean electron energy for oxygen.

References

1. G.J.M. Hagelaar and L.C. Pitchford, "Solving the Boltzmann Equation to Obtain Electron Transport Coefficients and Rate Coefficients for Fluid Models," *Plasma Sources Science and Technology*, vol. 14, pp. 722–733, 2005.

2. J. Dutton, "A Survey of Electron Swarm Data," *J. Phys. Chem. Ref. Data*, vol. 4, pp. 577–866, 1975.

Application Library path: `Plasma_Module/Two-Term_Boltzmann_Equation/boltzmann_oxygen`

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 **1D**.

2 In the **Select Physics** tree, select **Plasma>Boltzmann Equation, Two-Term Approximation (be)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Mean Energies**.

6 Click **Done**.

GEOMETRY 1

Notice that COMSOL generates the geometry and mesh for the **Boltzmann Equation, Two-Term Approximation** interface. The geometry and mesh almost never need to be modified.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Boltzmann Equation, Two-Term Approximation (be)**.

2 In the **Settings** window for **Boltzmann Equation, Two-Term Approximation**, locate the **Cross Section Import** section.

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `02_xsecs.txt`.

5 Locate the **Electron Energy Distribution Function Settings** section. From the **Electron energy distribution function** list, choose **Boltzmann**.

6 Locate the **Boltzmann Properties** section. From the **Electron-electron collisions** list, choose **On**.

Boltzmann Model 1

1 In the **Model Builder** window, expand the **Boltzmann Equation, Two-Term Approximation (be)** node, then click **Boltzmann Model 1**.

2 In the **Settings** window for **Boltzmann Model**, locate the **Mole Fraction Settings** section.

3 In the x_{O2a1d} text field, type `1.5E-5`.

4 In the x_{O245} text field, type `5E-6`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Boltzmann Equation, Two-Term Approximation (be)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the ε_0 text field, type `0.25`.

Zero Energy Flux 1

1 In the **Model Builder** window, right-click **Boltzmann Equation, Two-Term Approximation (be)** and choose **Zero Energy Flux**.

2 Select Boundary 1 only.

Zero Probability 1

1 Right-click **Boltzmann Equation, Two-Term Approximation (be)** and choose **Zero Probability**.

2 Select Boundary 2 only.

DEFINITIONS

Interpolation 1 (int1)

1 On the **Home** toolbar, click **Functions** and choose **Local>Interpolation**.

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

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `02_drift_velocity_expt.txt`.

6 Click **Import**.

7 Locate the **Units** section. In the **Arguments** text field, type `Td`.

8 In the **Function** text field, type `m/s`.

Interpolation 2 (int2)

1 On the **Home** toolbar, click **Functions** and choose **Local>Interpolation**.

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

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `02_Te_expt.txt`.

6 Click **Import**.

7 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

8 Locate the **Units** section. In the **Arguments** text field, type `Td`.

9 In the **Function** text field, type `V`.

STUDY 1

Step 1: Mean Energies

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Mean Energies**.

2 In the **Settings** window for **Mean Energies**, locate the **Study Settings** section.

3 In the **Mean energies** text field, type `range(0.25,0.25,10)`.

Solution 1 (sol1)

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

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

3 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Stationary Solver 1**.

4 In the **Settings** window for **Stationary Solver**, locate the **General** section.

5 From the **Linearity** list, choose **Nonlinear**.

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

RESULTS

EEDF (be)

1 In the **Model Builder** window, under **Results** click **EEDF (be)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Parameter selection (freq)** list, choose **From list**.

4 In the **Parameter values (freq (V))** list, choose **2**, **3**, **4**, **5**, and **6**.

5 Click to expand the **Axis** section. Select the **Manual axis limits** check box.

6 In the **x minimum** text field, type `-2`.

7 In the **x maximum** text field, type `40`.

8 In the **y minimum** text field, type `1e-8`.

9 In the **y maximum** text field, type `10`.

10 On the **EEDF (be)** toolbar, click **Plot**.

1D Plot Group 4

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

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Reduced electric field (Td)`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `Drift velocity (m/s)`.

7 Click to expand the **Legend** section. From the **Position** list, choose **Upper left**.

Global 1

1 Right-click **1D Plot Group 4** 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
`be.w`	`m/s`	`Computed drift velocity`

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 Locate the **x-axis data** section. Click **be.EN - Reduced electric field** in the upper-right corner of the section. Locate the **x-Axis Data** section. From the **Unit** list, choose **Td**.

6 On the **1D Plot Group 4** toolbar, click **Plot**.

Global 2

1 In the **Model Builder** window, under **Results** right-click **1D Plot Group 4** 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
`int1(be.EN)`		`Experimental drift velocity`

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 Locate the **x-axis data** section. Click **be.EN - Reduced electric field** in the upper-right corner of the section. Locate the **x-Axis Data** section. From the **Unit** list, choose **Td**.

6 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

7 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

8 In the **Number** text field, type `25`.

9 In the **Width** text field, type `3`.

10 On the **1D Plot Group 4** toolbar, click **Plot**.

1D Plot Group 5

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

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Reduced electric field (Td)`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `D/\mu (eV)`.

Global 1

1 Right-click **1D Plot Group 5** 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
`be.DeN/be.muN`	`Wb`	`Computed D/\mu`

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 Locate the **x-axis data** section. Click **be.EN - Reduced electric field** in the upper-right corner of the section. Locate the **x-Axis Data** section. From the **Unit** list, choose **Td**.

6 On the **1D Plot Group 5** toolbar, click **Plot**.

1D Plot Group 5

1 In the **Model Builder** window, under **Results** click **1D Plot Group 5**.

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

3 From the **Position** list, choose **Upper left**.

Global 2

1 Right-click **Results>1D Plot Group 5** 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
`int2(be.EN)`		`Experimental D/\mu`

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 Locate the **x-axis data** section. Click **be.EN - Reduced electric field** in the upper-right corner of the section. Locate the **x-Axis Data** section. From the **Unit** list, choose **Td**.

6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

7 Find the **Line markers** subsection. From the **Marker** list, choose **Diamond**.

8 In the **Number** text field, type `25`.

9 In the **Width** text field, type `3`.

10 On the **1D Plot Group 5** toolbar, click **Plot**.

1D Plot Group 6

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

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Mean electron energy (eV)`.

Global 1

1 Right-click **1D Plot Group 6** 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
be.xi_1	1	Fractional power loss
be.xi_2	1	Fractional power loss
be.xi_3	1	Fractional power loss
be.xi_4	1	Fractional power loss
be.xi_5	1	Fractional power loss
be.xi_6	1	Fractional power loss
be.xi_7	1	Fractional power loss
be.xi_8	1	Fractional power loss
be.xi_9	1	Fractional power loss
be.xi_10	1	Fractional power loss
be.xi_11	1	Fractional power loss
be.xi_12	1	Fractional power loss
be.xi_13	1	Fractional power loss
be.xi_14	1	Fractional power loss

Expression	Unit	Description
be.xi_15	1	Fractional power loss
be.xi_16	1	Fractional power loss
be.xi_17	1	Fractional power loss
be.xi_18	1	Fractional power loss

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

5 Click to expand the **Legends** section. Find the **Include** subsection. Select the **Expression** check box.

6 Clear the **Description** check box.

7 On the **1D Plot Group 6** toolbar, click **Plot**.

1D Plot Group 7

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

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Mean electron energy (eV)`.

5 Locate the **Axis** section. Select the **Manual axis limits** check box.

6 In the **x minimum** text field, type `-0.2375`.

7 In the **x maximum** text field, type `3`.

8 In the **y minimum** text field, type `1e-24`.

9 In the **y maximum** text field, type `4.052e-18`.

Global 1

1 Right-click **1D Plot Group 7** 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
be.alpha_1	m^2	Townsend coefficient
be.alpha_2	m^2	Townsend coefficient
be.alpha_3	m^2	Townsend coefficient
be.alpha_4	m^2	Townsend coefficient
be.alpha_5	m^2	Townsend coefficient
be.alpha_6	m^2	Townsend coefficient

Expression	Unit	Description
be.alpha_7	m^2	Townsend coefficient
be.alpha_8	m^2	Townsend coefficient
be.alpha_9	m^2	Townsend coefficient
be.alpha_10	m^2	Townsend coefficient
be.alpha_11	m^2	Townsend coefficient
be.alpha_12	m^2	Townsend coefficient
be.alpha_13	m^2	Townsend coefficient
be.alpha_14	m^2	Townsend coefficient
be.alpha_15	m^2	Townsend coefficient
be.alpha_16	m^2	Townsend coefficient
be.alpha_17	m^2	Townsend coefficient
be.alpha_18	m^2	Townsend coefficient

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

5 Locate the **Legends** section. Find the **Include** subsection. Select the **Expression** check box.

6 Clear the **Description** check box.

7 Click the **y-Axis Log Scale** button on the **Graphics** toolbar.

8 On the **1D Plot Group 7** toolbar, click **Plot**.

9 Click the **Zoom Extents** button on the **Graphics** toolbar.

Benchmark Model of a Capacitively Coupled Plasma

Introduction

The underlying physics of a capacitively coupled plasma is rather complicated, even for rather simple geometric configurations and plasma chemistries. This model benchmarks the COMSOL Multiphysics Plasma Module Capacitively Coupled Plasma interface against many different codes, the results of which are taken from Ref. 1.

Model Definition

The model geometry consists of a 1D gap of 0.067 m. A plasma forms in the gap provided the driving voltage and fill pressure are high enough. The driving frequency in this model is 13.56 MHz. Helium chemistry is used, as was the case in Ref. 1.

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/m^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $C^{1/2}/kg^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

In Ref. 1 the ion diffusivity is defined as:

$$D = 0.10901(a\lambda^3)^{\frac{1}{2}}$$

and the mobility, μ as:

$$\mu E = 0.79788(a\lambda)^{\frac{1}{2}}$$

where $a = qE/m$ and λ is the charge exchange mean free path. The same ion mobility and diffusivity models can be set in COMSOL. With that objective choose **Specify mobility, compute diffusivity** and **Use local field approximation** in the section **Mobility and Diffusivity Expressions** on the ion species node. After, go to the **Mobility Specification** and chose the **High field** ion mobility model with a **Cross section** σ equal to 3.10^{-19} m^2 to reproduce the same ion mobility and diffusivity as in Ref. 1.

BOUNDARY CONDITIONS

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the following boundary condition for the electron flux

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1-r}{1+r}\right)\left(\frac{1}{2}\nu_{e,\,\mathrm{th}} n_e\right) \tag{1}$$

and the electron energy flux

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{1-r}{1+r}\right)\left(\frac{5}{6}\nu_{e,\,\mathrm{th}} n_\varepsilon\right) \tag{2}$$

In order to make the COMSOL Multiphysics implementation of the electron losses to the wall consistent with the reference, the value of r must be set to $5/11$. The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the secondary electrons. For the helium ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

Surface charge accumulation is added to the dielectric surface by way of the following boundary condition:

$$\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

where ρ_s is the surface charge density, which is computed by solving the following distributed ODE on the surfaces:

$$\frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e$$

where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density at the wall, and $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density at the wall.

The discharge is driven by a sinusoidal total current applied to the exterior boundary of the dielectric plate:

$$I = I_0 \cos(\omega t)$$

where ω is the angular frequency. This boundary condition is not possible to implement directly — COMSOL Multiphysics requires that a voltage is specified on the driven electrode. In order to be able to apply a voltage to the driven electrode, a differential algebraic equation is added to the model. This differential algebraic equation then adjusts the voltage on the electrode at each time step such that the above current constraint is satisfied. The equation solved for the unknown electrode potential, V_{in}, is hence, in weak form:

$$\left(\frac{\partial D}{\partial t} - I_0 \cos(\omega t)\right) \overline{V}_{in} = 0$$

where the bar denotes test function. This is implemented as a bidirectional weak constraint in COMSOL Multiphysics.

PLASMA CHEMISTRY

The reference paper suggests a simplistic plasma chemistry for helium consisting of only 3 reactions and 4 species:

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon$(eV)
1	e+He=>e+He	Elastic	0
2	e+He=>e+Hes	Excitation	19.5
3	e+Hes=>e+He+	Ionization	24.5

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

TABLE 2: TABLE OF SURFACE REACTIONS.

REACTION	FORMULA	STICKING COEFFICIENT
1	Hes=>He	1
2	He+=>He	0

When a metastable helium atom makes contact with the wall, it reverts to the ground state helium atom with some probability (the sticking coefficient).

Results and Discussion

The time averaged ion current density is plotted in Figure 1. The peak ion current density occurs on the electrodes, at a value of around $0.2 A/m^2$. At lower pressures the ion current density profile is more smooth across the gap. At 300mtorr there is a pronounced flattening off of the ion current density in the plasma sheath. These results agree well with those presented in Figure 9 of Ref. 1.

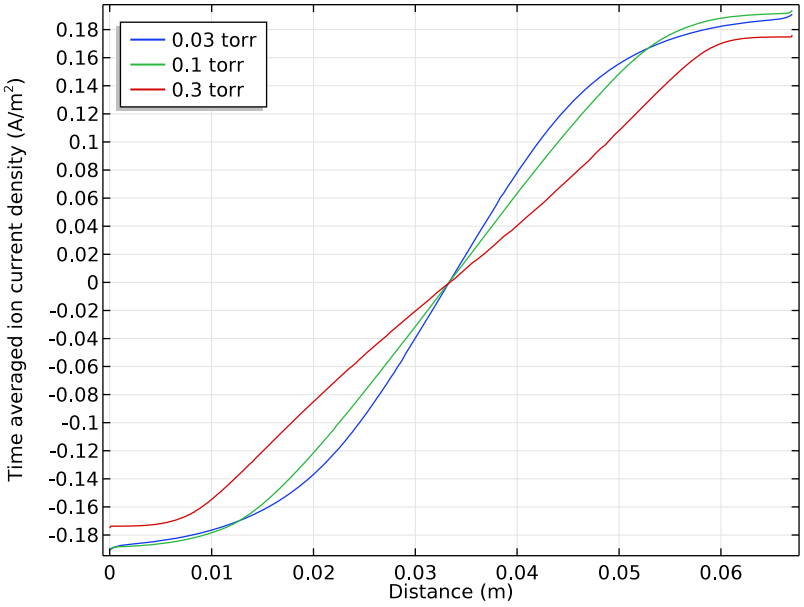

Figure 1: Plot of the time averaged ion current as a function of the distance from the left electrode.

The time averaged excitation and ionization rates are plotted in Figure 2 and Figure 3.

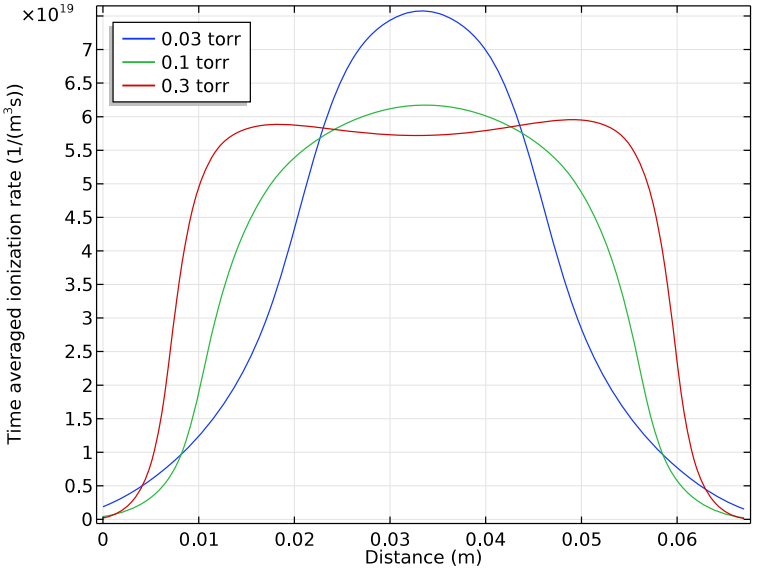

Figure 2: Plot of the time averaged ionization rate as a function of the distance from the left electrode.

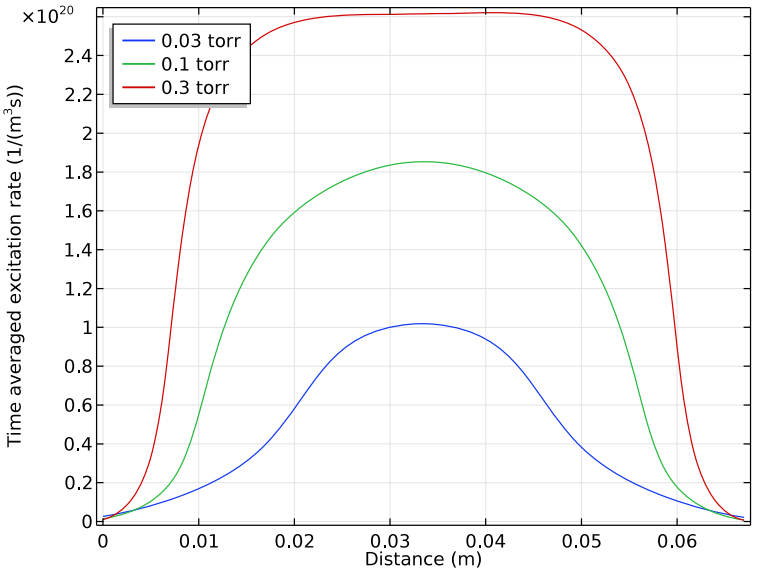

Figure 3: Plot of the time averaged excitation rate as a function of the distance from the left electrode.

The results for the ionization and excitation rates agree well with Ref. 1 in both absolute value and spatial distribution. The time averaged electron power deposition is plotted in Figure 4. The COMSOL results are again, in good agreement with the reference paper.

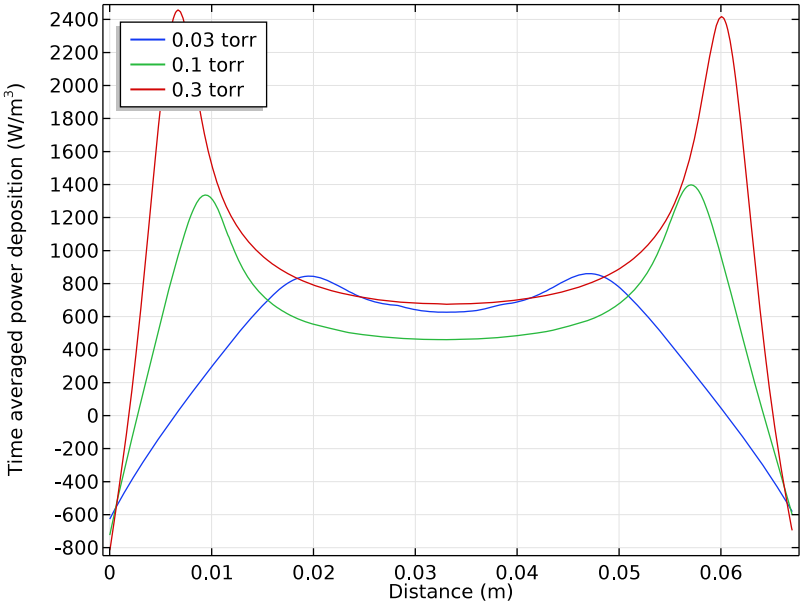

Figure 4: Plot of the time averaged electron power deposition as a function of the distance from the left electrode.

Figure 5 and Figure 6 plot the time averaged electron and ion density at different operating pressures. The electron and ion density is the same in the plasma bulk but the ion density is higher in the plasma sheath. This creates a net positive space charge density in the plasma sheath which tends to hold electrons in the plasma and accelerate ions towards the wall via the plasma potential.

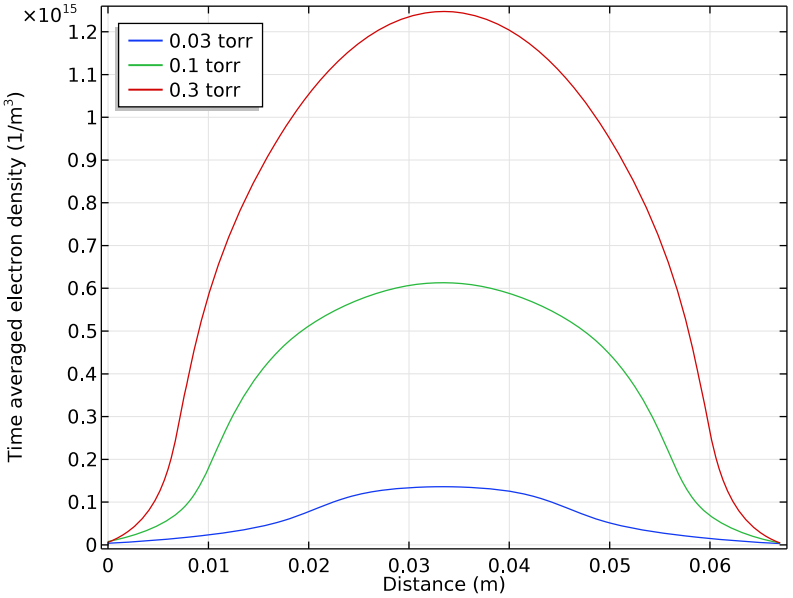

Figure 5: Plot of the time averaged electron density at different operating pressures.

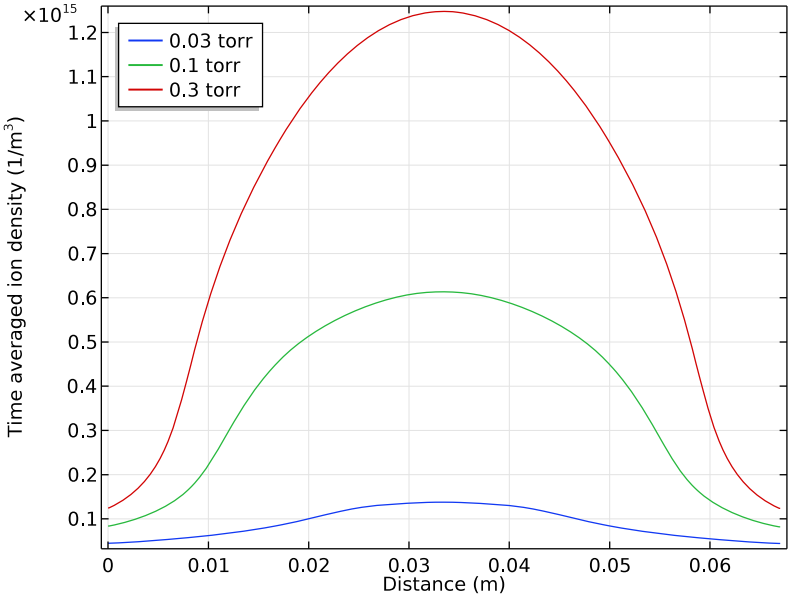

Figure 6: Plot of the time averaged ion density for different operating pressures.

Ref. 1 tabulates a wide range of lumped parameters for the discharge. These same parameters for the COMSOL model are shown in Table 3. There is good agreement between the COMSOL model and the values quoted in Ref. 1.

TABLE 3: RESULTS FROM THE DISCHARGE MODEL

P (MTORR)	$V_{rf}(V)$	$n_e(\mathrm{cm}^{-3})$	$\bar{\varepsilon}(\mathrm{eV})$	$P_{\mathrm{tot}}(\mathrm{mWcm}^2)$	$j_{\mathrm{pos}}(\mathrm{mAcm}^2)$	$I_{rf}(\mathrm{mAcm}^2)$
30	392.5	1.38×10^8	14.7	2.92	0.019	1.00
100	220.0	6.19×10^8	7.3	4.0	0.0195	1.00
300	165.0	1.25×10^9	5.5	6.46	0.0175	1.00

Reference

1. M. Surendra, "Radiofrequency discharge benchmark model comparison," *Plasma Sources Sci. Technol,* vol. 4, pp 56–73, 1995.

Application Library path: `Plasma_Module/Capacitively_Coupled_Plasmas/ccp_benchmark`

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 **1D**.

2 In the **Select Physics** tree, select **Plasma>Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

7 In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.

8 In the **Model Builder** window's toolbar, click the **Show** button and select **Equation View** in the menu.

GEOMETRY 1

Interval 1 (i1)

1 On the **Geometry** toolbar, click **Interval**.

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

3 In the **Right endpoint** text field, type `0.067`.

Interval 2 (i2)

1 On the **Geometry** toolbar, click **Interval**.

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

3 In the **Left endpoint** text field, type `0.067`.

4 In the **Right endpoint** text field, type `0.077`.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
p0	0.3[torr]	40 Pa	Gas pressure
T0	300[K]	300 K	Gas temperature
freq	13.56[MHz]	1.356E7 Hz	RF frequency
omega	2*pi*freq	8.52E7 Hz	Angular frequency
J0	1[mA/cm^2]	10 A/m²	Current density

DEFINITIONS

Variables 1

1 On the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
I_sp	J0*cos(omega*t)*1[m^2]	A	Current setpoint
mue	3.33E24[1/(V*m*s)]/plas.Nn	$m^2/(V \cdot s)$	Electron mobility

Integration 1 (intop1)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

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

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

5 Select Boundary 3 only.

PLASMA (PLAS)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Plasma (plas)** node, then click **Plasma (plas)**.

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

3 From the **Diffusion model** list, choose **Fick's law**.

4 Locate the **Out-of-Plane Thickness** section. In the *d* text field, type `1[m^2]`.

5 In the **Model Builder** window's toolbar, click the **Show** button and select **Stabilization** in the menu.

6 Click to expand the **Stabilization** section. Clear the **Reaction source stabilization** check box.

7 Clear the **Source stabilization** check box.

Cross Section Import 1

1 Right-click **Plasma (plas)** 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 `He_xsecs.txt`.

Species: He

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: He**.

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. In the D_f text field, type `0.8`.

5 From the **Preset species data** list, choose **He**.

Species: Hes

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hes**.

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

3 In the x_0 text field, type `1E-6`.

4 In the D_f text field, type `0.8`.

5 From the **Preset species data** list, choose **He**.

Species: He+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: He+**.

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 **He**.

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

6 Click to expand the **Mobility specification** section. Locate the **Mobility Specification** section. From the **Specify using** list, choose **High field**.

7 In the σ text field, type `3e-19[m^2]`.

8 Locate the **Mobility and Diffusivity Expressions** section. From the **Ion temperature** list, choose **Use local field approximation**.

Plasma Model 1

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

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

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

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

5 Locate the **Electron Density and Energy** section. In the μ_e text field, type `mue`.

Surface Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

2 Select Boundaries 1 and 2 only.

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

4 In the **Formula** text field, type `Hes=>He`.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

2 Select Boundaries 1 and 2 only.

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

4 In the **Formula** text field, type `He+=>He`.

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

Charge Conservation 1

1 Right-click **Plasma (plas)** and choose the domain setting **Electrostatics> Charge Conservation**.

2 Select Domain 2 only.

MATERIALS

Material 1 (mat1)

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

2 Select Domain 2 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permittivity	epsilonr	`4.2`	1	Basic

PLASMA (PLAS)

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E14`.

4 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

5 In the V text field, type `1e-6[V/m]*x`.

Wall 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

2 Select Boundaries 1 and 2 only.

3 In the **Settings** window for **Wall**, locate the **General Wall Settings** section.

4 In the r_e text field, type `5/11`.

Ground 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

2 Select Boundary 1 only.

Surface Charge Accumulation 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics> Surface Charge Accumulation**.

2 Select Boundary 2 only.

Terminal 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>More> Terminal**.

2 Select Boundary 3 only.

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

4 From the **Terminal type** list, choose **Current**.

5 In the I_0 text field, type `I_sp`.

6 Click to expand the **Constraint settings** section. Locate the **Constraint Settings** section. Select the **Use weak constraints** check box.

MESH 1

Edge 1

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

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

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

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

5 Select Domain 1 only.

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Distribution**.

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

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

4 In the **Number of elements** text field, type 200.

5 In the **Element ratio** text field, type 10.

6 From the **Distribution method** list, choose **Geometric sequence**.

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

Size 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Edge**.

2 Right-click **Edge 2** and choose **Size**.

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

4 From the **Predefined** list, choose **Extremely fine**.

5 Click **Build All**.

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

GEOMETRY 1

Click the **Zoom Extents** button on the **Graphics** toolbar.

MESH 1

Click the **Zoom Extents** button on the **Graphics** toolbar.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

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

3 Click **Range**.

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

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

6 In the **Stop** text field, type `200/13.56e6`.

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

8 Click **Replace**.

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

10 Click **Range**.

11 In the **Range** dialog box, type `200/13.56e6` in the **Start** text field.

12 In the **Stop** text field, type `201/13.56e6`.

13 In the **Number of values** text field, type `51`.

14 Click **Add**.

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

16 In the **Settings** window for **Study**, locate the **Study Settings** section.

17 Clear the **Generate convergence plots** check box.

18 Clear the **Generate default plots** check box.

Parametric Sweep

1 On 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
p0	`0.03[torr] 0.1[torr] 0.3[torr]`	

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

RESULTS

In the **Model Builder** window, expand the **Results** node.

1D Plot Group 1

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

2 In the **Settings** window for **1D Plot Group**, type `Time Averaged Ion Current Density` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

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

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `Distance (m)`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `Time averaged ion current density (A/m<sup>2</sup>)`.

9 Click to expand the **Title** section. From the **Title type** list, choose **None**.

10 Click to expand the **Legend** section. From the **Position** list, choose **Upper left**.

Line Graph 1

1 Right-click **Time Averaged Ion Current Density** and choose **Line Graph**.

2 Select Domain 1 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `timeavg(200/freq,201/freq, pprint(plas.Jix_wHe_1p),1e-3)`.

5 Click to expand the **Legends** section. Select the **Show legends** check box.

6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
0.03 torr
0.1 torr
0.3 torr

8 On the **Time Averaged Ion Current Density** toolbar, click **Plot**.

9 Click the **Zoom Extents** button on the **Graphics** toolbar.

Time Averaged Ion Current Density 1

1 In the **Model Builder** window, under **Results** right-click **Time Averaged Ion Current Density** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Time Averaged Ionization Rate` in the **Label** text field.

3 Locate the **Plot Settings** section. In the **x-axis label** text field, type `Distance (m)`.

4 In the **y-axis label** text field, type `Time averaged ionization rate (1/(m<sup>3</sup>s))`.

Line Graph 1

1 In the **Model Builder** window, expand the **Results>Time Averaged Ionization Rate** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `timeavg(200/freq,201/freq,plas.r_3*N_A_const,1e-3)`.

4 On the **Time Averaged Ionization Rate** toolbar, click **Plot**.

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

Time Averaged Ionization Rate 1

1 In the **Model Builder** window, under **Results** right-click **Time Averaged Ionization Rate** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Time Averaged Excitation Rate` in the **Label** text field.

3 Locate the **Plot Settings** section. In the **x-axis label** text field, type `Distance (m)`.

4 In the **y-axis label** text field, type `Time averaged excitation rate (1/(m<sup>3</sup>s))`.

Line Graph 1

1 In the **Model Builder** window, expand the **Results>Time Averaged Excitation Rate** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `timeavg(200/freq,201/freq,plas.r_2*N_A_const,1e-3)`.

4 On the **Time Averaged Excitation Rate** toolbar, click **Plot**.

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

Time Averaged Excitation Rate 1

1 In the **Model Builder** window, under **Results** right-click **Time Averaged Excitation Rate** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Time Averaged Power Deposition` in the **Label** text field.

3 Locate the **Plot Settings** section. In the **x-axis label** text field, type `Distance (m)`.

4 In the **y-axis label** text field, type `Time averaged power deposition (W/m<sup>3</sup>)`.

Line Graph 1

1. In the **Model Builder** window, expand the **Results>Time Averaged Power Deposition** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3. In the **Expression** text field, type `timeavg(200/freq,201/freq, pprint(plas.Pcap),1e-3)`.
4. On the **Time Averaged Power Deposition** toolbar, click **Plot**.
5. Click the **Zoom Extents** button on the **Graphics** toolbar.

Time Averaged Power Deposition 1

1. In the **Model Builder** window, under **Results** right-click **Time Averaged Power Deposition** and choose **Duplicate**.
2. In the **Settings** window for **1D Plot Group**, type `Time Averaged Electron Density` in the **Label** text field.
3. Locate the **Plot Settings** section. In the **y-axis label** text field, type `Time averaged electron density (1/m<sup>3</sup>)`.

Line Graph 1

1. In the **Model Builder** window, expand the **Results>Time Averaged Electron Density** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3. In the **Expression** text field, type `timeavg(200/freq,201/freq,plas.ne,1e-3)`.
4. On the **Time Averaged Electron Density** toolbar, click **Plot**.
5. Click the **Zoom Extents** button on the **Graphics** toolbar.

Time Averaged Electron Density 1

1. In the **Model Builder** window, under **Results** right-click **Time Averaged Electron Density** and choose **Duplicate**.
2. In the **Settings** window for **1D Plot Group**, type `Time Averaged Ion Density` in the **Label** text field.
3. Locate the **Plot Settings** section. In the **y-axis label** text field, type `Time averaged ion density (1/m<sup>3</sup>)`.

Line Graph 1

1. In the **Model Builder** window, expand the **Results>Time Averaged Ion Density** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `timeavg(200/freq,201/freq,plas.n_wHe_1p,1e-3)`.

4 On the **Time Averaged Ion Density** toolbar, click **Plot**.

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

Cut Point 1D 1

1 On the **Results** toolbar, click **More Data Sets** and choose **Cut Point 1D**.

2 In the **Settings** window for **Cut Point 1D**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

4 Locate the **Point Data** section. In the **X** text field, type `0.067/2`.

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

1D Plot Group 7

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

2 In the **Settings** window for **1D Plot Group**, type `Electric Potential on Electrode` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

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

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 `200/13.56e6`.

8 In the **Stop** text field, type `201/13.56e6`.

9 In the **Number of values** text field, type `51`.

10 Click **Replace**.

Point Graph 1

1 Right-click **Electric Potential on Electrode** and choose **Point Graph**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `V`.

5 On the **Electric Potential on Electrode** toolbar, click **Plot**.

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

Point Evaluation 1

1 On the **Results** toolbar, click **Point Evaluation**.

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

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

5 From the **Table columns** list, choose **Time**.

6 From the **Data set** list, choose **Cut Point 1D 1**.

7 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1>Plasma (Drift Diffusion)>Electron density>plas.ne - Electron density**.

8 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
plas.ne	1/cm^3	Electron density

9 Click **Evaluate**.

Point Evaluation 2

1 Right-click **Point Evaluation 1** and choose **Duplicate**.

2 In the **Settings** window for **Point Evaluation**, click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1>Plasma (Drift Diffusion)>Electron energy density>plas.ebar - Mean electron energy**.

3 Click **Table 1 - Point Evaluation 1 (plas.ne)**.

Point Evaluation 3

1 On the **Results** toolbar, click **Point Evaluation**.

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

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

5 From the **Table columns** list, choose **Time**.

6 Select Boundary 2 only.

7 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1>Plasma (Heavy Species Transport)>Current>plas.nJt - Total ion current density on wall**.

8 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
plas.nJt	mA/cm^2	Total ion current density on wall

9 Click **Table 1 - Point Evaluation 1 (plas.ne)**.

Global Evaluation 1

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

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

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 `200/13.56e6`.

8 In the **Stop** text field, type `201/13.56e6`.

9 In the **Number of values** text field, type `51`.

10 Click **Replace**.

11 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

12 From the **Table columns** list, choose **Time**.

13 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1>Plasma>Power and collisions>plas.Pcap_tot - Total capacitive power deposition**.

14 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`1e-4*plas.Pcap_tot`	`mW`	

15 Locate the **Data Series Operation** section. From the **Operation** list, choose **Average**.

16 Click **New Table**.

Chlorine Discharge Global Model

Introduction

Plasma discharges containing Chlorine are commonly used to etch semiconductors and metals in microelectronics fabrication. Cl_2 has low dissociation energy and very low threshold energy for dissociative attachment, and atomic chlorine has large electron affinity. As a consequence a Cl_2 plasma has substantial levels of electronegativity and dissociation. Quantification of the negative ion and atomic chlorine density is important to understand the reactor operation. In particular Chlorine atoms are accepted to be a main reactant for plasma etching.

In this study are presented model results of chlorine and electron density for absorbed powers between 25 and 600 W and for working pressures between 1 and 100 mTorr. To explore such a large parametric region it is used a global (volume-averaged) model since it can run simulations in a fraction of the time of a space dependent model while retaining the tendencies of volume-averaged physical quantities.

Model results of several relevant quantities such as atomic chlorine density, electron density, and electron temperature are in good agreement with measurements performed in inductively coupled plasma reactors found in the literature.

The reader can found more information about global models and Chlorine plasmas in Ref. 1, Ref. 2, and Ref. 3 and in the references therein.

Model Definition

The model used in this work considers that the spatial information of the different quantities in the plasma reactor can be treated as uniform or can be introduce using analytic models. Without the spatial derivatives the numerical solution of the equation set becomes considerably simpler and the computational time is reduced. In the following it is taken advantage of the fast computational time to investigate a broad region of parameters with a complex plasma chemistry.

When using a plasma global model the species densities and the electron temperature are treated as volume-averaged quantities. Detailed information on the global model can be found in the section Theory for Global Models in the *Plasma Module User's Guide*. For heavy species the following equation is solved for the mass fraction

$$V\rho\frac{d}{dt}(w_k) = m_f w_{f,k} - m_o w_k + VR_k + \sum_l h_l A_l R_{surf,k,l} M_k - w_k \sum_l h_l A_l M_{f,l}$$

where ρ is the mass density (SI unit: kg/m^3), w_k is the mass fraction, $w_{f,k}$ is the mass fraction in the feed, m_f and m_o are the mass-flow rates of the total feed and outlet, and R_k is the rate expression (SI unit: kg/(m^3.s)). The forth term on the right hand side accounts for surface losses and creation, where A_l is the surface area, h_l is a dimensionless correction

term, V is the reactor volume, M_k is the species molar mass (SI unit: kg/mol) and $R_{surf,k,l}$ is the surface rate expression (SI unit: mol/(m^2.s)) at a surface l. The last term is introduce because the species mass balance equations are written in the non-conservative form and it was used the mass-continuity equation to replace for the mass density time derivative. In the last term $M_{f,l}$ is the inward mass flux of surface l (SI unit: kg/(m^2·s)). The sum in the last two terms is over all surfaces where there are surface reactions.

To take into account possible variations of the system total mass or pressure the mass-continuity equation can also be solved

$$V\frac{d\rho}{dt} = m_f - m_o + \sum_l h_l A_l M_{f,l}\,.$$

The electron number density is obtained from electroneutrality

$$n_e = \sum_{k=1}^{N} Z_k n_k$$

and electron energy density n_ε (unit: V/ m^3) is computed from

$$V\frac{dn_\varepsilon}{dt} = VR_\varepsilon + \frac{P_{abs}}{e} + \sum_l \sum_{ions} h_l A_l R_{surf,k,l} N_a(\varepsilon_e + \varepsilon_i)$$

where R_ε is the electron energy loss due to inelastic and elastic collisions, P_{abs} is the power absorbed by the electrons (SI unit: W), and e is the elementary charge. The last term on the rhs accounts for the kinetic energy transported to the surface by electrons and ions. The summation is over all positive ions, ε_e is the mean kinetic energy lost per electron lost, ε_i is the mean kinetic energy lost per ion lost, and N_a is the Avogadro's number.

In this work are simulated cylindrical reactors with several dimensions corresponding to inductively coupled plasma reactors used by different experimental groups. The simulations are performed for a reactor operating at constant pressure. Moreover, the mass-flow rate of the outlet is found by assuming that the feed and the surface reactions can not change the total mass of the system

$$m_o = m_f + \sum_l h_l A_l M_{f,l}\ .$$

Note that the surface reactions used in these simulations do not change the mass of the system.

However the mass-continuity equation is not solved, the mass density can still change as a result of a change in the mean molar mass, thus accounting for changes in the number density (due to dissociation and association) to maintaining a constant pressure.

The expressions used for the mean kinetic energy lost per electron lost and the mean kinetic energy lost per ion lost are deduced from theory and numerical solution and are explained in Ref. 1and references therein. The gas temperature is a function of pressure and absorbed power and is based on experiential data Ref. 1.

PLASMA CHEMISTRY

It is used the plasma chemistry suggested in Ref. 2 and presented in Table 1that consists of 10 species and 44 reactions.

TABLE I: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\varepsilon(eV)$
1	e+Cl2=>e+Cl2	Momentum	0
2	e+Cl=>e+Cl	Momentum	0
3	e+Cl2=>Cl+Cl+e	Dissociation	4
4	e+Cl2=>2e+Cl2+	Ionization	11.5
5	e+Cl2=>2e+Cl+Cl+	Ionization	14.25
6	e+Cl2=>3e+2Cl+	Ionization	28.5
7	e+Cl2=>Cl+Cl-	Attachment	0
8	e+Cl2v1=>Cl+Cl-	Attachment	0
9	e+Cl2v2=>Cl+Cl-	Attachment	0
10	e+Cl2v3=>Cl+Cl-	Attachment	0
11	e+Cl2=>Cl++Cl-+e	Ionization/Attachment	14.25
12	e+Cl2=>e+Cl2v1*	Excitation	0.07
13	e+Cl2=>e+Cl2v2*	Excitation	0.14
14	e+Cl2=>e+Cl2v3*	Excitation	0.21
15	e+Cl2v1=>e+Cl2v2*	Excitation	0.07
16	e+Cl2v2=>e+Cl2v3*	Excitation	0.07
17	e+Cl2v1=>e+Cl2v3*	Excitation	0.14
18	e+Cl2+=>2Cl	Excitation	0
19	e+Cl=>e+Cl12*	Excitation	1.35
20	e+Cl=>e+Cl52*	Excitation	10.17
21	e+Cl=>Cl++2e	Ionization	14.25

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\varepsilon(eV)$
22	e+Cl12=>Cl++2e	Ionization	10.18
23	e+Cl52=>Cl++2e	Ionization	4.08
24	e+Cl-=>Cl+2e	Ionization	2.36
25	e+Cl-=>Cl++3e	Ionization	16.61
26	Cl52=>Cl	Radiation decay	0
27	Cl2++Cl-=>3Cl	Ion-ion recombination	0
28	Cl2++Cl-=>Cl+Cl2	Ion-ion recombination	0
29	Cl++Cl-=>2Cl	Ion-ion recombination	0
30	Cl2+Cl+=>Cl+Cl2+	Charge exchange	0
31	Cl2v1+Cl+=>Cl+Cl2+	Charge exchange	0
32	Cl2v2+Cl+=>Cl+Cl2+	Charge exchange	0
33	Cl2v3+Cl+=>Cl+Cl2+	Charge exchange	0
34	2Cl+Cl2=>2Cl2	Association	0
35	2Cl+Cl=>Cl2+Cl	Association	0
36	Cl+Cl2v3=>Cl+Cl2v2	Deexcitation	0
37	Cl+Cl2v2=>Cl+Cl2v1	Deexcitation	0
38	Cl+Cl2v1=>Cl+Cl2v0	Deexcitation	0

*The reaction set includes the inverse reaction with the rate coefficient obtained by detailed balance.

The model also include the surface reactions presented in Table 2.

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Cl2+=>Cl2	1
2	Cl+=>Cl	1
3	Cl2v1=>Cl2	1
4	Cl2v2=>Cl2	1
5	Cl2v3=>Cl2	1
6	Cl12=>Cl	1
7	Cl52=>Cl	1
8	Cl=>0.5Cl2	Ref. 1

The rate at which positive ions are lost to the wall is computed from the Bohm velocity and the density that an ion have near the surface. The ion density at the surface is estimated

from theory Ref. 1 and Ref. 3 and is introduce in the model using the correction factor h_l. Negative ions are assumed to be confined in the plasma bulk.

The rate at which neutral species are lost to the wall involves the information of diffusional losses, of the particle mean velocity, and of the sticking coefficient Ref. 1 and Ref. 3. The wall recombination of neutral chlorine atoms is an important aspect of chlorine containing discharges since it influences the degree of dissociation of the discharge. The sticking coefficient for the recombination of Cl at the surface is obtained by fitting experimental data Ref. 1. All other neutral excited species revert to ground state with sticking coefficient equal to one.

Results and Discussion

In this section are presented simulations results that can be compared with measurements and simulations reported in Ref. 1. The measurements are for inductively coupled plasma reactors with radius R and length L, operate at a given volumetric flow (Q_f), and sweep either the input power or the pressure. The power absorbed by the plasma that is used in the simulations is estimated in Ref. 1. The parameters used in the simulations are summarized in Table 3, and are labeled with the name of the authors that perform the measurements. Overall the numeric results are consistent with those of Ref. 1 and agree well for most experimental conditions.

TABLE 3: REACTOR PARAMETERS.USED IN THE SIMULATIONS.

AUTHOR	$R(cm)$	$L(cm)$	$Q_f(sccm)$	$P_{abs}(W)$	$P(mTorr)$
Corr *et al*	10	8.5	10	25-300 300	10 1-100
Malyshev and Donnelly	18.5	20	100	50-650	10
Efremov *et al*	15	14	20	300	1-100

Figure 1 and Figure 2 present electron and Cl number density as a function of the absorbed power for the experimental conditions of Corr *et al* and Malyshev and Donnelly. The atomic Chlorine density for the conditions of Corr *et al* and the electron density for the conditions of Malyshev and Donnelly (Figure 2) agree well with measurements. The electron density for the conditions o Corr *et al* (Figure 1) is highly overestimated when compared with measurements but is consistent with the simulation results of Ref. 1. The electronegativity, also presented in Figure 1, only agrees well with measurements at higher absorbed powers.

Figure 3 presents electron and Cl number density as a function of the reactor pressure for the experimental conditions of Corr *et al.* There is a fair agreement for all conditions with the model capturing the tendencies but slightly underestimating the Cl density and overestimating the electron density.

Figure 4 presents the electron temperature as a function of the reactor pressure for the experimental conditions of Efremov *et al.* The model agrees well with measurements capturing the decrease of the electron temperature with pressure. However, the measured temperature decreases at a faster rate with pressure at higher pressures.

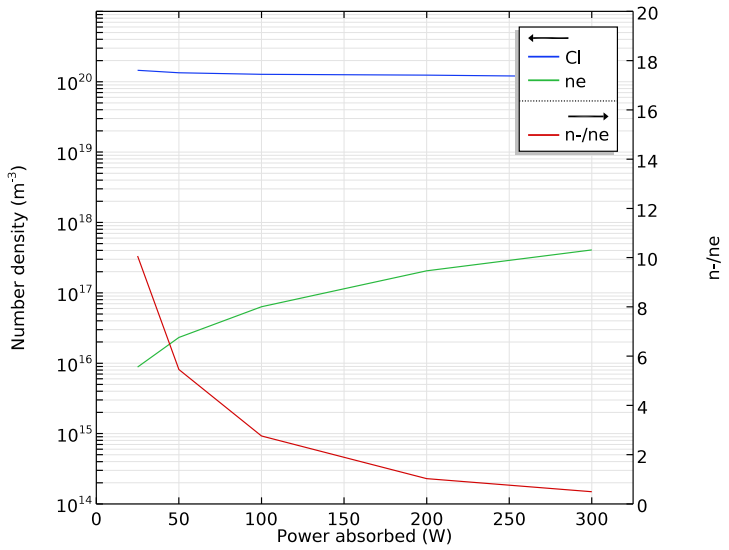

Figure 1: Model results for the electron and Cl densities, and for the electronegativity as a function of the absorbed power for the conditions of Corr et al: P=10 mTorr, Q_f=10 sccm, R=10 cm, and L=8.5 cm.

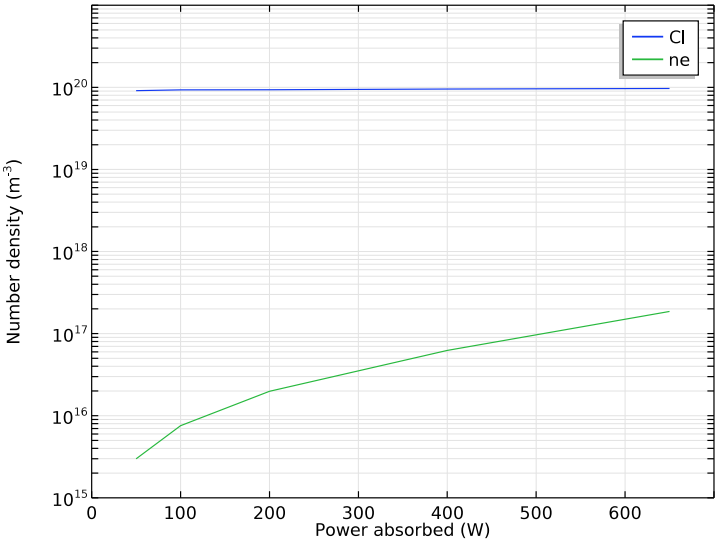

Figure 2: Model results for the electron and Cl densities as a function of the absorbed power for the conditions of Malyshev and Donnelly: P=10 mTorr, Q_f=100 sccm, R=8.5 cm, and L=20 cm.

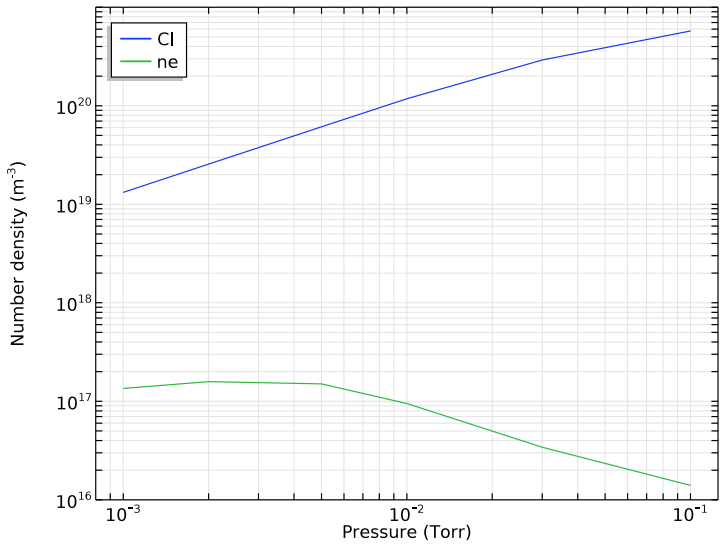

Figure 3: Model results for the electron and Cl densities as a function of pressure. The Cl density is for the conditions of Corr et al: P_{abs}=300 W, Q_f=10 sccm, R=10 cm, and L=8.5 cm. The electron density is for the conditions of Efremov et al: P_{abs}=300 W, Q_f=20 sccm, R=25 cm, and L=14 cm.

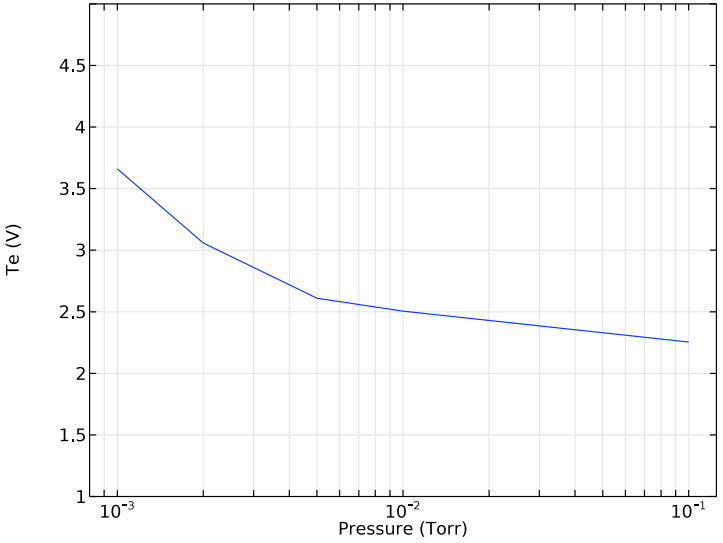

Figure 4: Model results for the electron temperature as a function of pressure for the conditions of Efremov et al: P_{abs}=300 W and Q_f=20 sccm, R=15 cm, and L=14 cm.

Reference

1. E. G. Thorsteinsoon, and J. T. Gudmundsson, "A global (volume averaged) model of a chlorine discharge," *Plasma Sources Sci. Technol.*, vol. 19, p. 015001 (15pp), 2010.

2. E. Kemaneci, E. Carbone, J-P. Booth, W. Graef, J. van Dijk, and G. Kroesen, "Global (volume-averaged) model of inductively coupled chlorine plasma: influence of Cl wall recombination and external heating on continuous and pulse-modulated plasmas," *Plasma Sources Sci. Technol.*, vol. 23, p. 045002 (14pp), 2014.

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

Application Library path: `Plasma_Module/Global_Discharges/chlorine_global_model`

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 **2D Axisymmetric**.
2. In the **Select Physics** tree, select **Plasma>Plasma (plas)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies>Time Dependent**.
6. Click **Done**.

ROOT

Construct a cylindrical reactor with radius Rad and length L. The values of Rad and L are set in the **Parameters** node.

GEOMETRY 1

Rectangle 1 (r1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `Rad`.

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

GLOBAL DEFINITIONS

Add parameters to be used in the simulations. The pressure and absorbed power need to be set here to be available to do a parameter sweep.

The different studies performed use different parameters so that before each new study (after the first study) it is necessary to change some of the parameters values.

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	10[cm]	0.1 m	
L	8.5[cm]	0.085 m	
Pabs	25[W]	25 W	
Qfeed	10	10	
p0	0.01[Torr]	1.333 Pa	

DEFINITIONS

Import the file containing the energy levels to be used when defining the reactions.

Variables 1

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

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

3 Click **Load from File**.

4 Browse to the application's Application Libraries folder and double-click the file `chlorine_global_model_variables_1.txt`.

Import the file containing the variables used to define the gas temperature, the plasma and sheath potential, and the h_l correction factors.

Variables 2

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

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

3 Click **Load from File**.

4 Browse to the application's Application Libraries folder and double-click the file `chlorine_global_model_variables_2.txt`.

Choose to use a global model for the following simulations and set the model to work at constant pressure.

PLASMA (PLAS)

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

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

3 From the **Diffusion model** list, choose **Global**.

4 Locate the **Reactor** section. From the **Reactor type** list, choose **Constant pressure**.

Set the background gas temperature, the working pressure, the total mass flow, the power absorbed, the mean kinetic energy lost per ion and electron lost.

The mole fraction of each species in the mass flow is set later in the species node.

Plasma Model 1

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

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

3 In the T text field, type `Th`.

4 In the p_{A} text field, type `p0`.

5 Locate the **Total Mass Flow** section. In the Q_{sccm} text field, type `Qfeed`.

6 Locate the **Mean Electron Energy** section. In the P_{abs} text field, type `Pabs`.

7 In the ε_e text field, type `Epsilon_e`.

8 In the ε_i text field, type `Epsilon_p+Epsilon_s`.

Add reactions relevant for the Chlorine plasma chemistry. There are about 40 volume reactions that need to be added.

For electron impact reactions it is needed to set the collision type, the rate constant and the energy loss in the collision.

For reactions between heavy species it is only necessary to set the rate constant.

Electron Impact Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport>Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>Cl+Cl+e`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the $\Delta\varepsilon$ text field, type `ediss`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `1.04e-13* plas.Te^(-0.29)*exp(-8.84/plas.Te)*N_A_const`.

Electron Impact Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>2e+Cl2+`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the $\Delta\varepsilon$ text field, type `eionCl2`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `5.12e-14* plas.Te^(0.48)*exp(-12.34/plas.Te)*N_A_const`.

Electron Impact Reaction 3

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>2e+Cl+Cl+`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the $\Delta\varepsilon$ text field, type `eionCl`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `2.14e-13* plas.Te^(-0.07)*exp(-25.26/plas.Te)*N_A_const`.

Electron Impact Reaction 4

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.
2. In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `e+Cl2=>3e+2Cl+`.
4. Locate the **Collision Type** section. From the list, choose **Ionization**.
5. In the $\Delta\varepsilon$ text field, type `2*eionCl`.
6. Locate the **Reaction Parameters** section. In the k^{f} text field, type `2.27e-16*plas.Te^(1.92)*exp(-21.26/plas.Te)*N_A_const`.

Electron Impact Reaction 5

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.
2. In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `e+Cl2=>Cl+Cl-`.
4. Locate the **Collision Type** section. From the list, choose **Attachment**.
5. Locate the **Reaction Parameters** section. In the k^{f} text field, type `(3.43e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 3.05e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 6

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.
2. In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `e+Cl2v1=>Cl+Cl-`.
4. Locate the **Collision Type** section. From the list, choose **Attachment**.
5. Locate the **Reaction Parameters** section. In the k^{f} text field, type `(14.06e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 12.51e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 7

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.
2. In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `e+Cl2v2=>Cl+Cl-`.
4. Locate the **Collision Type** section. From the list, choose **Attachment**.

5 Locate the **Reaction Parameters** section. In the k^f text field, type `(30.18e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 26.84e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 8

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v3=>Cl+Cl-`.

4 Locate the **Collision Type** section. From the list, choose **Attachment**.

5 Locate the **Reaction Parameters** section. In the k^f text field, type `(46.31e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 41.18e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 9

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>Cl++Cl-+e`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the $\Delta\varepsilon$ text field, type `eionCl`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `2.94e-16*plas.Te^(0.19)*exp(-18.79/plas.Te)*N_A_const`.

Electron Impact Reaction 10

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>e+Cl2v1`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the $\Delta\varepsilon$ text field, type `ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.99e-12*plas.Te^(-1.5)*exp(-7.51/plas.Te-0.0001/plas.Te^2)*N_A_const`.

Electron Impact Reaction 11

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>e+Cl2v2`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `ev2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3.28e-17*plas.Te^(-1.12)*exp(-0.37/plas.Te) + 2.86e-17*exp(-(log(plas.Te)+0.99)^2/(2*1.06^2)))*N_A_const`.

Electron Impact Reaction 12

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>e+Cl2v3`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `ev3`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.3e-17*plas.Te^(-1.24)*exp(-0.41/plas.Te) + 6.08e-18*exp(-(log(plas.Te)+0.94)^2/(2*1.02^2)))*N_A_const`.

Electron Impact Reaction 13

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v1=>e+Cl2v2`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `ev2-ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const`.

Electron Impact Reaction 14

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v2=>e+Cl2v3`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `ev3-ev2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const`.

Electron Impact Reaction 15

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v1=>e+Cl2v3`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `ev3-ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.25e-16*plas.Te^(-1.13)*exp(-0.36/plas.Te) + 1.06e-16*exp(-(log(plas.Te)+1.01)^2/(2*1.06^2)))*N_A_const`.

Electron Impact Reaction 16

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2+=>2Cl`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-eionCl2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `9e-14*plas.Te^(-0.5)*N_A_const`.

Electron Impact Reaction 17

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl=>e+Cl12`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `eCl12`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `4.55e-14*plas.Te^(-0.46)*exp(-2.01/plas.Te-0.001/plas.Te^2)*N_A_const`.

Electron Impact Reaction 18

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl=>e+Cl52`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `eCl52`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(7.03e-17* plas.Te^(0.55)*exp(-2.15/plas.Te-1.5/plas.Te^2-2.05/plas.Te^3))* N_A_const`.

Electron Impact Reaction 19

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl=>Cl++2e`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the Δε text field, type `eionCl`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.17e-14* plas.Te^(0.53)*exp(-13.29/plas.Te)*N_A_const`.

Electron Impact Reaction 20

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl12=>Cl++2e`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the Δε text field, type `eionCl-eCl12`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.17e-14* plas.Te^(0.53)*exp(-13.29/plas.Te)*N_A_const`.

Electron Impact Reaction 21

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl52=>Cl++2e`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the Δε text field, type `eionCl-eCl52`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(4.33e-14*plas.Te^(0.55)*exp(-0.15/plas.Te-0.85/plas.Te^2))*N_A_const`.

Electron Impact Reaction 22

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl-=>Cl+2e`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the Δε text field, type `eatt`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `9.02e-15*plas.Te^(0.92)*exp(-4.88/plas.Te)*N_A_const`.

Electron Impact Reaction 23

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl-=>Cl++3e`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the Δε text field, type `eatt+eionCl`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.62e-15*plas.Te^(0.72)*exp(-25.38/plas.Te)*N_A_const`.

Electron Impact Reaction 24

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v1=>e+Cl2`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.99e-12*plas.Te^(-1.5)*exp(-7.51/plas.Te-0.0001/plas.Te^2)*N_A_const*exp(ev1/plas.Te)`.

Electron Impact Reaction 25

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v2=>e+Cl2`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-ev2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3.28e-17*plas.Te^(-1.12)*exp(-0.37/plas.Te) + 2.86e-17*exp(-(log(plas.Te)+0.99)^2/(2*1.06^2)))*N_A_const*exp(ev2/plas.Te)`.

Electron Impact Reaction 26

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v3=>e+Cl2`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-ev3`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.3e-17*plas.Te^(-1.24)*exp(-0.41/plas.Te) + 6.08e-18*exp(-(log(plas.Te)+0.94)^2/(2*1.02^2)))*N_A_const*exp(ev3/plas.Te)`.

Electron Impact Reaction 27

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v2=>e+Cl2v1`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-(ev2-ev1)`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const*exp((ev2-ev1)/plas.Te)`.

Electron Impact Reaction 28

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v3=>e+Cl2v2`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-(ev3-ev2)`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const*exp((ev3-ev2)/plas.Te)`.

Electron Impact Reaction 29

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2v3=>e+Cl2v1`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-(ev3-ev1)`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.25e-16*plas.Te^(-1.13)*exp(-0.36/plas.Te) + 1.06e-16*exp(-(log(plas.Te)+1.01)^2/(2*1.06^2)))*N_A_const*exp((ev3-ev1)/plas.Te)`.

Electron Impact Reaction 30

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl12=>e+Cl`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-eCl12`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `4.55e-14*plas.Te^(-0.46)*exp(-2.01/plas.Te-0.001/plas.Te^2)*N_A_const*exp((eCl12)/plas.Te)`.

Electron Impact Reaction 31

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl52=>e+Cl`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-eCl52`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(7.03e-17*plas.Te^(0.55)*exp(-2.15/plas.Te-1.5/plas.Te^2-2.05/plas.Te^3))*N_A_const*exp((eCl52)/plas.Te)`.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `Cl52=>Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1e5`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `Cl2++Cl-=>3Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5e-14*(300/Th)^0.5*N_A_const`.

Reaction 3

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `Cl2++Cl-=>Cl+Cl2`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5e-14[m^3/s]*N_A_const`.

Reaction 4

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `Cl++Cl-=>2Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5e-14*(300/Th)^0.5*N_A_const`.

Reaction 5

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Cl2+Cl+=>Cl+Cl2+`.
4. Locate the **Reaction Parameters** section. In the k^{f} text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 6

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Cl2v1+Cl+=>Cl+Cl2+`.
4. Locate the **Reaction Parameters** section. In the k^{f} text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 7

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Cl2v2+Cl+=>Cl+Cl2+`.
4. Locate the **Reaction Parameters** section. In the k^{f} text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 8

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Cl2v3+Cl+=>Cl+Cl2+`.
4. Locate the **Reaction Parameters** section. In the k^{f} text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 9

1. Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `2Cl+Cl2=>2Cl2`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `3.5e-45*exp(810/Th)*N_A_const`.

Reaction 10

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `2Cl+Cl=>Cl2+Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `8.75e-46*exp(810/Th)*N_A_const`.

Reaction 11

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `Cl+Cl2v3=>Cl+Cl2v2`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1.3e-17*(Th/300)^0.5*N_A_const`.

Reaction 12

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `Cl+Cl2v2=>Cl+Cl2v1`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1.3e-17*(Th/300)^0.5*N_A_const`.

Reaction 13

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

3 In the **Formula** text field, type `Cl+Cl2v1=>Cl+Cl2`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `1.3e-17*(Th/300)^0.5*N_A_const`.

This model has two electron impact reactions of the elastic type: one with molecular Chlorine and another with atomic Chlorine.

These two reactions are defined using collision cross section data that needs to be imported from files.

Electron Impact Reaction 32

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e+Cl2=>e+Cl2`.

4 Locate the **Collision Type** section. In the m_{r} text field, type `7.720e-6`.

5 Locate the **Collision** section. From the **Specify reaction using** list, choose **Cross section data**.

6 Locate the **Reaction Parameters** section. From the **Electron energy distribution function** list, choose **Maxwellian**.

7 Click **Load from File**.

8 Browse to the application's Application Libraries folder and double-click the file `Cl2_mom_xsec.txt`.

Electron Impact Reaction 33

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

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

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

4 Locate the **Collision Type** section. In the m_{r} text field, type `1.510e-5`.

5 Locate the **Collision** section. From the **Specify reaction using** list, choose **Cross section data**.

6 Locate the **Reaction Parameters** section. From the **Electron energy distribution function** list, choose **Maxwellian**.

7 Click **Load from File**.

8 Browse to the application's Application Libraries folder and double-click the file `Cl_mom_xsec.txt`.

In the species nodes (for heavy species) set the species data by choosing the atomic and molecular chlorine presets accordingly.

This information is used to compute the diffusion coefficients and the Bohm velocity that is used to estimate the surface losses of neutral species and positive ions, respectively.

Also for each species set the initial mole fraction (for neutrals) and the initial number density (for ions) in the reactor.

If the species is a neutral it is also possible to set the mole fraction of the total mass flow.

In this model the feed only contains molecular Chlorine so that the **Feed mole fraction** of Cl2 is set to 1.

Species: Cl2

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl2**.

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 **Cl2**.

5 In the x_{feed} text field, type `1`.

Species: Cl

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl**.

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

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

Species: Cl2+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl2+**.

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

3 From the **Preset species data** list, choose **Cl2**.

4 In the n_0 text field, type `1E16[1/m^3]`.

Species: Cl+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl+**.

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

3 In the n_0 text field, type `1E14[1/m^3]`.

4 From the **Preset species data** list, choose **Cl**.

Species: Cl-

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl-**.

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

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

4 In the n_0 text field, type `1E14[1/m^3]`.

Species: Cl2v1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl2v1**.

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

3 From the **Preset species data** list, choose **Cl2**.

Species: Cl2v2

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl2v2**.

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

3 From the **Preset species data** list, choose **Cl2**.

Species: Cl2v3

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl2v3**.

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

3 From the **Preset species data** list, choose **Cl2**.

Species: Cl12

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl12**.

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

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

Species: Cl52

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Cl52**.

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

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

Add surface reactions to estimate the losses at the walls.

Neutral species are estimated to be lost with the same frequency at all boundaries. In Contrast, the surface losses of positive ions in this model are different at radial and longitudinal boundaries.

For each ion two surface reactions are created: one selects longitudinal boundaries and sets the longitudinal correction factor, the other select the radial boundary and sets the radial correction factor.

Surface Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

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

3 In the **Formula** text field, type `Cl2+=>Cl2`.

4 From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_l text field, type `hRCl2`.

6 Select Boundary 4 only.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

3 In the **Formula** text field, type `Cl=>0.5Cl2`.

4 From the **Specify reaction using** list, choose **Sticking coefficient and diffusion**.

5 Locate the **Reaction Parameters** section. In the γ_f text field, type `gammaCl_steel`.

6 In the Λ_{eff} text field, type `Lambda_diff`.

7 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

Surface Reaction 3

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

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

4 From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_l text field, type `hRCl`.

6 Select Boundary 4 only.

Surface Reaction 4

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

3 In the **Formula** text field, type `Cl2v1=>Cl2`.

4 From the **Specify reaction using** list, choose **Sticking coefficient and diffusion**.

5 Locate the **Reaction Parameters** section. In the Λ_{eff} text field, type `Lambda_diff`.

6 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

5: Cl2v1=>Cl2

1 Right-click **Component 1 (comp1)>Plasma (plas)>Surface Reaction 4** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl2v2=>Cl2`.

6: Cl2v2=>Cl2

1 Right-click **Component 1 (comp1)>Plasma (plas)>5: Cl2v1=>Cl2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl2v3=>Cl2`.

7: Cl2v3=>Cl2

1 Right-click **Component 1 (comp1)>Plasma (plas)>6: Cl2v2=>Cl2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl12=>Cl`.

8: Cl12=>Cl

1 Right-click **Component 1 (comp1)>Plasma (plas)>7: Cl2v3=>Cl2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl52=>Cl`.

Surface Reaction 9

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

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

3 In the **Formula** text field, type `Cl2+=>Cl2`.

4 From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `hLCl2`.

6 Select Boundaries 2 and 3 only.

Surface Reaction 10

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

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

4 From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `hLCl`.

6 Select Boundaries 2 and 3 only.

PLASMA (PLAS)

1 In the **Model Builder** window, collapse the **Component 1 (comp1)>Plasma (plas)** node.

In the following create and run four separate studies that will do parametric sweeps.

The studies are labeled with the names of the authors that made the measurements.

Since each study needs a different set of parameters after the first study it is necessary to change some parameters such as the reactor radius and length, the absorbed power, and the total mass flow.

STUDY 1

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

2 In the **Settings** window for **Study**, type `Corr power sweep` in the **Label** text field.

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

4 Clear the **Generate convergence plots** check box.

Solution 1 (sol1)

On the **Study** toolbar, click **Show Default Solver**.

CORR POWER SWEEP

Solution 1 (sol1)

1 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

Set the **Jacobian update** to **Minimal** to decrease the computational time.

2 In the **Model Builder** window, expand the **Corr power sweep>Solver Configurations> Solution 1 (sol1)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

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

4 Locate the **Method and Termination** section. From the **Jacobian update** list, choose **Minimal**.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Corr power sweep** click **Step 1: Time Dependent**.

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

3 In the **Times** text field, type `0 10^{range(-12,0.1,2)}`.

Parametric Sweep

1 On 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
Pabs	25 50 100 200 300	W

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

CORR POWER SWEEP

In the **Model Builder** window, collapse the **Corr power sweep** node.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	18.5[cm]	0.185 m	
L	20[cm]	0.2 m	
Qfeed	100	100	

ADD STUDY

1 On 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**.

4 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

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

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

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

3 In the **Times** text field, type `0 10^{range(-12,0.1,2)}`.

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

5 In the **Settings** window for **Study**, type `Malyshev and Donnelly power sweep` in the **Label** text field.

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

7 Clear the **Generate convergence plots** check box.

Parametric Sweep

On the **Study** toolbar, click **Parametric Sweep**.

MALYSHEV AND DONNELLY POWER SWEEP

Parametric Sweep

1 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

2 Click **Add**.

3 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Pabs	50 100 200 400 650	W

Solution 8 (sol8)

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

2 In the **Model Builder** window, expand the **Solution 8 (sol8)** node.

3 In the **Model Builder** window, expand the **Malyshev and Donnelly power sweep> Solver Configurations>Solution 8 (sol8)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, locate the **Method and Termination** section.

5 From the **Jacobian update** list, choose **Minimal**.

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

MALYSHEV AND DONNELLY POWER SWEEP

In the **Model Builder** window, collapse the **Malyshev and Donnelly power sweep** node.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	10[cm]	0.1 m	
L	8.5[cm]	0.085 m	
Pabs	300[W]	300 W	
Qfeed	10	10	

ADD STUDY

1 Go to the **Add Study** window.

2 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

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

STUDY 3

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 3** click **Step 1: Time Dependent**.

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

3 In the **Times** text field, type `0 10^{range(-12,0.1,2)}`.

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

5 In the **Settings** window for **Study**, type `Corr pressure sweep` in the **Label** text field.

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

7 Clear the **Generate convergence plots** check box.

Parametric Sweep

On the **Study** toolbar, click **Parametric Sweep**.

CORR PRESSURE SWEEP

Parametric Sweep

1 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

2 Click **Add**.

3 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
p0	1e-3 2e-3 5e-3 10e-3 30e-3 100e-3	Torr

Solution 15 (sol15)

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

2 In the **Model Builder** window, expand the **Solution 15 (sol15)** node.

3 In the **Model Builder** window, expand the **Corr pressure sweep>Solver Configurations> Solution 15 (sol15)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, locate the **Method and Termination** section.

5 From the **Jacobian update** list, choose **Minimal**.

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

CORR PRESSURE SWEEP

In the **Model Builder** window, collapse the **Corr pressure sweep** node.

GLOBAL DEFINITIONS

Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	15[cm]	0.15 m	
L	14[cm]	0.14 m	
Qfeed	20	20	

ADD STUDY

1 Go to the **Add Study** window.

2 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.

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

STUDY 4

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 4** click **Step 1: Time Dependent**.

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

3 In the **Times** text field, type `0 10^{range(-12,0.1,2)}`.

4 In the **Model Builder** window, click **Study 4**.

5 In the **Settings** window for **Study**, type `Efremov pressure sweep` in the **Label** text field.

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

7 Clear the **Generate convergence plots** check box.

Parametric Sweep

On the **Study** toolbar, click **Parametric Sweep**.

EFREMOV PRESSURE SWEEP

Parametric Sweep

1 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

2 Click **Add**.

3 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
p0	1e-3 2e-3 5e-3 10e-3 30e-3 100e-3	Torr

Solution 23 (sol23)

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

2 In the **Model Builder** window, expand the **Solution 23 (sol23)** node.

3 In the **Model Builder** window, expand the **Efremov pressure sweep>Solver Configurations> Solution 23 (sol23)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, locate the **Method and Termination** section.

5 From the **Jacobian update** list, choose **Minimal**.

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

EFREMOV PRESSURE SWEEP

1 In the **Model Builder** window, collapse the **Efremov pressure sweep** node.

Create 4 plots that show the results from the previous simulations. Each plot is labeled with the name of the authors that performed the measurements.

First create a plot with the data from the Corr study that shows the electron density, the atomic chlorine density, and the electronegativity as a function of the absorbed power.

RESULTS

1D Plot Group 1

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

2 In the **Settings** window for **1D Plot Group**, type `Corr power sweep` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Corr power sweep/ Parametric Solutions 1 (sol2)**.

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

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Plot Settings** section. Select the **x-axis label** check box.

7 In the associated text field, type `Power absorbed (W)`.

8 Select the **y-axis label** check box.

9 In the associated text field, type `Number density (m<sup>-3</sup>)`.

10 Select the **Two y-axes** check box.

11 Select the **Secondary y-axis label** check box.

12 In the associated text field, type `n-/ne`.

13 Locate the **Axis** section. Select the **Manual axis limits** check box.

14 In the **x minimum** text field, type `0`.

15 In the **x maximum** text field, type `325`.

16 In the **y minimum** text field, type `1e14`.

17 In the **y maximum** text field, type `1e21`.

18 In the **Secondary y minimum** text field, type `0`.

19 In the **Secondary y maximum** text field, type `20`.

20 Select the **y-axis log scale** check box.

21 Locate the **Legend** section. From the **Position** list, choose **Upper right**.

Global 1

1 Right-click **Corr power sweep** 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
plas.n_wCl	1/m^3	Number density
plas.ne	1/m^3	Electron density

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

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

6 In the table, enter the following settings:

Legends
Cl
ne

Global 2

1 In the **Model Builder** window, under **Results** right-click **Corr power sweep** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis** section.

3 Select the **Plot on secondary y-axis** check box.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
alpha	1	

5 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Pabs**.

6 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
n-/ne

8 On the **Corr power sweep** toolbar, click **Plot**.

Create a second plot with the data from the Malyshev and Donnelly study that shows the electron density, and the atomic chlorine density as a function of the absorbed power.

1D Plot Group 2

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

2 In the **Settings** window for **1D Plot Group**, type `Malyshev and Donnelly power sweep` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Malyshev and Donnelly power sweep/Parametric Solutions 2 (sol9)**.

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

5 Locate the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Plot Settings** section. Select the **x-axis label** check box.

7 In the associated text field, type `Power absorbed (W)`.

8 Select the **y-axis label** check box.

9 In the associated text field, type `Number density (m<sup>-3</sup>)`.

10 Locate the **Axis** section. Select the **Manual axis limits** check box.

11 In the **x minimum** text field, type `0`.

12 In the **x maximum** text field, type `700`.

13 In the **y minimum** text field, type `1e15`.

14 In the **y maximum** text field, type `1e21`.

15 Select the **y-axis log scale** check box.

Global 1

1 Right-click **Malyshev and Donnelly power sweep** 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
`plas.n_wCl`	`1/m^3`	`Number density`
`plas.ne`	`1/m^3`	`Electron density`

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

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Cl`
`ne`

7 On the **Malyshev and Donnelly power sweep** toolbar, click **Plot**.

1D Plot Group 3

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

Create a third plot with the data from the Corr and Efremov studies that shows the electron density, and the atomic chlorine density as a function of the pressure.

2 In the **Settings** window for **1D Plot Group**, type `Corr and Efremov pressure sweep` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **None**.

4 Locate the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `Pressure (Torr)`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `Number density (m<sup>-3</sup>)`.

9 Locate the **Axis** section. Select the **Manual axis limits** check box.

10 In the **x minimum** text field, type `8e-4`.

11 In the **x maximum** text field, type `125e-3`.

12 In the **y minimum** text field, type `1e16`.

13 In the **y maximum** text field, type `1e21`.

14 Select the **x-axis log scale** check box.

15 Select the **y-axis log scale** check box.

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

Global 1

1 Right-click **Corr and Efremov pressure sweep** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Data set** list, choose **Corr pressure sweep/Parametric Solutions 3 (sol16)**.

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

5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`plas.n_wCl`	`1/m^3`	`Number density`

6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **p0**.

7 From the **Parameter** list, choose **Expression**.

8 In the **Expression** text field, type `p0`.

9 From the **Unit** list, choose **Torr**.

10 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
Cl

Global 2

1 In the **Model Builder** window, under **Results** right-click **Corr and Efremov pressure sweep** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Data set** list, choose **Efremov pressure sweep/Parametric Solutions 4 (sol24)**.

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

5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
plas.ne	1/m^3	Electron density

6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **p0**.

7 From the **Parameter** list, choose **Expression**.

8 In the **Expression** text field, type `p0`.

9 From the **Unit** list, choose **Torr**.

10 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
ne

12 On the **Corr and Efremov pressure sweep** toolbar, click **Plot**.

1D Plot Group 4

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

Create the fourth and last plot with the data from the Efremov study that shows the electron temperature as a function of the pressure.

2 In the **Settings** window for **1D Plot Group**, type `Efremov pressure sweep` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Efremov pressure sweep/ Parametric Solutions 4 (sol24)**.

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

5 Locate the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Plot Settings** section. Select the **x-axis label** check box.

7 In the associated text field, type `Pressure (Torr)`.

8 Select the **y-axis label** check box.

9 In the associated text field, type `Te (V)`.

10 Locate the **Axis** section. Select the **Manual axis limits** check box.

11 In the **x minimum** text field, type `8e-4`.

12 In the **x maximum** text field, type `125e-3`.

13 In the **y minimum** text field, type `1`.

14 In the **y maximum** text field, type `5`.

15 Select the **x-axis log scale** check box.

16 Locate the **Legend** section. Clear the **Show legends** check box.

Global 1

1 Right-click **Efremov pressure sweep** 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
`plas.Te`	`V`	`Electron temperature`

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **p0**.

5 From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `p0`.

7 From the **Unit** list, choose **Torr**.

8 On the **Efremov pressure sweep** toolbar, click **Plot**.

Atmospheric Pressure Corona Discharge

Introduction

This model simulates a corona discharge occurring between two co-axially fashioned conductors. The negative electric potential is applied to the inner conductor and the exterior conductor is grounded. The discharge gas simulated is argon at atmospheric pressure.

Model Definition

Figure 1 shows a cross section of the model. By considering a long and uniform coaxial conductor configuration, the model can be viewed as axisymmetric and thus simplified to a 1D problem.

The model presented in the following section is used to simulate the ionization of the neutral gas (Ar) as well as the flux of charged particles (Ar+ and electrons) when the negative electric potential is applied at the inner conductor (cathode). The high electric field generated by the combination of high potential and small conductor curvature radius (inner conductor, r_i) causes electron drift and ionization of the neutral gas surrounding the cathode. The resulting ions generate more electrons through secondary emission at the cathode surface. These electrons are accelerated through a small region away from the cathode, where they can acquire significant energy. This can lead to ionization which creates new electron-ion pairs. The secondary ions migrate towards the cathode where they eject more secondary electrons. This process is responsible for sustaining the discharge.

The model is based on the fluid equations for electrons and ions as well as on Poisson's equation. Secondary electrons generated by ion bombardment of the cathode surface are taken into account. The model uses a Scharfetter-Gummel upwind scheme to eliminate numerical instabilities in the number density of the charged particles associated with the finite element method. This is needed, in particular close to the cathode, where the ion flux is particularly high.

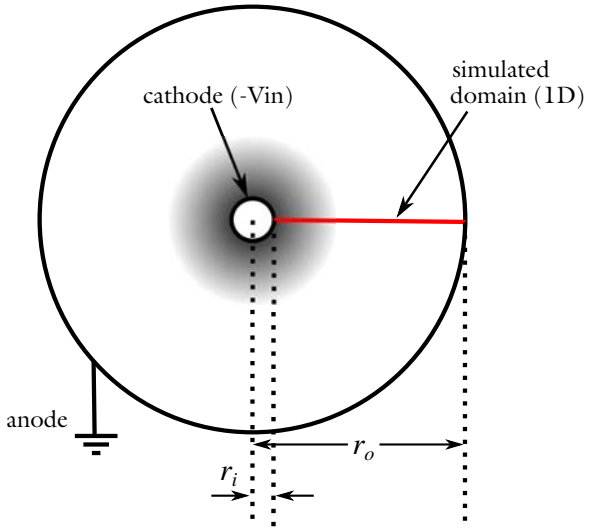

Figure 1: Not-to-scale cross section of the co-axial configuration. The negative potential ($-V_{in}$) is applied at the inner conductor (cathode) and the outer electrode is grounded (anode). The shaded area represents the ionization region created by the positive space charge distribution generated in the vicinity of the cathode.

DOMAIN EQUATIONS

The electron density and mean electron energy are computed by solving the drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For more detailed information on electron transport see the section Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using the relations

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \frac{5}{3}\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth

or decay of electron density and P inelastic electron-neutral collisions. In general $P \gg M$. In the case of rate coefficients, the electron source term is given by

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

Here $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross-section data as the integrals

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\mathrm{C}^{1/2}/\mathrm{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is the energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case, a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species:

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

For detailed information on the transport of the non-electron species see the section Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

The electrostatic field is computed using the equation

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

Boundary Conditions

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the boundary condition

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} v_{e,\,\mathrm{th}} n_e\right) - \sum_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{1}$$

for the electron flux and

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6} v_{e,\,\mathrm{th}} n_\varepsilon\right) - \sum_p \varepsilon_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{2}$$

for the electron energy flux. The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

The discharge is driven by the electric potential applied to the inner conductor of the coaxial geometry (at coordinate $r = r_i$).

$$V = V_0 \tanh\left(\frac{t}{\tau}\right)$$

where the function $\tanh(t/\tau)$ is used to generate the voltage step function (−1000 V). The other boundary (at coordinate $r = r_o$) is grounded.

Note that, during the simulation, the cathode is submitted to an intense flux of ions that generate an important amount of secondary electrons which, in turn, increase the cathode ion bombardment and so on. In order to prevent this avalanche from increasing indefinitely, a RC circuit has been added in series with the system. In order to model the

circuit addition, the voltage at the inner conductor is modified using the differential equation

$$V = V_0 - \left(I_p R_b + R_b C_b \frac{\partial V}{\partial t}\right)$$

where I_p is defined as

$$I_p = -\int \left(\mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e + \frac{\partial}{\partial t}(\mathbf{n} \cdot \mathbf{D})\right) dS$$

and where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density at the wall, $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density at the wall, and $\mathbf{n} \cdot \mathbf{D}$ the normal electrical displacement at the surface.

PLASMA CHEMISTRY

Argon is an attractive gas to use in a benchmark problem because only a handful of reactions and a few species need to be considered. Table 1 lists the chemical reactions considered.

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

Reaction	Formula	Type	$\Delta\varepsilon$ (eV)	k_f (m^3/(s·mol))
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	Ar+Ars=>Ar+Ar	Reaction	-	1807
7	Ars+Ars=>Ars+Ar	Reaction	-	$2.3 \cdot 10^7$

Initially a small number of seed electrons are present. These are necessary in order to initiate the discharge. In addition to the volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS.

Reaction	Formula	Sticking coefficient
1	Ars=>Ar	1
2	Ar+=>Ar	1

When the ion atoms reach the wall, they are assumed to change back to neutral argon atoms and donate their charge to the wall. Note that the secondary emission coefficient is

set to 0.2 on the cathode boundary (at coordinate $r = r_i$) and to 0 at the outer electrode (at coordinate $r = r_o$). The mean electron energy of the secondary electron is set to 4 eV.

Results and Discussion

When solving the problem, you can choose to plot the electron and ion density as the solver runs. Doing so allows the behavior of the charged species to be observed as the model is solving.

Looking at the evolution of the densities during the solving process shows that the gas is initially weekly ionized (electrons and ions having relatively low densities compared to neutral atoms). As the negative voltage is applied to the cathode, the highly mobile electrons are accelerated towards the anode leaving behind a positively charged gas in the cathode vicinity. With increasing negative potential, ion bombardment becomes more persistent on the cathode surface, which generates more secondary electrons, ionizing more neutral atoms, and engendering greater ion current. As the negative potential rises, the population of charged particles becomes larger as a consequence of this avalanche effect.

As the ion current becomes more significant, the RC circuit reduces the cathode negative potential such that an equilibrium is reached between the generation of the charged particles, preventing the transition of the plasma into an arcing regime.

Figure 2 shows the electron and ion densities at the end of the simulation ($t = 0.1$ s). Note that the figure is plotted on a log-log scale. In the figure, one can see that the ion density is approximately three orders of magnitude higher than the electron density in the vicinity of the cathode. The tiny positive space charge distribution generated by the ion density defines an ionization region that screens the cathode potential from the anode. This can be observed by displaying the electric potential along the radius of the coaxial assembly; see Figure 3.

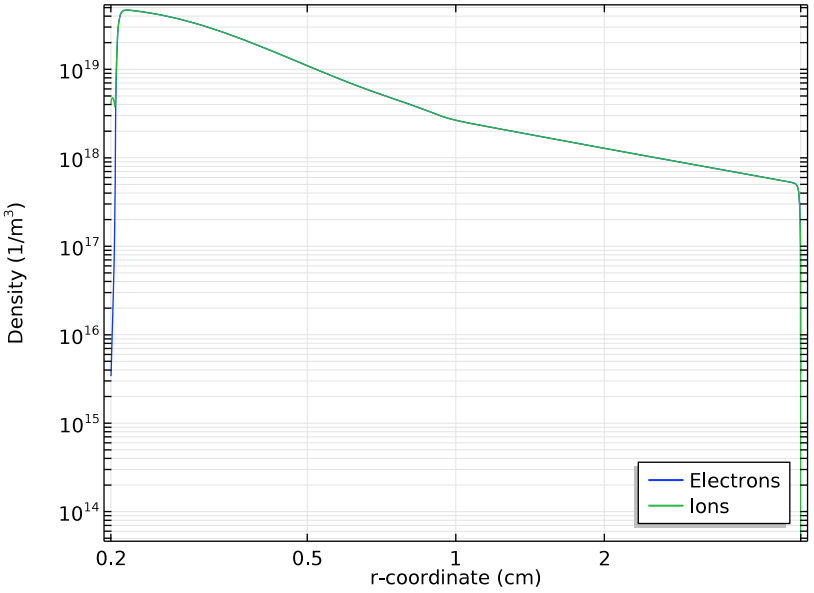

Figure 2: Plot of electron (blue) and ion (green) number density at the end of the simulation (t = 0.1 s).

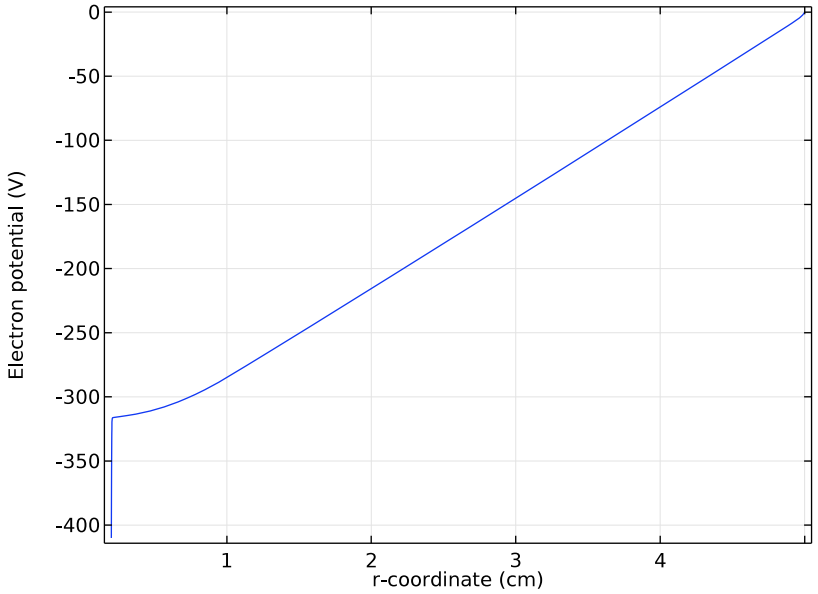

Figure 3: Electric potential along the radius of the coaxial assembly at the end of the simulation (t = 0.1 s).

The high voltage and important current density at the cathode enhance the electron temperature near the electrode, thus boosting ionization of the neutral atoms in the ionization zone. This can be seen in Figure 4, which displays the electron temperature at the end of the simulation.

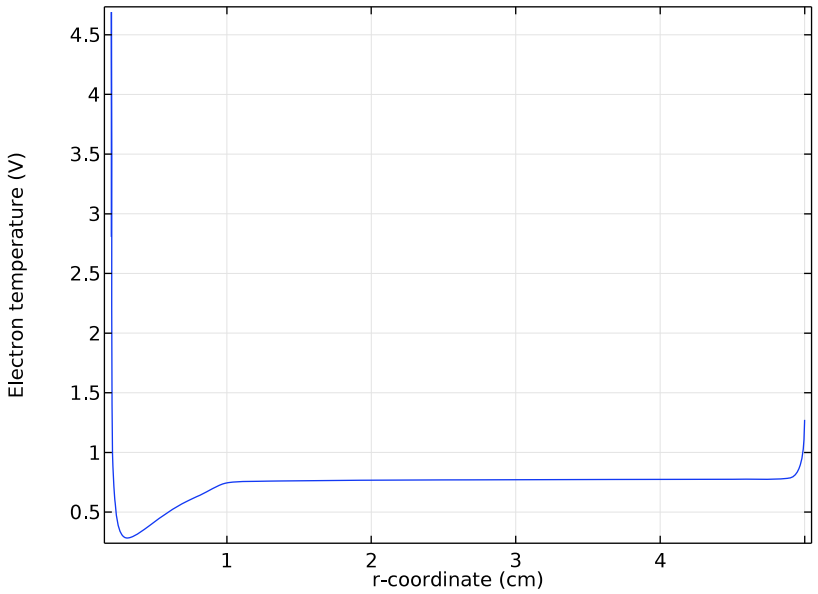

Figure 4: Electron temperature along the radius of the assembly at the end of the simulation (t = 0.1 s).

To see the effect of the RC circuit on the system, plot the secondary electron flux as a function of time at the cathode surface; see Figure 5. A close look at the figure shows a rapid rise of the flux that tends to stabilize as the circuit sees higher currents. Figure 6 also shows the potential at both electrodes as a function of time. Comparing figure Figure 5 with Figure 6 reveals the effect of the circuit on both potential and secondary emission at the cathode surface. One can also observe a similar effect by plotting the electron current density at the electrodes, Figure 6. Doing so shows a direct relation between the cathode secondary emission (positive current flow), the anode recombination (negative flow), and the RC circuit. Figure 7 displays a surface plot of the logarithm of the electron density at the last time step.

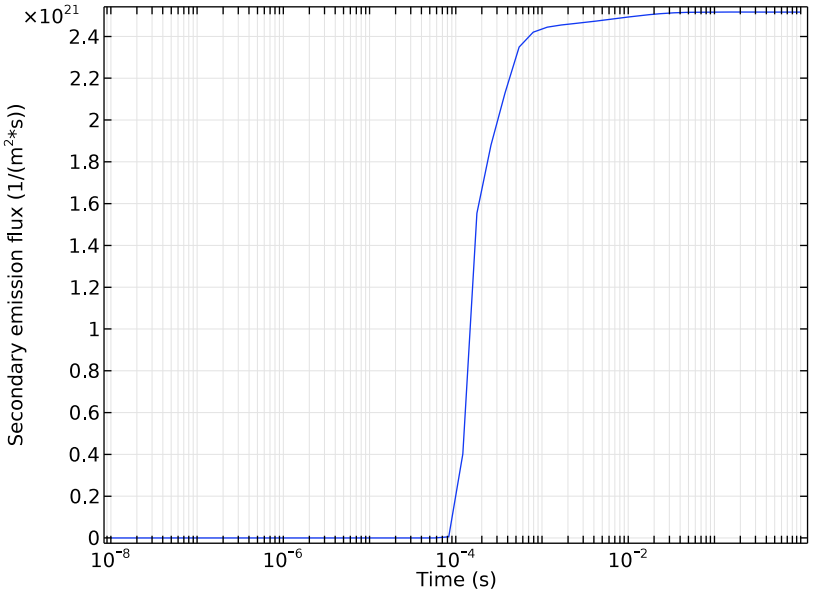

Figure 5: Secondary emission flux along time at the cathode.

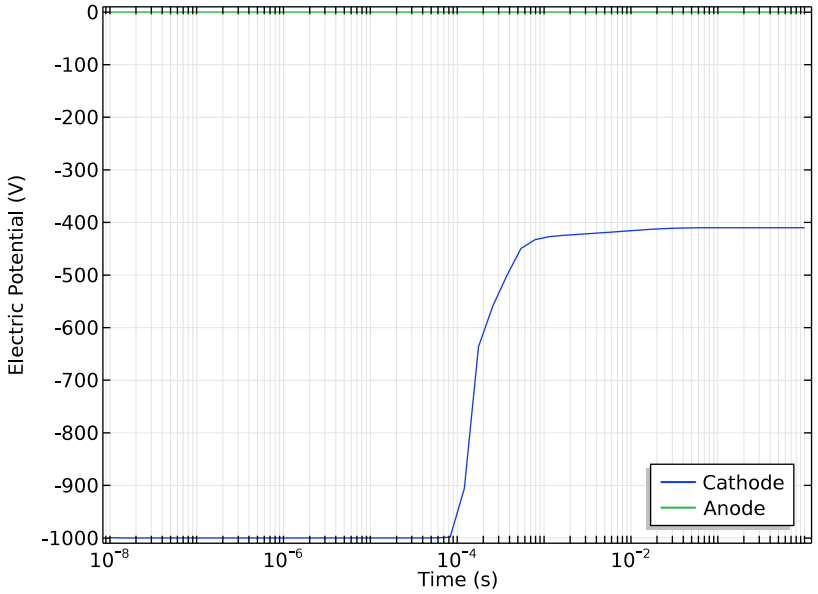

Figure 6: Potential at the electrodes as a function of time.

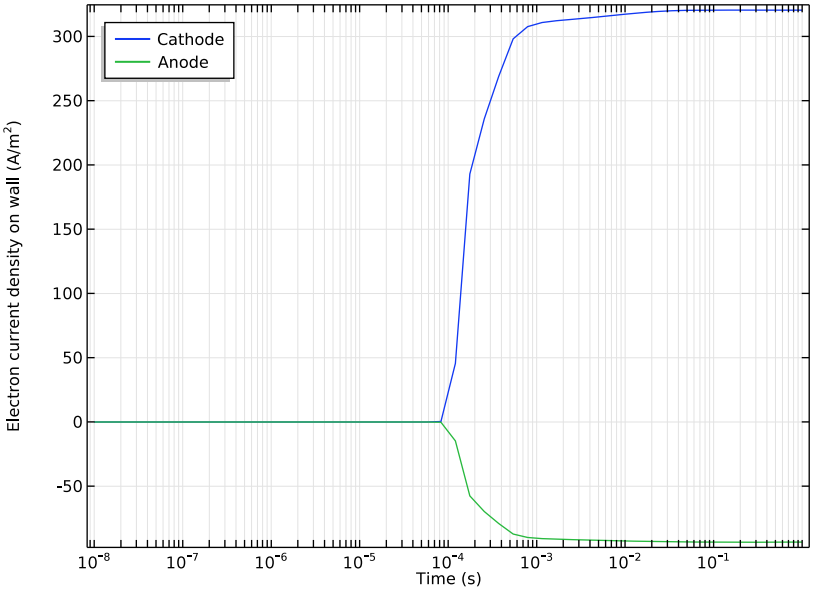

Figure 7: Electron current density at the electrodes as a function of time.

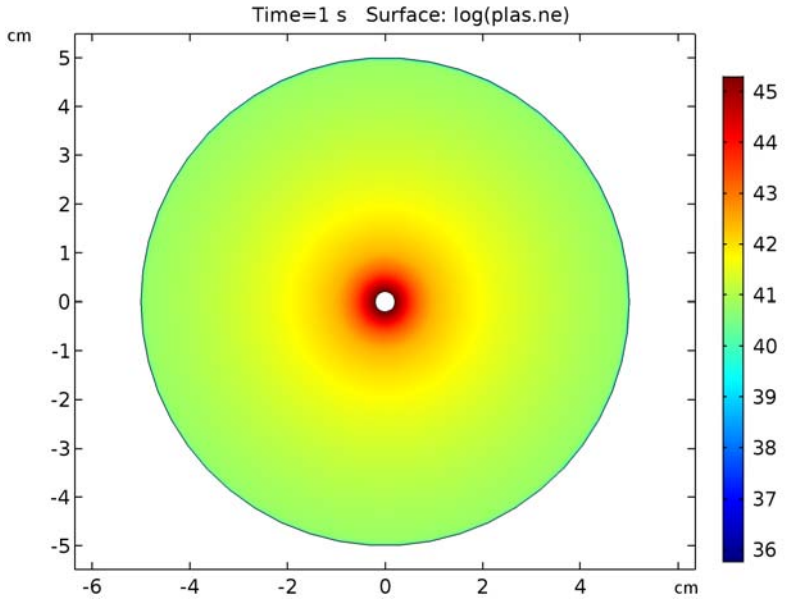

Figure 8: 2D electron density (log of n_e) at the last time step.

Application Library path: `Plasma_Module/Direct_Current_Discharges/corona_discharge_1d`

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 **1D Axisymmetric**.

2 In the **Select Physics** tree, select **Plasma>Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

To set up this model, you need access to some advanced settings.

PLASMA (PLAS)

Solve this model using the finite volume method and a Scharfetter-Gummel scheme. You can switch from the finite element method to the finite volume method by suitable choices in the **Discretization** section.

1 In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

2 In the **Model Builder** window, under **Component 1 (comp1)** click **Plasma (plas)**.

3 In the **Settings** window for **Plasma**, click to expand the **Discretization** section.

4 From the **Formulation** list, choose **Finite volume (constant shape function)**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
V0	1000[V]	1000 V	Voltage

GEOMETRY 1

Follow the steps below to create the model geometry: a simple 1D geometry consisting of a single domain bounded by the cathode (left, inner conductor) and the anode (right, outer conductor).

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

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

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

Interval 1 (i1)

1 On the **Geometry** toolbar, click **Interval**.

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

3 In the **Left endpoint** text field, type `0.2`.

4 In the **Right endpoint** text field, type `5`.

5 Click **Build All Objects**.

PLASMA (PLAS)

Load the argon cross sections from file. They form the basis of the plasma chemistry under investigation. To fix the species data, load the argon preset for each species.

Cross Section Import 1

1 On 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`.

When solving any type of reacting flow problem one species must always be chosen to fulfill the mass constraint. This should be taken as the species with the largest mass fraction.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar**.

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

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

When solving a plasma problem the plasma must initially be charge neutral. COMSOL automatically computes the initial concentration of a selected ionic species such that the initial electroneutrality constraint is satisfied. Now let the initial number density of argon ions be the same as the initial number of electrons. This forces the plasma to be initially charge neutral.

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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**.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar**.

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

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

Species: Ars

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ars**.

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

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

Now add two more regular reactions that describe how electronically excited argon atoms are consumed on the volumetric level. The rate coefficients for these reactions are taken from the literature.

Reaction 1

1 On 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 `Ar+Ars=>Ar+Ar`.

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

Reaction 2

1 On 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=>Ars+Ar`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `2.3e7`.

Surface reactions must always be included in a plasma model because they describe how ionic, excited, and radical species interact with the wall.

Surface Reaction 1

1 On 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 `Ars=>Ar`.

4 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

Secondary emission of electrons is important to sustain a DC discharge. In this example, add a secondary emission coefficient on the left wall (cathode).

Surface Reaction 2

1 On 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 Select Boundary 1 only.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0.2`.

6 In the ε_i text field, type `4`.

Surface Reaction 3

1 On 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 Select Boundary 2 only.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Plasma Properties** section.

7 Select the **Use reduced electron transport properties** check box.

8 Locate the **Out-of-Plane Thickness** section. In the d_z text field, type `0.02[m]`.

Plasma Model 1

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

2 In the **Settings** window for **Plasma Model**, locate the **Electron Density and Energy** section.

3 In the $\mu_e N_n$ text field, type `4e24`.

Ground 1

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

2 Select Boundary 2 only.

Now, add an RC circuit in series with the system. The role of the circuit is to limit the current at the cathode and avoid the arcing regime.

Metal Contact 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 In the V_0 text field, type `-V0`.

5 Locate the **Quick Circuit Settings** section. From the **Quick circuit type** list, choose **Series RC circuit**.

Wall 1

1 On 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**.

MESH 1

Meshing is a critical step in any plasma model. A fine mesh is needed close to the electrodes to capture the separation of space charge between the electrons and ions close to the wall.

Distribution 1

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

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

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

4 From the **Distribution properties** list, choose **Predefined distribution type**.

5 In the **Number of elements** text field, type `500`.

6 In the **Element ratio** text field, type `400`.

7 From the **Distribution method** list, choose **Geometric sequence**.

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

9 Click **Build All**.

STUDY 1

Compute an initial solution to generate the default plots and then set them up to show the electron and ion density while the solver runs.

1 In the **Model Builder** window, right-click **Study 1** and choose **Get Initial Value for Step**.

RESULTS

Electron Density (plas)

Set up an electron and ion density plot.

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

2 Select the **x-axis label** check box.

3 Select the **y-axis label** check box.

4 In the associated text field, type `Density (1/m<sup>3</sup>)`.

5 Click to expand the **Legend** section. From the **Position** list, choose **Lower right**.

Line Graph 1

1 In the **Model Builder** window, expand the **Electron Density (plas)** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click to expand the **Legends** section.

3 Select the **Show legends** check box.

4 From the **Legends** list, choose **Manual**.

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Legends** section. In the table, enter the following settings:

Legends
Electrons

7 Right-click **Results>Electron Density (plas)>Line Graph 1** and choose **Rename**.

8 In the **Rename Line Graph** dialog box, type `Electrons` in the **New label** text field.

9 Click **OK**.

Electrons 1

1 Right-click **Results>Electron Density (plas)>Electrons** and choose **Duplicate**.

2 In the **Model Builder** window, under **Results>Electron Density (plas)** right-click **Electrons 1** and choose **Rename**.

3 In the **Rename Line Graph** dialog box, type `Ions` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

6 In the **Expression** text field, type `plas.n_wAr_1p`.

7 Locate the **Legends** section. In the table, enter the following settings:

Legends
Ions

Electron Density (plas)

1 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

3 Right-click **Results>Electron Density (plas)** and choose **Rename**.

4 In the **Rename 1D Plot Group** dialog box, type `Electron and Ion Number Density` in the **New label** text field.

5 Click **OK**.

6 Click the **y-Axis Log Scale** button on the **Graphics** toolbar.

7 Click the **x-Axis Log Scale** button on the **Graphics** toolbar.

Now set up the last two default plots.

Electron Temperature (plas)

1 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electron Temperature (plas)** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

Electric Potential (plas)

1 In the **Model Builder** window, under **Results** click **Electric Potential (plas)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electric Potential (plas)** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **y-Axis Data** section. Select the **Description** check box.

5 In the associated text field, type `Electron potential`.

STUDY 1

Step 1: Time Dependent

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

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

3 In the **Times** text field, type `0` .

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 `-8`.

7 In the **Stop** text field, type `0`.

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

9 From the **Function to apply to all values** list, choose **exp10**.

10 Click **Add**.

11 In the **Settings** window for **Time Dependent**, click to expand the **Results while solving** section.

12 Locate the **Results While Solving** section. Select the **Plot** check box.

13 On the **Home** toolbar, click **Compute**.

RESULTS

Electric Potential (plas)

Now plot the electric potential on the electrodes.

Point Graph 1

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

2 In the **Model Builder** window, right-click **1D Plot Group 4** and choose **Point Graph**.

3 In the **Settings** window for **Point Graph**, locate the **Selection** section.

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

5 Locate the **y-Axis Data** section. In the **Expression** text field, type V.

6 Click to expand the **Legends** section. Select the **Show legends** check box.

7 From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
Cathode
Anode

9 Locate the **y-Axis Data** section. Select the **Description** check box.

10 In the associated text field, type `Electric potential`.

11 Click to expand the **Title** section. From the **Title type** list, choose **None**.

1D Plot Group 4

1 In the **Model Builder** window, under **Results** click **1D Plot Group 4**.

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

3 From the **Position** list, choose **Lower right**.

4 Right-click **Results>1D Plot Group 4** and choose **Rename**.

5 In the **Rename 1D Plot Group** dialog box, type `Electric Potential on Electrodes` in the **New label** text field.

6 Click **OK**.

7 Click the **x-Axis Log Scale** button on the **Graphics** toolbar.

8 On the **Electric Potential on Electrodes** toolbar, click **Plot**.

Electric Potential on Electrodes

1 In the **Model Builder** window, collapse the **Results>Electric Potential on Electrodes** node.

Plot the electron current density on the electrodes as follows:

Point Graph 1

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

2 In the **Model Builder** window, right-click **1D Plot Group 5** and choose **Point Graph**.

3 In the **Settings** window for **Point Graph**, locate the **Selection** section.

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

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.nJe`.

6 Locate the **Legends** section. Select the **Show legends** check box.

7 From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
Cathode
Anode

9 Locate the **Title** section. From the **Title type** list, choose **None**.

1D Plot Group 5

1 In the **Model Builder** window, under **Results** click **1D Plot Group 5**.

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

3 From the **Position** list, choose **Upper left**.

4 Right-click **Results>1D Plot Group 5** and choose **Rename**.

5 In the **Rename 1D Plot Group** dialog box, type `Electron Current Density on Electrodes` in the **New label** text field.

6 Click **OK**.

7 Click the **x-Axis Log Scale** button on the **Graphics** toolbar.

8 On the **Electron Current Density on Electrodes** toolbar, click **Plot**.

Electron Current Density on Electrodes

1 In the **Model Builder** window, collapse the **Results>Electron Current Density on Electrodes** node.

Next, plot the secondary electron emission at the cathode.

Point Graph 1

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

2 In the **Model Builder** window, right-click **1D Plot Group 6** and choose **Point Graph**.

3 Select Boundary 1 only.

4 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

5 In the **Expression** text field, type `plas.sflux`.

6 Locate the **Title** section. From the **Title type** list, choose **None**.

1D Plot Group 6

1 In the **Model Builder** window, under **Results** right-click **1D Plot Group 6** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Secondary Emission Flux` in the **New label** text field.

3 Click **OK**.

Secondary Emission Flux

1 In the **Model Builder** window, collapse the **Results>Secondary Emission Flux** node.

2 Click the **x-Axis Log Scale** button on the **Graphics** toolbar.

3 On the **Secondary Emission Flux** toolbar, click **Plot**.

Finally, create a nice plot for the model thumbnail.

Data Sets

1 On the **Results** toolbar, click **More Data Sets** and choose **Revolution 1D**.

2 In the **Model Builder** window, collapse the **Results>Data Sets** node.

RESULTS

Surface 1

1 On the **Results** toolbar, click **2D Plot Group**.

2 In the **Model Builder** window, right-click **2D Plot Group 7** and choose **Surface**.

3 In the **Settings** window for **Surface**, locate the **Expression** section.

4 In the **Expression** text field, type `log(plas.ne)`.

2D Plot Group 7

1 In the **Model Builder** window, under **Results** right-click **2D Plot Group 7** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `Log of Electron Density` in the **New label** text field.

3 Click **OK**.

Log of Electron Density

1 In the **Model Builder** window, collapse the **Results>Log of Electron Density** node.

2 On the **Log of Electron Density** toolbar, click **Plot**.

3 Click the **Zoom Extents** button on the **Graphics** toolbar.

Atmospheric Pressure Corona Discharge in Air

Introduction

This example presents a study of a co-axial DC corona discharge in dry air at atmospheric pressure. The dimensions and operation conditions are similar to the ones found in electrostatic precipitators with wire-to-plate configuration. The inner electrode has 100 μm radius and the gap between electrodes is 10 cm. The simulations presented are for steady state regimes with the discharge sustained with 10s kV applied to the inner electrode while the exterior electrode is grounded. Emphasis is placed on the charged particles creation and transport and how that translates into the current-voltage characteristic of the discharge.

Model Definition

Figure 1 shows a cross section of the model geometry. The discharge is assumed to be diffuse and uniform in the radial direction. The model is one dimensional in the radial direction between the electrodes and describes the behavior of charged species using fluid-type equations. We Assume that the gas temperature and air number density are constant. The gas temperature is kept at 600 K.

The model solves the electron and ions continuity and momentum equations, in the drift-diffusion approximation, self-consistently coupled with Poisson's equation. The local field approximation is used, which means that transport and source coefficients are assumed to be well parametrized through the reduced electric field ($\boldsymbol{E}/\boldsymbol{N}$). In the local field approximation the fluid equation for the mean electron energy is not solved, which reduces significantly the complexity of the numerical problem.

The local field approximation is valid in a situation where the rate of electron energy gain from the electric field is locally balanced by the energy loss rate. When this condition is met the electrons are said to be in local equilibrium with the electric field and the electron mean properties can be expressed as a function the reduced electric field.

The model presented in the following section is used to simulate the ionization of the neutral gas as well as the flux of charged particles when the negative electric potential is applied at the inner conductor (cathode). The high electric field generated by the combination of high potential and small conductor curvature radius (inner conductor, r_{i}) causes electron drift and ionization of the neutral gas surrounding the cathode. The resulting positive ions generate more electrons through secondary emission at the cathode surface. These electrons are accelerated through a small region away from the cathode, where they can acquire significant energy. This can lead to ionization which creates new

electron-ion pairs. The secondary ions migrate towards the cathode where they eject more secondary electrons. This process is responsible for sustaining the discharge.

The model uses a Scharfetter-Gummel upwind scheme to eliminate numerical instabilities in the number density of the charged particles associated with the finite element method. This is needed, in particular close to the cathode, where the ion flux is particularly high.

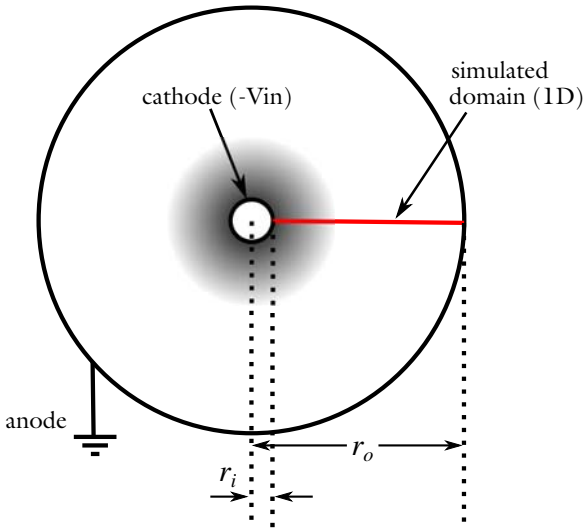

Figure 1: Not-to-scale cross section of the co-axial configuration. The negative potential ($-V_{in}$) is applied at the inner conductor (cathode) and the outer electrode is grounded (anode). The shaded area represents the ionization region created by the positive space charge distribution generated in the vicinity of the cathode.

DOMAIN EQUATIONS

The electron density is computed by solving the drift-diffusion equation for the electron density.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e \qquad (1)$$

Convection of electrons due to fluid motion is neglected. For more detailed information on electron transport see the section Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

When using the local field approximation the electron density equation is not solved and the transport and source coefficients are mapped by the reduced electric field. In practice,

when using the local field approximation or the local energy approximation, the transport and source coefficients are still given as a function of the mean electron energy. When using the local field approximation however, it must be provided a function that relates the mean electron energy and the reduced electric field

$$\varepsilon = F(E/N)\,. \tag{2}$$

The electron source R_e is defined later. The electron diffusivity is computed from the electron mobility using the relation

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e \tag{3}$$

The source coefficients in the above equation is determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general $P \gg M$. In the case of rate coefficients, the electron source term is given by

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e \tag{4}$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). For DC discharges it is better practice to use Townsend coefficients instead of rate coefficients to define reaction rates. Townsend coefficients provide a better description of what happens in the cathode fall region Ref. 1. When Townsend coefficients are used, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j \alpha_j N_n |\boldsymbol{\Gamma}_e| \tag{5}$$

where α_j is the Townsend coefficient for reaction j (m^2) and Γ_e is the electron flux as defined above ($1/(\mathrm{m}^2{\cdot}\mathrm{s})$). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges.

For non-electron species, the following equation is solved for the mass fraction of each species:

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u}\cdot\nabla)w_k = \nabla\cdot\mathbf{j}_k + R_k \tag{6}$$

For detailed information on the transport of the non-electron species see the section Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

The electrostatic field is computed using the equation

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho \tag{7}$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right) \tag{8}$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

Boundary Conditions

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the boundary condition for the electron flux

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} \nu_{e,\,\mathrm{th}} n_e\right) - \sum_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{9}$$

The second term on the right-hand side of Equation 9 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0] \tag{10}$$

The discharge is driven by a DC electric potential (V_0) applied to the inner conductor of the co-axial geometry (at coordinate $r = r_\mathrm{i}$). The other boundary (at coordinate $r = r_\mathrm{o}$) is grounded. To facilitate the beginning of the numerical simulation a step function is used to modulate V_0 with the transient applied potential assuming the form

$$V = V_0 \tanh\left(\frac{t}{\tau}\right). \tag{11}$$

This numeric technique does not interfere with the results at steady state, which are the ones of interest in this work.

PLASMA CHEMISTRY

The chemistry of a plasma sustained in air can be very complex and a detailed study of the main excited states could easily have hundreds of reactions. The main goal of this model is to study the charge particle density profiles and currents. With that in mind it is used a simplified set of reactions that describes correctly the creation and destruction of charged species in a background of dry air.

Table 1 lists the chemical reactions considered Ref. 2. In the fluid equations Nitrogen and Oxygen are not treated separately as in a detailed chemistry. Instead a general species A is used for the background gas. A can be ionized forming positive ions p, and A can attach electrons forming negative ions n.

The creation and destruction of electrons in the volume is described by ionization and attachment Townsend coefficients, and by rate constants for a three-body attachment and electron-ion recombination. The Townsend coefficients are obtained as a function of the mean electron energy by suitably averaging over the electron energy distribution computed using a Boltzmann solver with a consistent set of electron scattering collisions cross sections of Nitrogen and Oxygen Ref. 3. It is used a mixture of 80% Nitrogen and 20% Oxygen. The relation between the mean electron energy and the reduced electric field is also obtain from the Boltzmann solver and is given in Figure 2.

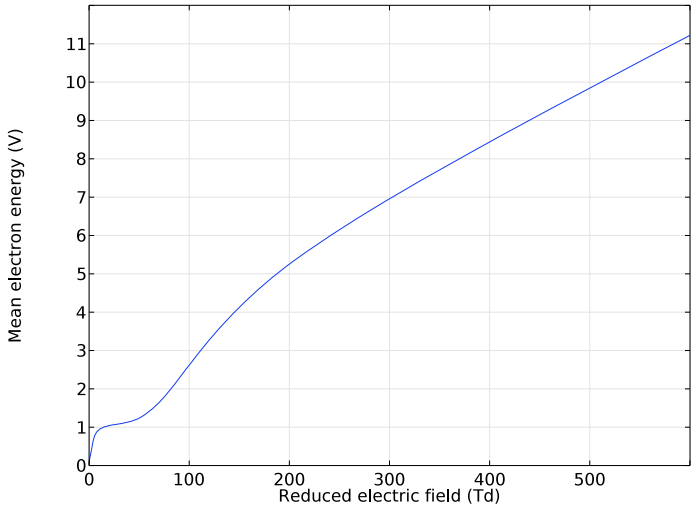

Figure 2: Mean electron energy as a function of the reduced electric field for a mixture of 80% Nitrogen and 20% Oxygen.

For detailed information on how to compute source coefficients from a Boltzmann solver see the section The Boltzmann Equation, Two-Term Approximation Interface in the *Plasma Module User's Guide*.

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

Reaction	**Formula**	**Type**	$\Delta\varepsilon$ **(eV)**	k_f **(m^3/s)**
1	e+A=>p+2e	Ionization	15	-
2	e+A=>n	Attachment	-	-
3	e+2A=>n+A	Attachment	-	-
4	e+p=>A	Reaction	-	$5\cdot10^{-14}$
5	n+p=>2A	Reaction	-	$5\cdot10^{-12}$

At steady state the plasma main charged species are ions. For this reason the initial conditions have an equal density of positive and negative ions and a small density of electrons. These initial conditions preserve charge neutrality as it is important for numerical reasons.

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

TABLE 2: TABLE OF SURFACE REACTIONS.

Reaction	Formula	Sticking coefficient
1	p=>A	1
2	n=>A	1

When the ions reach the wall, they are assumed to change back to neutral atoms. Note that the secondary emission coefficient for positive ions is set to 0.05 on the cathode boundary (at coordinate $r = r_i$) and to 0 at the outer electrode (at coordinate $r = r_o$). The mean electron energy of the secondary electron is set to 4 eV. When using the local field approximation the mean energy of the secondary electron is only used in post-processing.

Results and Discussion

Throughout most of this section, results are presented and discussed for a DC negative corona sustained with -45 kV applied to the inner electrode. At the end, the current-voltage characteristic of the discharge are presented. The background gas is kept at a constant density as obtained by the ideal gas law at atmospheric pressure and at a temperature of 600 K. All results presented and discussed correspond to a steady state operation.

When comparing with corona discharges sustained in noble gases, air corona discharges need much higher voltage to breakdown the background gas and to sustain a discharge. There are two main reasons for this: (i) the electron collision frequency in air is higher (in part due to rotational and vibrational interactions) making it more difficult to accelerate electrons; and (ii) oxygen is electronegative.

Figure 3 presents the spatial profiles of the charged species. The discharge can be separated in two regions: (a) corresponding to a region of less than 1 mm near the cathode where most of the ionization occurs; and (b) the rest of the volume that reaches to the ground electrode.

The strongly negative potential at the inner electrode accelerates positive ions towards it and repeals negative charged particles. The result is a region of positive charge separation (region (a)) where strong electric fields exist and the electrons are accelerated to energies capable of ionizing the background gas. The electron temperature, the electric potential, and the reduced electric field are represented in Figure 4, Figure 5, and Figure 6. As can be seen, region (b) has weak electric field and consequent electron temperatures. In this region, electrons have not enough energy to ionize and are efficiently attached forming negative ions. The result is a long spatial portion of the discharge dominated by negative

ions that drift towards the ground electrode. Note also that in region (b) the charge separation barely deforms the applied potential.

Figure 7, Figure 8 and Figure 9 are 2D representations (obtained by a revolution of the 1D solution) of the charged species number density. A representation of the charge distribution with distances in linear scale helps to build a more realistic image of this type of discharges. Notice how small is the inner electrode and the ionization region, and how most of the volume is filled with negative ions drifting in the directions of the anode. This observation does not mean that region (a) should be neglected. In fact, it is in region (a) that the mechanisms that sustain the discharge occur.

Comparing with corona discharges in noble gases, this type of corona discharges have a much higher resistivity because the charged particle number density is much lower, and ions, much less mobile than electrons, are the main charge carriers.

Figure 10 shows the absolute value of the total ion current at the ground electrode as a function of the absolute value of the applied voltage at the inner electrode. The current-voltage characteristic follows a quadratic law as expected. The values of current density obtained are also coherent with the ones find in this type of discharges.

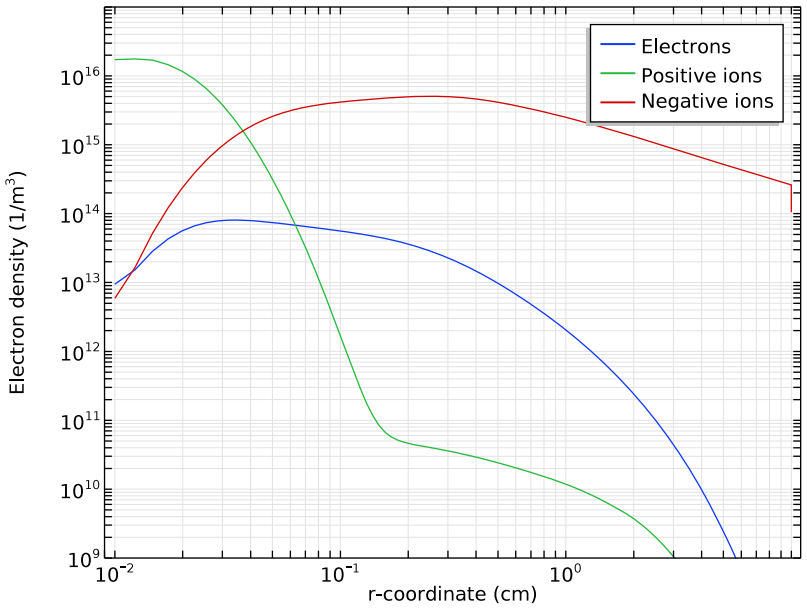

Figure 3: Spatial profiles of the charged species number density at steady state: electrons (blue), positive ions (green), and negative ions (red).

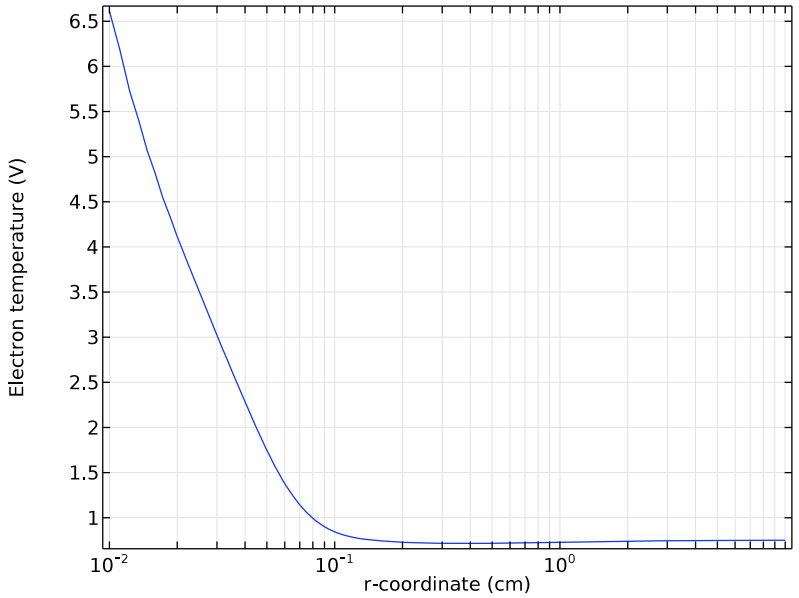

Figure 4: Spatial profile of the electron temperature.

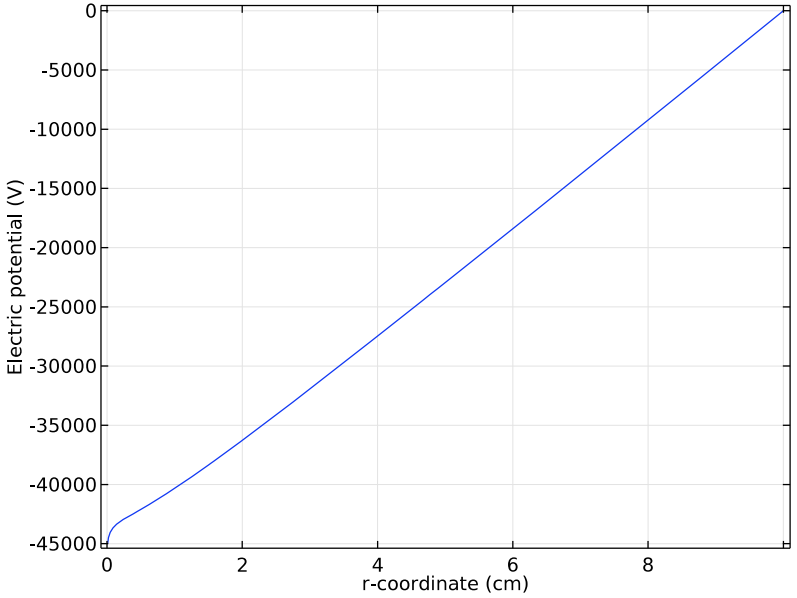

Figure 5: Spatial profile of the electric potential.

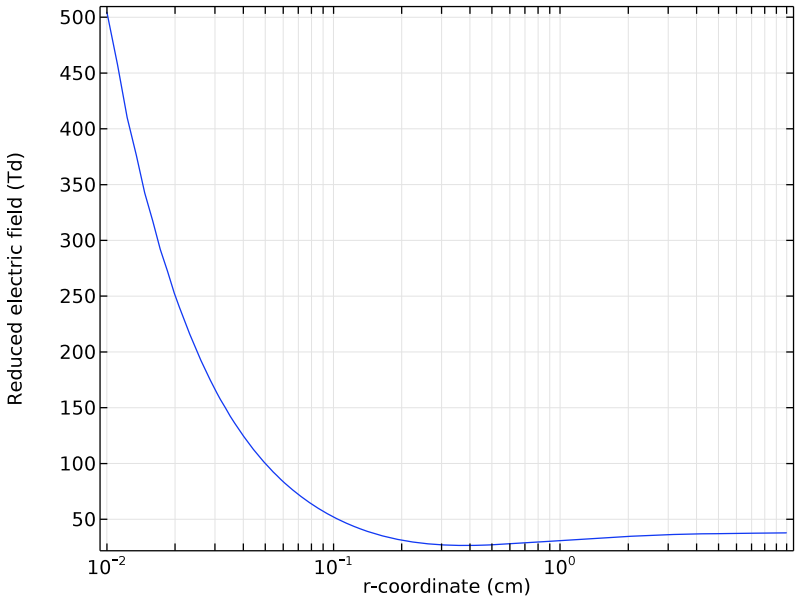

Figure 6: Spatial profile of the reduced electric field

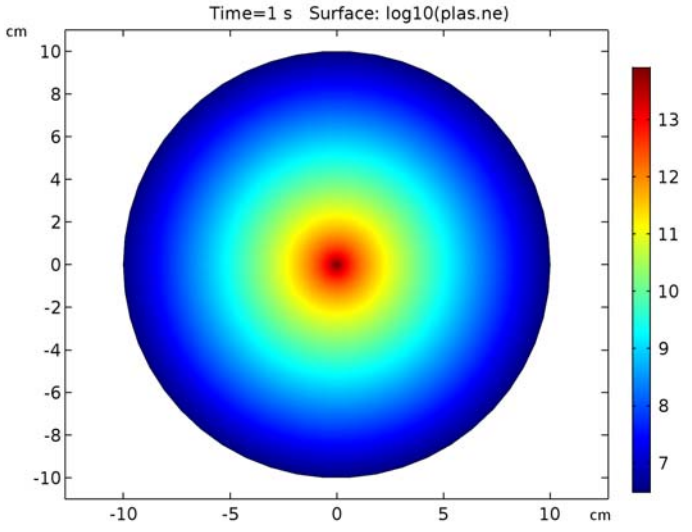

Figure 7: 2D representation of the electron density (the scale is in log base 10).

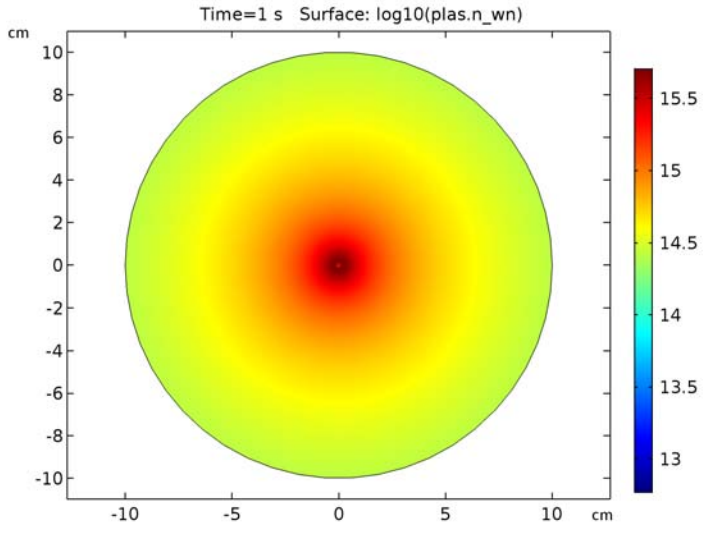

Figure 8: 2D representation of the negative ion density (the scale is in log base 10).

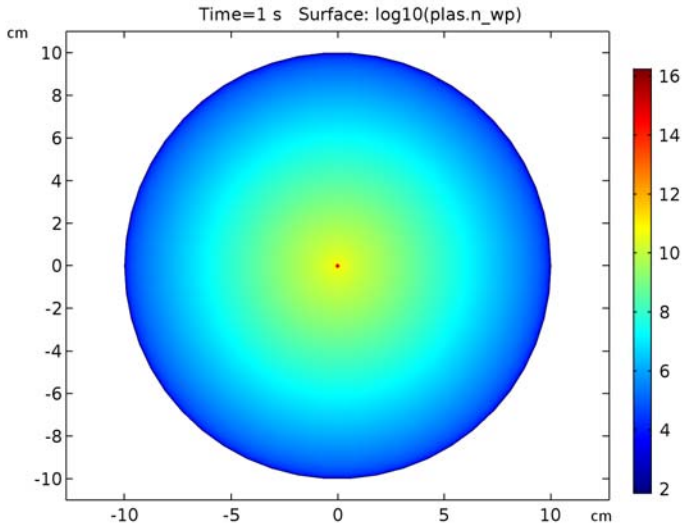

Figure 9: 2D representation of the positive ion density (the scale is in log base 10).

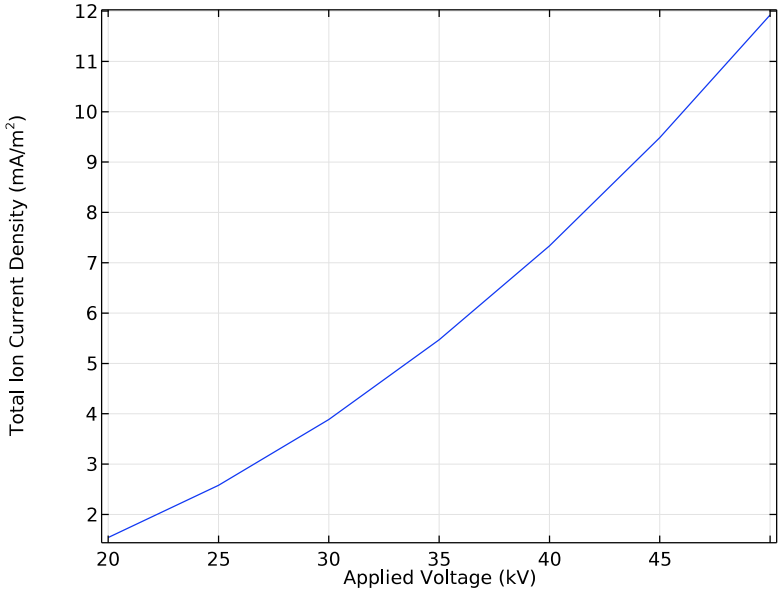

Figure 10: Total ion current density (absolute value) at the ground electrode as a function of the applied voltage (absolute value) at the inner electrode.

Reference

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

2. A. A. Kulikovsky, "Positive streamer between parallel plate electrode in atmospheric pressure air", *J. Phys. D: Appl. Phys.*, vol. 30, pp. 441–450, 1997.

3. LXCAT, see http://fr.lxcat.net for Phelps database (2016).

Application Library path: `Plasma_Module/Direct_Current_Discharges/corona_discharge_air_1d`

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 **1D Axisymmetric**.

2 In the **Select Physics** tree, select **Plasma>Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GEOMETRY 1

Follow the steps below to create the model geometry: a simple 1D geometry consisting of a single domain bounded by the cathode (left, inner conductor) and the anode (right, outer conductor).

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

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

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

Interval 1 (i1)

1 On the **Geometry** toolbar, click **Interval**.

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

3 In the **Left endpoint** text field, type `10`.

4 In the **Right endpoint** text field, type `0.01`.

5 Click **Build All Objects**.

DEFINITIONS

Variables 1

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

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
mueN	3.74e24*(plas.Erd*1e21)^-0.22[1/(V*m*s)]		Reduced electron mobility
muiN	6e21[1/(V*s*m)]	1/(V·m·s)	Reduced ion mobility
rnp	2e-6[cm^3/s]	m^3/s	ion-ion recombination
rei	5e-8[cm^3/s]	m^3/s	electron-ion recombination
Vapp	-V0*ramp		Applied Voltage
ramp	tanh(1e5*t)		
p0	760[torr]	Pa	Gas pressure
t0	600[K]	K	Gas temperature
ni0	1e17[m^-3]	$1/m^3$	Initial ion number density
ne0	1e10[m^-3]	$1/m^3$	Initial electron number density

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
V0	45[kV]	4.5E4 V	

PLASMA (PLAS)

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

2 In the **Settings** window for **Plasma**, locate the **Out-of-Plane Thickness** section.

3 In the d_z text field, type `1[m]`.

4 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** check box.

This model uses the local field approximation to parametrize in space source and trasnport coefficients

5 From the **Mean electron energy** list, choose **Local field approximation**.

Solve this model using the finite volume method and a Scharfetter-Gummel scheme. You can switch from the finite element method to the finite volume method by suitable choices in the **Discretization** section.

6 In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

7 Click to expand the **Discretization** section. From the **Formulation** list, choose **Finite volume (constant shape function)**.

Electron Impact Reaction 1

1 Right-click **Component 1 (comp1)>Plasma (plas)** and choose the domain setting **Heavy Species Transport>Electron Impact Reaction**.

Add an ionization reaction.

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

3 In the **Formula** text field, type `A+e=>p+2e`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the Δε text field, type `15`.

Import the ionization Townsend coefficient

6 Locate the **Collision** section. From the **Specify reaction using** list, choose **Use lookup table**.

7 Locate the **Reaction Parameters** section. From the **Rate constant form** list, choose **Townsend coefficient**.

8 Click **Load from File**.

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

Electron Impact Reaction 2

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport>Electron Impact Reaction**.

Add an attachment reaction.

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

3 In the **Formula** text field, type `A+e=>n`.

4 Locate the **Collision Type** section. From the list, choose **Attachment**.

Import the attachment Townsend coefficient.

5 Locate the **Collision** section. From the **Specify reaction using** list, choose **Use lookup table**.

6 Locate the **Reaction Parameters** section. From the **Rate constant form** list, choose **Townsend coefficient**.

7 Click **Load from File**.

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

Electron Impact Reaction 3

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Electron Impact Reaction**.

Add a 3-body attachment reaction.

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

3 In the **Formula** text field, type `A + A + e => n + A`.

4 Locate the **Collision Type** section. From the list, choose **Attachment**.

5 Locate the **Reaction Parameters** section. In the k^f text field, type `1.4e-41*(0.026/plas.Te)*exp(100/t0-0.061/plas.Te)*N_A_const^2*0.1`.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

Add electron-ion recombination.

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

3 In the **Formula** text field, type `e+p=>A`.

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

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

Add ion-ion recombination.

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

3 In the **Formula** text field, type `n+p=>A+A`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `rnp*N_A_const`.

Species: A

When solving any type of reacting flow problem one species must always be chosen to fulfill the mass constraint. This should be taken as the species with the largest mass fraction.

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: A**.

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 **N2**.

Species: p

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: p**.

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

3 From the **Species type** list, choose **Ion**.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **N2**.

5 In the z text field, type `1`.

6 In the n_0 text field, type `ni0`.

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

8 Click to expand the **Mobility specification** section. Locate the **Mobility Specification** section. In the u_{m} text field, type `muiN/plas.Nn`.

Species: n

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: n**.

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

3 From the **Species type** list, choose **Ion**.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **N2**.

5 In the z text field, type `-1`.

6 In the n_0 text field, type `ni0`.

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

8 Click to expand the **Mobility specification** section. Locate the **Mobility Specification** section. In the u_{m} text field, type `muiN/plas.Nn`.

Surface Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

Surface reactions must always be included in a plasma model because they describe how ions, excited, and radical species interact with the wall. Secondary emission of electrons is important to sustain a DC discharge. In this example, add a secondary emission coefficient on the left wall (cathode).

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

3 In the **Formula** text field, type `p=>A`.

4 Select Boundary 1 only.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0.05`.

6 In the ε_i text field, type `4`.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

3 In the **Formula** text field, type `p=>A`.

4 Select Boundary 2 only.

Surface Reaction 3

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

3 In the **Formula** text field, type `n=>A`.

4 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

Plasma Model 1

Set up the background gas information, the electron mobility and import the table that gives the relation between the mean electron energy and the reduced electric field.

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

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

3 In the T text field, type `t0`.

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

5 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `mueN`.

6 Click to expand the **Mean electron energy specification** section. Locate the **Mean Electron Energy Specification** section. From the **Specify using** list, choose **Use lookup table**.

7 Click **Load from File**.

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

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,\,0}$ text field, type `ne0`.

Ground 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

2 Select Boundary 2 only.

Metal Contact 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics> Metal Contact**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

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

Wall 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

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

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

MESH 1

Meshing is a critical step in any plasma model. A fine mesh is needed close to the electrodes to capture the separation of space charge between the electrons and ions close to the wall.

Distribution 1

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edge**.
2. Right-click **Edge 1** and choose **Distribution**.
3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. From the **Distribution properties** list, choose **Predefined distribution type**.
5. In the **Number of elements** text field, type 200.
6. In the **Element ratio** text field, type 100.
7. From the **Distribution method** list, choose **Geometric sequence**.
8. Select the **Symmetric distribution** check box.
9. Click **Build All**.

STUDY 1

Step 1: Time Dependent

1. In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
2. In the **Times** text field, type `0 10^{range(-8,8/49,0)}`.
3. Click to expand the **Results while solving** section. Locate the **Results While Solving** section. Select the **Plot** check box.

Solution 1 (sol1)

1. On the **Study** toolbar, click **Show Default Solver**.
2. In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

   Set the Jacobian update to minial to decrease the computational time.
3. In the **Model Builder** window, expand the **Study 1>Solver Configurations> Solution 1 (sol1)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.
4. In the **Settings** window for **Fully Coupled**, click to expand the **Method and termination** section.
5. Locate the **Method and Termination** section. From the **Jacobian update** list, choose **Minimal**.

   Get the initial values to generate the default plots and then set them up to show the electron and ion densities while the solver runs.

Electron Density (plas)

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

RESULTS

Electron Density (plas)

1. In the **Settings** window for **1D Plot Group**, type `Electron and Ion Number Density` in the **Label** text field.
2. Click to expand the **Title** section. From the **Title type** list, choose **None**.
3. Locate the **Data** section. From the **Time selection** list, choose **Last**.
4. Locate the **Plot Settings** section. Select the **x-axis label** check box.
5. Select the **y-axis label** check box.
6. Locate the **Axis** section. Select the **Manual axis limits** check box.
7. In the **x minimum** text field, type `0.009`.
8. In the **x maximum** text field, type `11`.
9. In the **y minimum** text field, type `1e9`.
10. In the **y maximum** text field, type `1e17`.
11. Select the **x-axis log scale** check box.
12. Select the **y-axis log scale** check box.

Line Graph 1

1. In the **Model Builder** window, expand the **Results>Electron and Ion Number Density** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, type `Electrons` in the **Label** text field.
3. Click to expand the **Legends** section. Select the **Show legends** check box.
4. From the **Legends** list, choose **Manual**.
5. In the table, enter the following settings:

Legends
Electrons

6. Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

Electrons 1

1. Right-click **Results>Electron and Ion Number Density>Electrons** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, type `Positive ions` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.n_wp`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Positive ions

Positive ions 1

1 Right-click **Results>Electron and Ion Number Density>Positive ions** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `Negavtive ions` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.n_wn`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Negative ions

Electron Temperature (plas)

1 In the **Model Builder** window, under **Results** click **Electron Temperature (plas)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

4 Locate the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Axis** section. Select the **x-axis log scale** check box.

Electric Potential (plas)

1 In the **Model Builder** window, under **Results** click **Electric Potential (plas)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

4 Locate the **Title** section. From the **Title type** list, choose **None**.

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

Electric Potential (plas) 1

1 Right-click **Electric Potential (plas)** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Reduced Electric Field` in the **Label** text field.

3 Locate the **Axis** section. Select the **x-axis log scale** check box.

Line Graph 1

1 In the **Model Builder** window, expand the **Results>Reduced Electric Field** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `plas.Erd`.

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

5 On the **Reduced Electric Field** toolbar, click **Plot**.

2D Plot Group 5

1 On the **Results** toolbar, click **More Data Sets** and choose **Revolution 1D**.

2 On the **Results** toolbar, click **2D Plot Group**.

3 In the **Settings** window for **2D Plot Group**, type `Log of Electron Density` in the **Label** text field.

Surface 1

1 Right-click **Log of Electron Density** and choose **Surface**.

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

3 In the **Expression** text field, type `log10(plas.ne)`.

4 On the **Log of Electron Density** toolbar, click **Plot**.

Log of Electron Density 1

1 In the **Model Builder** window, under **Results** right-click **Log of Electron Density** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Log of Negative Ion Density` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Log of Negative Ion Density** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `log10(plas.n_wn)`.

4 On the **Log of Negative Ion Density** toolbar, click **Plot**.

Log of Negative Ion Density 1

1 In the **Model Builder** window, under **Results** right-click **Log of Negative Ion Density** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Log of Positive Ion Density` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Log of Positive Ion Density** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `log10(plas.n_wp)`.

4 On the **Log of Positive Ion Density** toolbar, click **Plot**.

STUDY 1

Prepare a parametrization of the applied volatge.

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

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

3 Clear the **Generate default plots** check box.

4 Clear the **Generate convergence plots** check box.

Parametric Sweep

1 On the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 Click to select row number 1 in the table.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V0	20 25 30 35 40 45 50	kV

Step 1: Time Dependent

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

2 In the **Settings** window for **Time Dependent**, click to expand the **Results while solving** section.

3 Locate the **Results While Solving** section. Clear the **Plot** check box.

Parametric Sweep

On the **Study** toolbar, click **Compute**.

RESULTS

1D Plot Group 8

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

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

Point Graph 1

1 Right-click **1D Plot Group 8** and choose **Point Graph**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Current>plas.nJt - Total ion current density on wall**.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `abs(plas.nJt)`.

5 In the **Unit** field, type `mA/m^2`.

6 Select the **Description** check box.

7 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **V0**.

8 From the **Parameter** list, choose **Expression**.

9 In the **Expression** text field, type `V0`.

10 From the **Unit** list, choose **kV**.

11 Select the **Description** check box.

12 In the associated text field, type `Applied Voltage`.

1D Plot Group 8

1 In the **Model Builder** window, under **Results** click **1D Plot Group 8**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **y-axis label** check box.

4 In the associated text field, type `Total Ion Current Density (mA/m<sup>2</sup>)`.

5 On the **1D Plot Group 8** toolbar, click **Plot**.

Dipolar Microwave Plasma Source

Introduction

This model presents a 2D axisymmetric dipolar microwave plasma source sustained through resonant heating of the electrons. This is known as electron cyclotron resonance (ECR), which occurs when a suitable high magnetic flux density is present along with the microwaves.

This is an advanced model that showcases many of the features that make COMSOL unique, including:

- Infinite elements for the magnetostatic model.
- Functional-based mesh adaption to create a fine mesh on the ECR surface.
- PMLs for the electromagnetic waves to represent infinite space.
- Degrees of freedom for all 3 components of the high-frequency electric field despite the fact that the problem is geometrically axisymmetric.
- Full anisotropic tensors for the plasma conductivity and charged particle transport properties.
- Resonant power absorption in the ECR surface by the electrons.
- Equation-based modeling using integrated quantities to fix the total absorbed power.
- Solver sequencing to first compute the static magnetic field, then solve for all the plasma components.

Note: This application requires the Plasma Module, AC/DC Module, and RF Module.

Model Definition—Static Magnetic Field

For the static magnetic field, Ampère's law governs the azimuthal component of the magnetic vector potential:

$$\nabla \times \mu_r^{-1} \mu_0^{-1} (\nabla \times A_\varphi) = J_\varphi$$

where the external current density, J_φ only has an azimuthal component and is defined in the coil as:

$$J_\varphi = \frac{NI}{A}$$

where N is the number of turns in the coil I is the total current and A is the cross sectional area. To represent the fact that the coil is in free space, infinite elements are used far away from the coil, as shown in Figure 1. A stationary study type is used to compute the static magnetic field. This field is then fed into a self consistent model for the plasma.

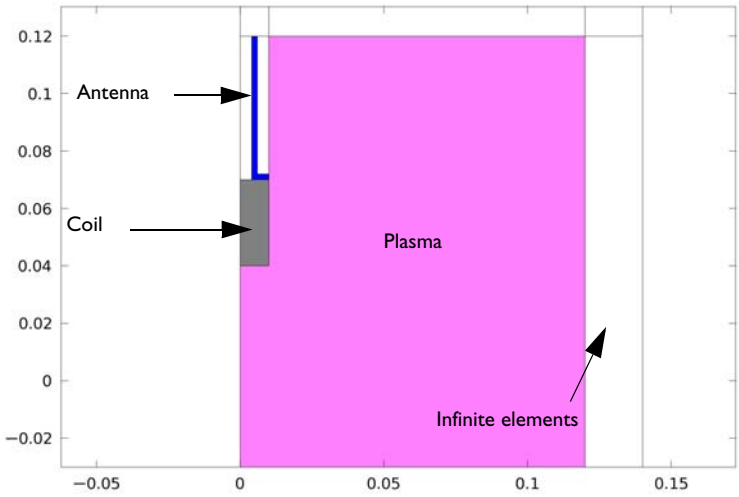

Figure 1: Basic concept for the plasma source. A stationary azimuthal current flows in the coil which generates a static magnetic field in the surroundings. Resonant heating of the electrons occurs on the contour of the critical magnetic flux density.

The plasma conductivity becomes a full tensor in the presence of a static magnetic field. At some critical magnetic field the electrons continually gain energy from both the electric and magnetic fields over one RF cycle. This leads to a resonance zone in the plasma where the incoming electromagnetic wave is completely absorbed over a very short distance. The critical magnetic field is only dependent on the angular frequency, the electron mass and charge:

$$B_{\mathrm{cr}} = \frac{\omega m_e}{q}$$

At 2.45 GHz the critical magnetic flux density is 875 gauss or 0.0875 T. Therefore you can use functional-based mesh adaption to ensure that the ECR surface is adequately meshed for the plasma model. The functional is somewhat arbitrary; it is chosen such that it is zero everywhere but becomes large at the resonant magnetic flux density. In this model, use the functional

$$f = \frac{1}{|\|\mathbf{B}\| - 0.0875| + \delta} \tag{1}$$

where δ is a small number to prevent division by zero.

Model Definition—Microwave Plasma

In this example, you solve the following wave equation for the high-frequency component of the electric field in the frequency domain:

$$\nabla \times \mu_0^{-1}(\nabla \times \mathbf{E}) - k_0^2\left(\varepsilon_r - \frac{j\boldsymbol{\sigma}}{\omega\varepsilon_0}\right) \cdot \mathbf{E} = 0$$

Here σ is the plasma conductivity, which is a full tensor and a function of the electron density, collision frequency, and the static magnetic flux density. Using the definitions

$$\alpha = \frac{q}{m_e(\nu_e + j\omega)} \tag{2}$$

where q is the electron charge, m_e is the electron mass, ν_e is the electron-neutral collision frequency, and ω is the angular frequency. The inverse of the plasma conductivity is defined as

$$qn_e\boldsymbol{\sigma}^{-1} = \begin{bmatrix} 1 & -\alpha B_z & \alpha B_y \\ \alpha B_z & 1 & -\alpha B_x \\ -\alpha B_y & \alpha B_x & 1 \end{bmatrix} \tag{3}$$

where n_e is the electron number density. Using the inverse of the plasma conductivity is convenient because it can be written in a compact form. COMSOL automatically computes the tensor form of the plasma conductivity for you by inverting Equation 3. Because the plasma conductivity tensor is a full tensor, all three components of the electric field are computed despite the fact that the only excitation from the coaxial port occurs in the rz-plane. The nonlinearity in the plasma conductivity can be seen in Figure 2. The surface represents four of the components of the nondimensional plasma conductivity versus the r- and z-components of the magnetic flux density (indicated by the x-axis and y-axis, respectively) on a log scale. At the resonant flux density (0.0875 T) the plasma conductivity is more than 10^6 higher than the case where no static magnetic field is present.

In Ref. 1 the size of the resonance is smoothed over a distance which can be resolved by the mesh. It is argued that this has a physical basis corresponding to collision-less heating.

In Ref. 2 the physical reasoning behind the broadening of the resonance zone is Doppler shifting of the electrons into resonance. The same smoothing used in Ref. 1 is available in COMSOL by selecting the **Doppler broadening** check box in the Microwave Plasma interface properties. In this case, the collision frequency, ν_e in Equation 2 is replaced by an effective collision frequency:

$$\tilde{\nu}_e = \nu_e + \frac{\omega}{\delta} \tag{4}$$

where δ is chosen to be 20. This is very simple from an implementation point of view but does lead to unphysical power absorption away from the resonance zone. The approach taken in Ref. 2 leads to the ECR surface being broadened only at the resonance zone.

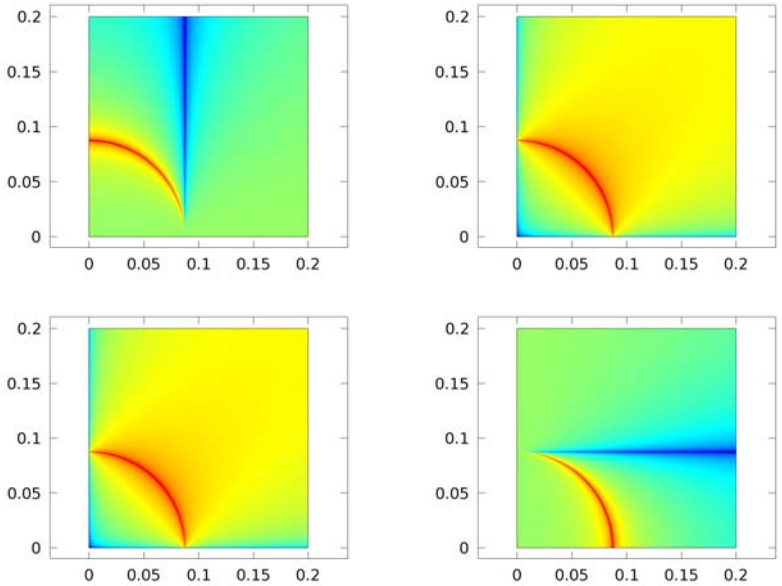

Figure 2: Plots of the four components of the plasma conductivity tensor.

Compute the electron number density and electron energy density by solving a pair of drift-diffusion equations:

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility and energy diffusivity are calculated from the electron mobility using

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The electron transport properties are, like the plasma conductivity, full tensors. The electron mobility in the direction of the magnetic field lines is up to 8 orders of magnitude higher than the cross-field electron mobility. As such, electrons are only transported along magnetic field lines. The inverse of the electron mobility can be written in compact form as

$$\boldsymbol{\mu}_e^{-1} = \begin{bmatrix} \frac{1}{\mu_{dc}} & -B_z & B_y \\ B_z & \frac{1}{\mu_{dc}} & -B_x \\ -B_y & B_x & \frac{1}{\mu_{dc}} \end{bmatrix} \tag{5}$$

where μ_{dc} is the electron mobility in the absence of a magnetic field. COMSOL automatically inverts the matrix in Equation 5 for you. The source coefficients in the above equations are determined by the plasma chemistry and are written using rate coefficients. Suppose that there are M reactions which contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general $P >> M$. In the case of rate coefficients, the electron source term is given by

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (m^3/s), and N_n is the total neutral number density ($1/\mathrm{m}^3$).The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (V). The electron source and inelastic energy loss are automatically computed by the multiphysics interface. The rate coefficients may be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ ($C^{1/2}/kg^{1/2}$), m_e is the electron mass (kg), ε is energy (V), σ_k is the collision cross section (m^2), and f is the electron energy distribution function. In this model the distribution function is chosen to be Maxwellian:

$$f(\varepsilon) = \phi^{-3/2} \beta_1 \exp(-(\varepsilon \beta_2 / \phi))$$

where ϕ is the mean electron energy:

$$\phi = \frac{n_\varepsilon}{n_e}$$

and

$$\beta_1 = \Gamma(5/2)^{3/2} \Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2) \Gamma(3/2)^{-1}$$

where Γ is the gamma function. The heating term, $\mathbf{E} \cdot \Gamma_e$ has two components, one due to electron motion in the ambipolar field in the rz-plane and one due to heating of the electrons by the microwaves. Heating due to the microwaves is handled in the same way as described in Ref. 1. The power transferred from the electromagnetic field to the electrons is normalized so that 10 W of total power is absorbed by the electrons. This is accomplished by multiplying the heating term by a factor, α, which is defined as:

$$\alpha = \frac{10\ W}{\iiint Q_{\text{ind}} dV} \tag{6}$$

The result of this is that exactly 10 W of total power is transferred from the electromagnetic field to the electrons. If you did not apply this renormalization of the absorbed power then there would be nothing to stop the plasma from simply self-extinguishing or absorbing an inordinate amount of power. This approach is perfectly valid due to the fact that the microwave equations are linear. The only drawback from this method is that the S-parameters given on the coaxial port are not valid because the fields are decoupled from the plasma model. Furthermore, it is not possible to self-consistently compute the ratio of the absorbed and reflected power through the excitation port, a quantity that may be of interest.

For nonelectron species, the following equation is solved for the mass fraction of species k:

$$\rho\frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u}\cdot\nabla)w_k = \nabla\cdot\mathbf{j}_k + R_k \tag{7}$$

As with the electrons, the ion transport properties are functions of the static magnetic flux density. The magnetic force is included as it can generate a significant ion velocity in the azimuthal direction close to the antenna. The ion mobility is also a function of the ambipolar electric field and is specified as a look up table. The ion diffusion velocity, $\mathbf{v}_k$, is related to the diffusive flux via

$$\mathbf{j}_k = \rho\omega\mathbf{v}_k$$

where

$$\mathbf{v}_k = D_m\nabla\ln(w) + D_m\nabla\ln(M) + Z\mu(\mathbf{E} + \mathbf{v}_k\times\mathbf{B}) \tag{8}$$

Equation 7 can be re-arranged to give an expression for the diffusion velocity as a function of the other variables:

$$\mathbf{v}_k = \mathbf{A}^{-1}[D_m\nabla\ln(w) + D_m\nabla\ln(M) + Z\mu\mathbf{E}]$$

where

$$\mathbf{A} = \begin{bmatrix} 1 & -Z\mu B_z & Z\mu B_y \\ Z\mu B_z & 1 & -Z\mu B_x \\ -Z\mu B_y & Z\mu B_x & 1 \end{bmatrix}$$

COMSOL automatically inverts Equation 8 when defining the diffusion velocity for each of the ionic species. The electrostatic field is computed using the following equation:

$$-\nabla\cdot\varepsilon_0\varepsilon_r\nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

PLASMA CHEMISTRY

The model considers argon plasma chemistry with the following set of collisions including elastic, excitation, direct ionization and stepwise ionization. Penning ionization and metastable quenching are also included in the model.

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\varepsilon(\mathrm{eV})$
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	-

On surfaces, the following two reactions are considered:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ar+=>Ar	1
2	Ars=>Ar	1

BOUNDARY CONDITIONS

The above partial differential equations must be supplemented with a suitable set of boundary conditions. The coaxial port boundary condition is used to drive the electromagnetic waves. The port power is inconsequential due to the normalization scheme used on the absorbed power.

For the electrons, neglect reflection as well as secondary and thermal emission to get the following boundary condition on the electron flux:

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} \nu_{e,\,\mathrm{th}} n_e\right)$$

and the electron energy flux:

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6} \nu_{e,\,\mathrm{th}} n_\varepsilon\right)$$

Losses at the wall for the heavy species is due to surface reactions and migration due to the ambipolar field:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k [(\mathbf{A}^{-1} \cdot \mathbf{E}) \cdot \mathbf{n}][(Z_k \mu_k (\mathbf{A}^{-1} \cdot \mathbf{E}) \cdot \mathbf{n}) > 0]$$

The reactor walls are grounded.

Results and Discussion—Static Magnetic Field Model

Figure 3 and Figure 4 present the results from the first study step. As expected, the azimuthal current in the coil generates a static magnetic field that has a "3"-shaped contour at a flux density of 0.0875 T. The magnetic field lines form a circular pattern around the coil, which is important to bear in mind when discuss the transport of the charged particles later.

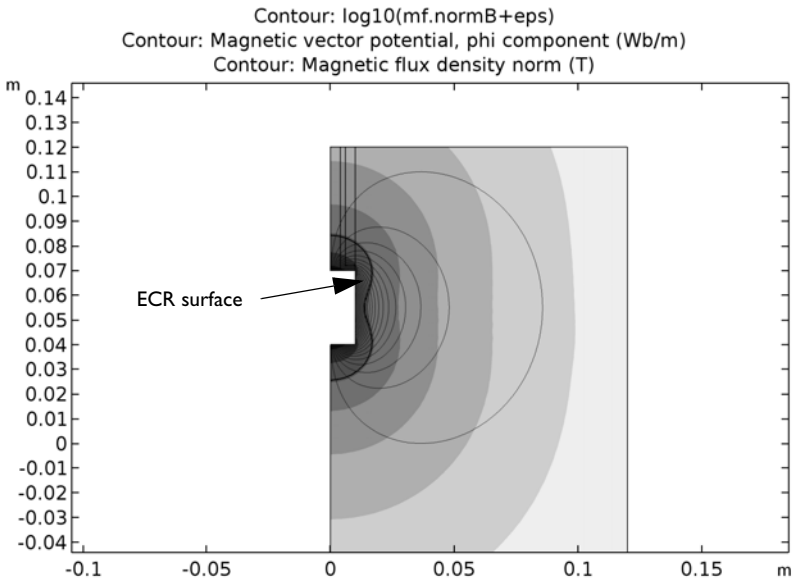

Figure 3: Plot of the static magnetic flux density on a log scale (filled contour), magnetic field lines (thin lines) and the ECR surface at 0.0875 T (thick black line).

In Figure 4 the mesh, which has adapted based on the functional given in Equation 1 is shown. The mesh has clearly been significantly refined around the contour of the resonant magnetic flux density. This is required to accurately resolve the region where all the power

deposition to the electrons occurs. Functional-based mesh adaption is a feature that makes the finite element approach more attractive than the finite difference approach for ECR modeling.

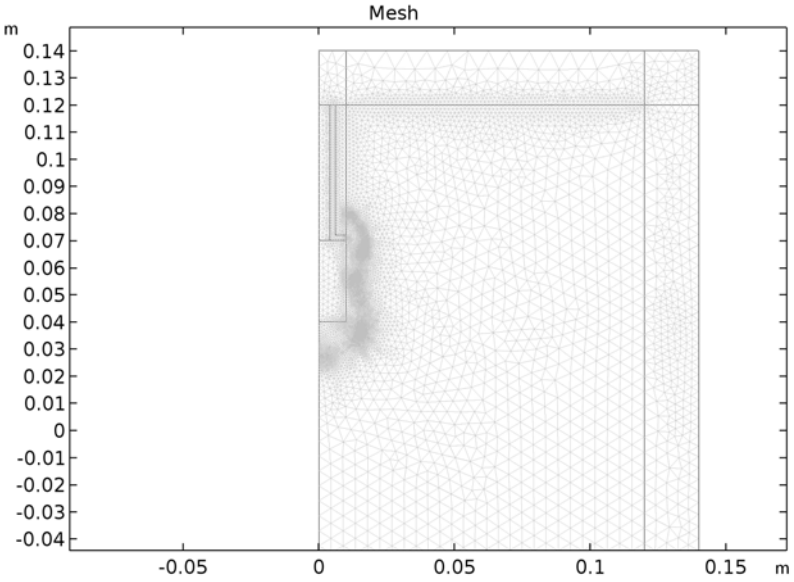

Figure 4: Mesh generated after one refinement using functional based mesh adaption. The mesh is very fine on the ECR surface and relatively coarse away from the resonance zone.

Results and Discussion—Microwave Plasma Model

The electron density at the quasi steady state solution is plotted in Figure 5. The peak electron density is around $5{\cdot}10^{16}$ m^{-3} and peaks radially outwards from the center of the coil. The magnitude of the electron number density and its profile agree well with the

results in Ref. 1.

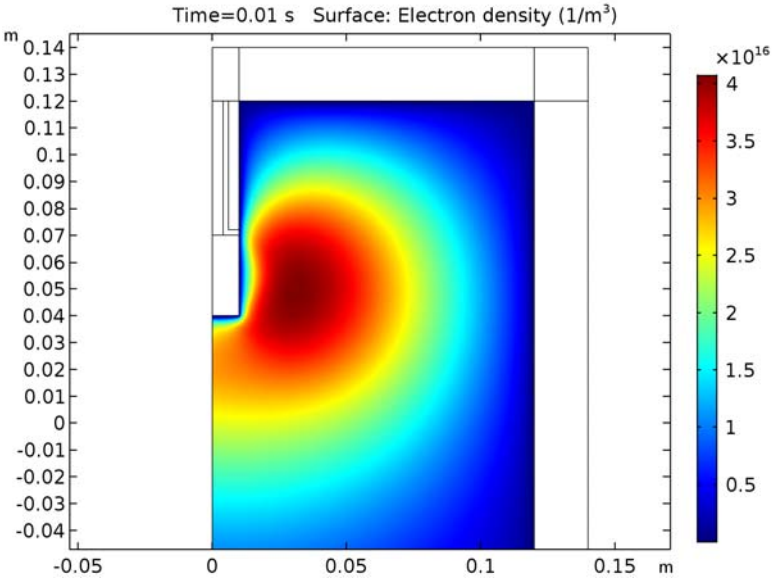

Figure 5: Plot of the electron density at the quasi steady state condition. The peak electron density is still below the critical electron density at the chosen operating frequency.

Despite the sharply peaked heating the electron temperature, plotted in Figure 6 does not show such peaks. Recall from Figure 3 that the magnetic field lines show the circular pattern away from the coil. This leads to strong energy transport along the field lines and very little transport across the magnetic field lines. Indeed the circular pattern along which the electron temperature is constant is consistent with the magnetic field lines. The peak electron temperature is around 3.8 eV and around 1.78 eV below the coil which is again, consistent with the results in Ref. 2.

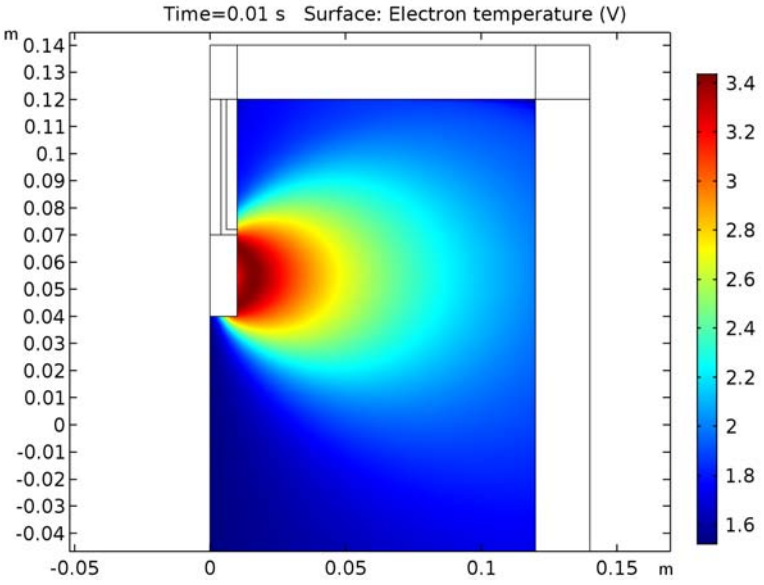

Figure 6: Plot of the electron temperature which peaks at around 3.8 eV

Despite the fact that power is only deposited to the plasma on the ECR surface, the electron temperature, plotted in Figure 6 is not sharply peaked at the critical magnetic flux density. Recall from Figure 3 that the magnetic field lines show the circular pattern away from the coil. The high degree of anisotropy in the electron transport properties results in strong energy transport along the magnetic field lines and little transport across the magnetic field lines. Indeed the circular pattern along which the electron temperature is constant is consistent with the magnetic field lines. The peak electron temperature is around 3.8 eV and around 1.78 eV below the coil which is again, consistent with the results in Ref. 2.

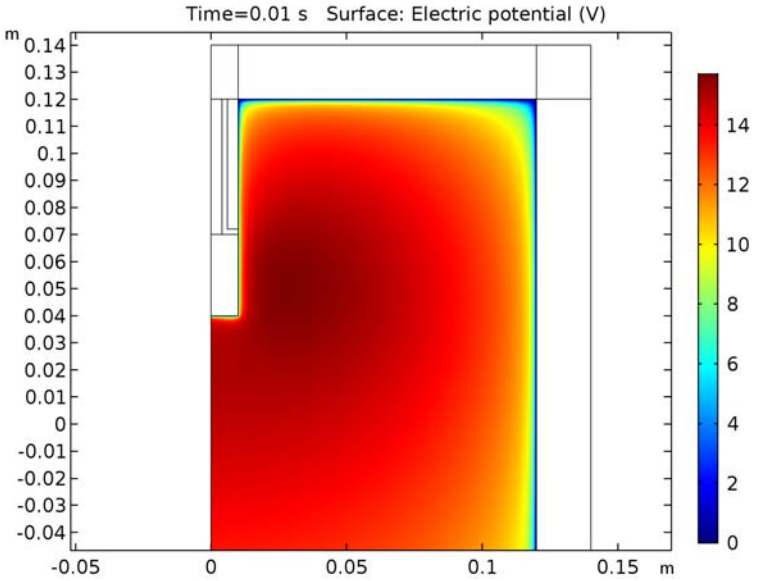

Figure 7: Plot of the plasma potential.

The electron density profile shows no signs of the resonance zone which is clearly seen in Figure 8. The power deposition is very high, peaking at 35 W/cm^3. All of the power deposition into the plasma from the electromagnetic field occurs in this resonance zone.

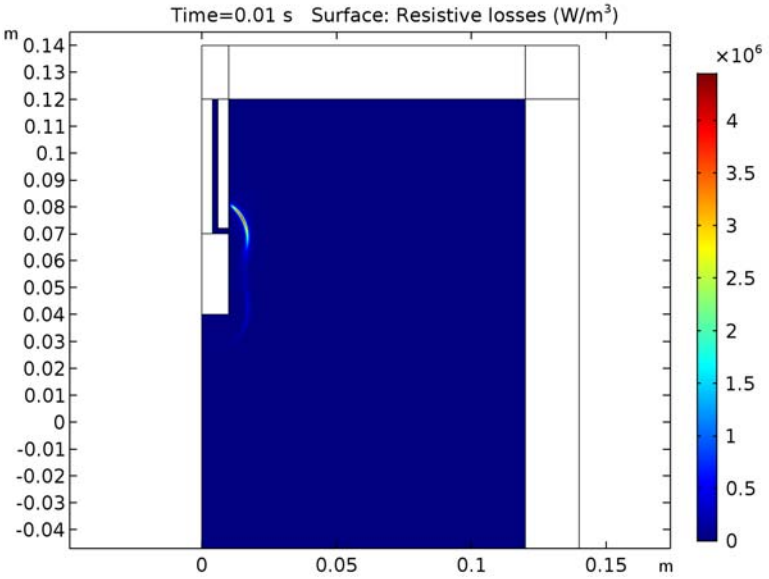

Figure 8: Plot of the power deposition into the plasma. Nearly all the power deposition occurs on the ECR surface.

The ionization source, plotted in Figure 9 is more highly localized around the coil. This corresponds to the region where the electron density and electron temperature are highest. Because the ionization rate scales linearly with the electron density and exponentially with the electron temperature this is to be expected.

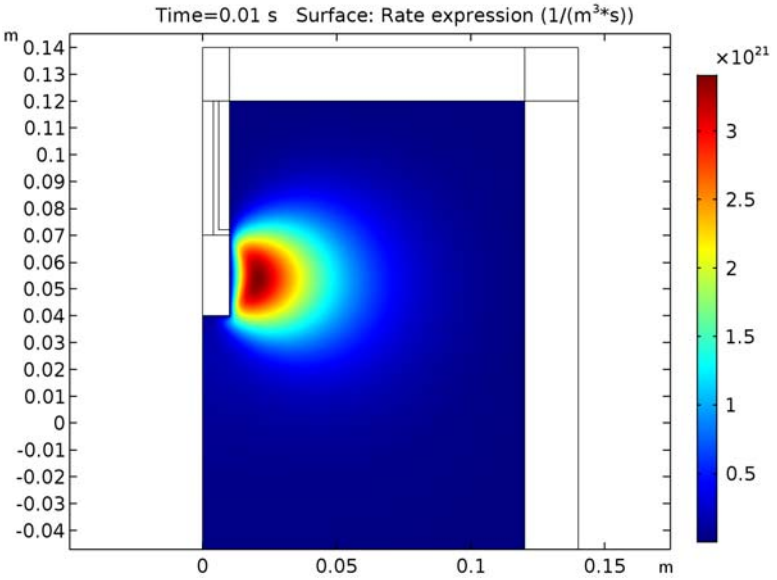

Figure 9: Plot of the rate expression for electrons generated via ionization.

The plasma potential, plotted in Figure 7, peaks at around 16 V. The plasma potential is uniform throughout the plasma, even though the electron temperature shows large variations. The physical basis for the flat plasma potential is explained in Ref. 1.

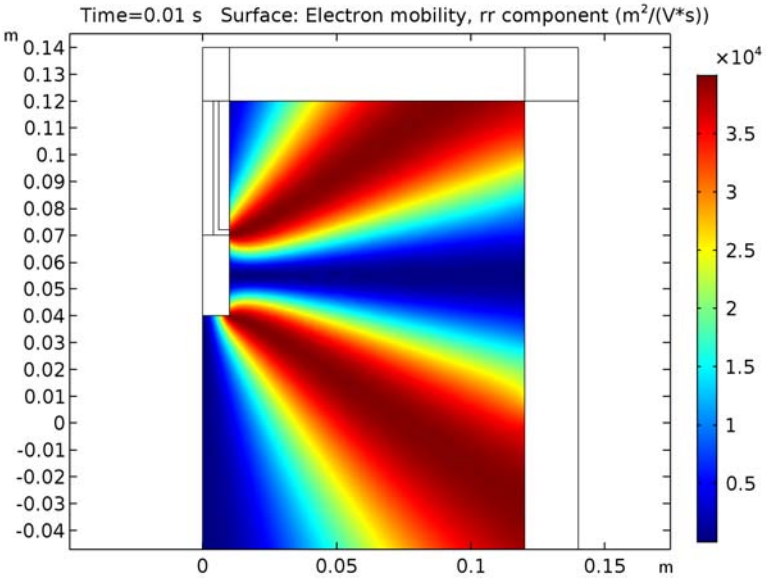

Figure 10: Plot of the electron mobility tensor's rr-component. The mobility varies by 8 orders of magnitude over the space of only a couple of centimeters.

The degree of anisotropy in the electron transport properties can be seen in Figure 10 and Figure 11. In Figure 10 the electron mobility varies by 8 orders of magnitude, it is $4{\cdot}10^4$ $m^2/(Vs)$ towards the coil edges and 10^{-4} $m^2/(Vs)$ radially outwards from the coil center. In Figure 11 the opposite is true, the electron mobility is very high in the z direction at the center of the coil, and very small towards the coil edges. This leads to migration of electrons along the magnetic field lines when they are produced in the ionization region, Figure 9.

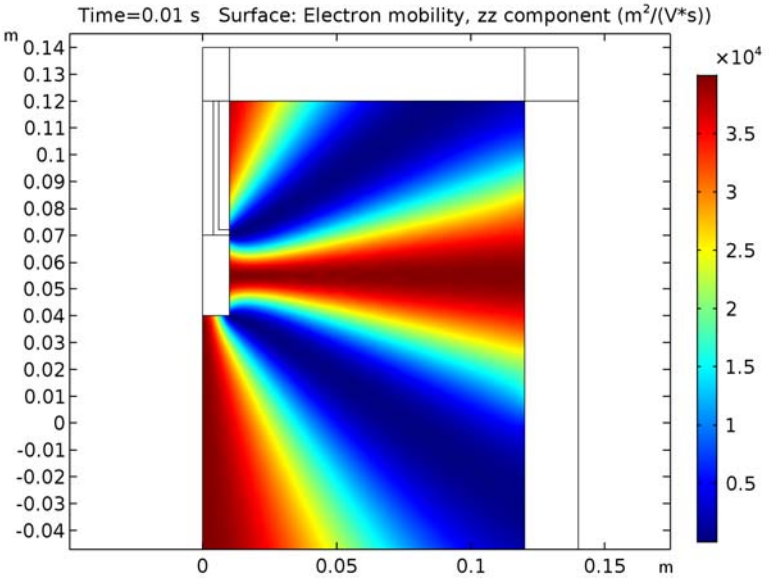

Figure 11: Plot of the electron mobility tensor's zz-component.

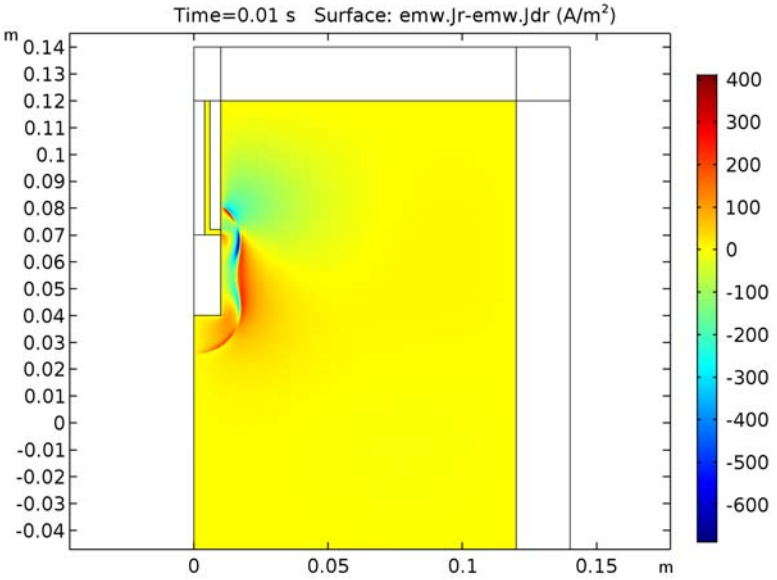

Figure 12: Unnormalized radial component of the microwave conduction current.

The conduction current due to the microwaves is plotted in Figure 12 - Figure 14. The largest component of the conduction current is actually in the azimuthal direction despite the coaxial port only propagating in the TM mode. Despite this, the heating (cooling) due to the dot product of the azimuthal components of the current and electric fields is small, due to the much lower value of the azimuthal component of the electric field.

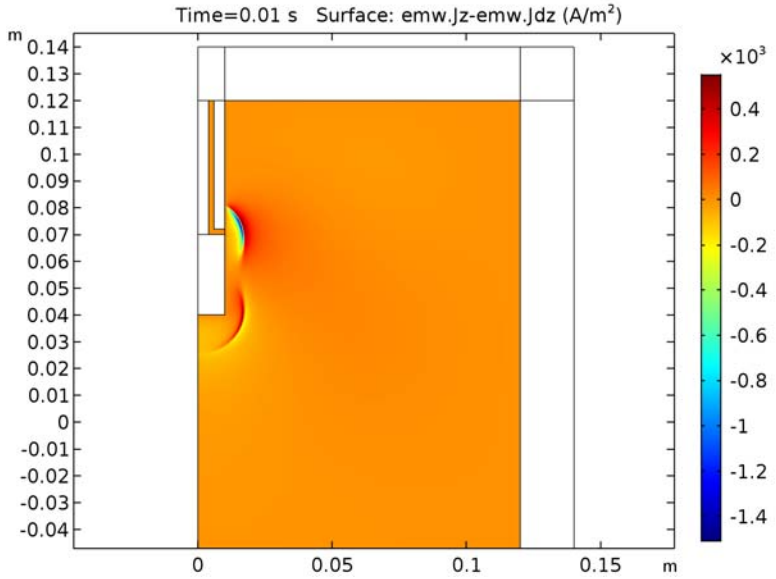

Figure 13: Unnormalized axial component of the microwave conduction current.

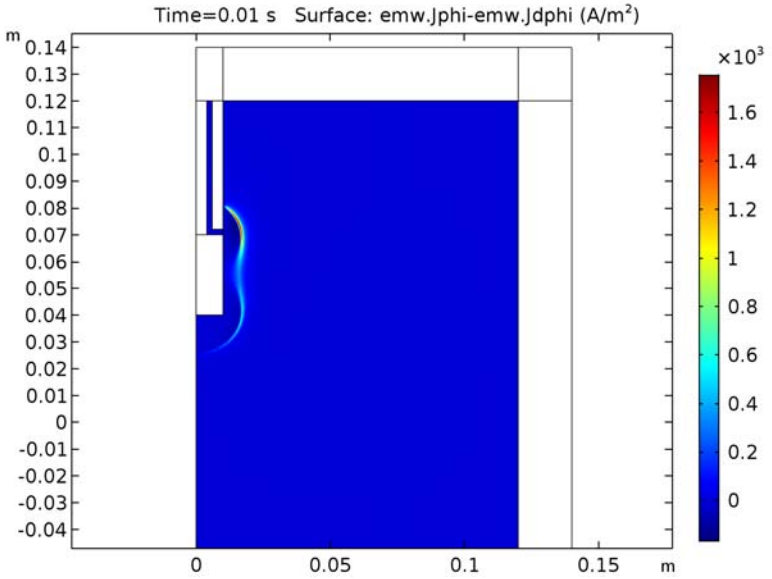

Figure 14: Unnormalized azimuthal component of the microwave conduction current.

Finally, the trace of the plasma conductivity is plotted in Figure 15. The resonance zone is evident and the locally high electrical conductivity leads to the propagating electromagnetic waves to be absorbed.

It is worth mentioning that the electron density in this example model is below the critical plasma density everywhere ($7.4{\cdot}10^{16}$ m^{-3} at 2.45 GHz). If either the pressure or the power is increased, the power absorption can shift from the ECR surface to the contour where the plasma density is equal to the critical plasma density. On this contour the phase velocity approaches infinity whereas the group velocity approaches zero. The numerical instabilities caused by this are also smoothed out by adding an effective collision frequency to the actual collision frequency using Equation 4.

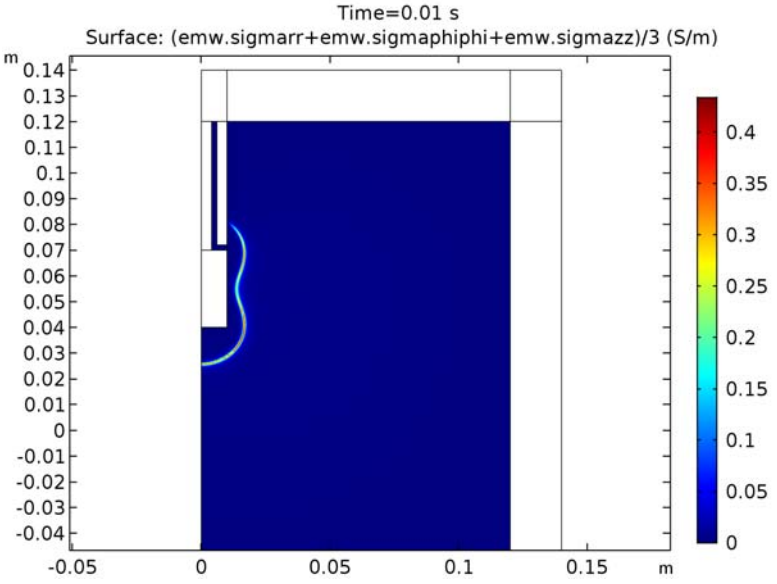

Figure 15: Plot of the trace of the plasma conductivity tensor.

Reference

1. G.J.M. Hagelaar, K. Makasheva, L. Garrigues, and J.-P. Boeuf, "Modelling of a dipolar microwave plasma sustained by electron cyclotron resonance," *J. Phys. D: Appl. Phys.*, vol. 42, p. 194019 (12pp), 2009.

2. R.L. Kinder and M.J. Kushner, "Consequences of mode structure on plasma properties in electron cyclotron resonance sources," *J. Vac. Sci. Technol. A*, vol. 175, Sep/Oct 1999.

Notes About the COMSOL Implementation

This problem is solved in two stages. First, compute the static magnetic field using adaptive mesh refinement. Then, in a separate study step, solve for the electron density, electron energy density, mass fraction of argon ions, and mass fraction of electronically excited argon atoms, as well as the plasma potential and the 3 components of the high-frequency electric field. The magnetic flux density computed in the first study step is used to define the tensor plasma conductivity as well as electron and ion transport properties.

Application Library path: `Plasma_Module/Wave-Heated_Discharges/dipolar_ecr_source`

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 **2D Axisymmetric**.
2. In the **Select Physics** tree, select **AC/DC>Magnetic Fields (mf)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies>Stationary**.
6. Click **Done**.
7. In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.

GLOBAL DEFINITIONS

Parameters

1. On the **Home** toolbar, click **Parameters**.
2. In the **Settings** window for **Parameters**, locate the **Parameters** section.
3. In the table, enter the following settings:

Name	Expression	Value	Description
r0	0.12	0.12	Plasma source radius
z0	0.24	0.24	Plasma source height
Psp	10[W]	10 W	Total power absorbed by the plasma setpoint

GEOMETRY 1

Rectangle 1 (r1)

1. On the **Geometry** toolbar, click **Primitives** and choose **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 `z0`.
5. Locate the **Position** section. In the **z** text field, type `-z0/2`.

Rectangle 2 (r2)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `0.01`.
4. In the **Height** text field, type `0.03`.
5. Locate the **Position** section. In the **z** text field, type `0.04`.

Rectangle 3 (r3)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `0.004`.
4. In the **Height** text field, type `0.048`.
5. Locate the **Position** section. In the **r** text field, type `0.006`.
6. In the **z** text field, type `0.072`.

Rectangle 4 (r4)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `0.004`.
4. In the **Height** text field, type `0.05`.
5. Locate the **Position** section. In the **z** text field, type `0.07`.

Rectangle 5 (r5)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `r0-0.01`.
4. In the **Height** text field, type `0.02`.

5 Locate the **Position** section. In the **r** text field, type `0.01`.

6 In the **z** text field, type `0.12`.

Rectangle 6 (r6)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.02`.

4 In the **Height** text field, type `0.02`.

5 Locate the **Position** section. In the **r** text field, type `r0`.

6 In the **z** text field, type `0.12`.

Rectangle 7 (r7)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.02`.

4 In the **Height** text field, type `z0`.

5 Locate the **Position** section. In the **r** text field, type `r0`.

6 In the **z** text field, type `-z0/2`.

Rectangle 8 (r8)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.02`.

4 In the **Height** text field, type `0.02`.

5 Locate the **Position** section. In the **r** text field, type `r0`.

6 In the **z** text field, type `-0.02-z0/2`.

Rectangle 9 (r9)

1 On the **Geometry** toolbar, click **Primitives** and choose **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 `0.02`.

5 Locate the **Position** section. In the **z** text field, type `-0.02-z0/2`.

Rectangle 10 (r10)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.01`.

4 In the **Height** text field, type `0.02`.

5 Locate the **Position** section. In the **z** text field, type `0.12`.

Bézier Polygon 1 (b1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Bézier Polygon**.

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

3 Find the **Added segments** subsection. Click **Add Linear**.

4 Find the **Control points** subsection. In row **1**, set **r** to `0.01` and **z** to `0.072`.

5 In row **2**, set **r** to `0.01` and **z** to `0.07`.

DEFINITIONS

In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.

Axis

1 Right-click **Definitions** and choose **View**.

2 In the **Model Builder** window, expand the **View 2** node, then click **Axis**.

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

4 In the **r minimum** text field, type `-0.05`.

5 In the **r maximum** text field, type `0.16`.

6 In the **z minimum** text field, type `-0.02`.

7 In the **z maximum** text field, type `0.12`.

8 Click **Update**.

View 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **View 2**.

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

3 Select the **Lock axis** check box.

Explicit 1

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

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

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

4 Select Boundaries 4, 6, 18–20, 22, and 26 only.

5 Right-click **Explicit 1** and choose **Rename**.

6 In the **Rename Explicit** dialog box, type `Walls` in the **New label** text field.

7 Click **OK**.

Infinite Element Domain 1 (ie1)

1 On the **Definitions** toolbar, click **Infinite Element Domain**.

2 In the **Settings** window for **Infinite Element Domain**, locate the **Geometry** section.

3 From the **Type** list, choose **Cylindrical**.

4 Select Domains 1, 5, and 8–11 only.

MATERIALS

Material 1 (mat1)

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

2 Select Domains 1, 2, 4, 5, and 7–11 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	1	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	1	1	Basic

Material 2 (mat2)

1 Right-click **Materials** and choose **Blank Material**.

2 Select Domain 3 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	1	Basic
Electrical conductivity	sigma	6e7	S/m	Basic
Relative permittivity	epsilonr	1	1	Basic

Material 3 (mat3)

1 Right-click **Materials** and choose **Blank Material**.

2 Select Domain 6 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	1	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	2	1	Basic

DEFINITIONS

Integration 1 (intop1)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 Select Domain 2 only.

MAGNETIC FIELDS (MF)

Coil 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Magnetic Fields (mf)** and choose the domain setting **Coil**.

2 Select Domain 3 only.

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

4 From the **Conductor model** list, choose **Homogenized multi-turn**.

5 Locate the **Homogenized Multi-Turn Conductor** section. In the N text field, type 5000.

6 Locate the **Coil** section. In the I_{coil} text field, type 14.

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

MESH 1

Edge 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **More Operations>Edge**.

2 Select Boundary 19 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Size**.

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

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

4 Click the **Custom** button.

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

6 In the associated text field, type `0.0005`.

Edge 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **More Operations>Edge**.

2 Select Boundaries 6, 18, 20, and 22 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 2** and choose **Size**.

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

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

4 Click the **Custom** button.

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

6 In the associated text field, type `0.0015`.

Free Triangular 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

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

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

4 Select Domain 2 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>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**.

Free Triangular 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

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

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

4 Select Domain 6 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Free Triangular 2** and choose **Size**.

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

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

4 Click the **Custom** button.

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

6 In the associated text field, type `0.001`.

Free Triangular 3

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Adaptation and error estimates** section.

3 Locate the **Adaptation and Error Estimates** section. From the **Adaptation and error estimates** list, choose **Adaptation and error estimates**.

4 From the **Error estimate** list, choose **Functional**.

5 From the **Functional type** list, choose **Manual**.

6 In the **Functional** text field, type `comp1.intop1(1/(abs(comp1.mf.normB-0.0875)+1e-4))`.

7 Find the **Mesh refinement** subsection. From the **Refinement method** list, choose **Mesh initialization**.

8 In the **Maximum number of refinements** text field, type `1`.

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

10 In the **Settings** window for **Study**, locate the **Study Settings** section.

11 Clear the **Generate default plots** check box.

12 On the **Home** toolbar, click **Compute**.

RESULTS

Reproduce the magnetic flux density plot in Figure 3 with the following steps.

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

Study 1/Solution 1 (sol1)

In the **Model Builder** window, expand the **Results>Data Sets** node, then click **Study 1/ Solution 1 (sol1)**.

Selection

1 On the **Results** toolbar, click **Selection**.

2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.

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

4 Select Domains 2, 4, 6, and 7 only.

2D Plot Group 1

1 On the **Results** toolbar, click **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Stationary Magnetic Flux Density` in the **Label** text field.

Contour 1

1 Right-click **Stationary Magnetic Flux Density** and choose **Contour**.

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

3 In the **Expression** text field, type `log10(mf.normB+eps)`.

4 Locate the **Levels** section. In the **Total levels** text field, type `8`.

5 Locate the **Coloring and Style** section. From the **Contour type** list, choose **Filled**.

6 From the **Color table** list, choose **GrayScale**.

7 Clear the **Color legend** check box.

8 Select the **Reverse color table** check box.

Contour 2

1 In the **Model Builder** window, under **Results** right-click **Stationary Magnetic Flux Density** and choose **Contour**.

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

3 In the **Expression** text field, type `Aphi`.

4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

5 From the **Color** list, choose **Black**.

6 Clear the **Color legend** check box.

Contour 3

1 Right-click **Results>Stationary Magnetic Flux Density>Contour 2** and choose **Duplicate**.

2 In the **Settings** window for **Contour**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Magnetic Fields>Magnetic> mf.normB - Magnetic flux density norm**.

3 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.

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 `0.086`.

7 In the **Stop** text field, type `0.089`.

8 In the **Number of values** text field, type `20`.

9 Click **Replace**.

10 On the **Stationary Magnetic Flux Density** toolbar, click **Plot**.

Next, visualize the refined mesh.

2D Plot Group 2

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

2 In the **Settings** window for **2D Plot Group**, type `Adpative Mesh` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Study 1/ Level 1 Refined Solution 2 (sol2)**.

Mesh 1

1 Right-click **Adpative Mesh** and choose **Mesh**.

2 In the **Settings** window for **Mesh**, locate the **Color** section.

3 From the **Element color** list, choose **None**.

4 From the **Wireframe color** list, choose **Custom**.

5 On Windows, click the colored bar underneath, or?if you are running the cross-platform desktop?the **Color** button.

6 Click **Define custom colors**.

7 Set the RGB values to 192, 192, and 192, respectively.

8 Click **Add to custom colors**.

9 Click **Show color palette only** or **OK** on the cross-platform desktop.

10 On the **Adpative Mesh** toolbar, click **Plot**.

Compare the result with the plot in Figure 4.

ADD PHYSICS

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

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

3 In the tree, select **Plasma>Microwave Plasma**.

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

PLASMA (PLAS)

On the **Physics** toolbar, click **Magnetic Fields (mf)** and choose **Plasma (plas)**.

1. On the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.
2. In the **Model Builder** window, under **Component 1 (comp1)** click **Plasma (plas)**.
3. Select Domains 1, 2, 5, 6, and 8–11 only.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EMW)

On the **Physics** toolbar, click **Plasma (plas)** and choose **Electromagnetic Waves, Frequency Domain (emw)**.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain (emw)**.
2. In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, locate the **Domain Selection** section.
3. Click **Clear Selection**.
4. Select Domains 2 and 6 only.

PLASMA (PLAS)

On the **Physics** toolbar, click **Electromagnetic Waves, Frequency Domain (emw)** and choose **Plasma (plas)**.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Plasma (plas)**.
2. In the **Settings** window for **Plasma**, locate the **Transport Settings** section.
3. Select the **Full expression for diffusivity** check box.
4. Select the **Compute tensor ion transport properties** check box.
5. Locate the **Plasma Properties** section. Select the **Compute tensor electron transport properties** check box.

MULTIPHYSICS

1. In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Plasma Conductivity Coupling 1 (pcc1)**.
2. In the **Settings** window for **Plasma Conductivity Coupling**, locate the **Compute Tensor Plasma Conductivity** section.
3. Select the **Compute tensor plasma conductivity** check box.
4. In the δ text field, type 20.

PLASMA (PLAS)

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

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

3 Click **Clear Selection**.

4 Select Domain 2 only.

Cross Section Import 1

1 In the **Model Builder** window, right-click **Plasma (plas)** 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`.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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 `3.734E8`.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ars**.

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

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

4 In the x_0 text field, type `1E-4`.

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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. Locate the **Mobility and Diffusivity Expressions** section. From the **Specification** list, choose **Specify mobility, compute diffusivity**.

6 Click to expand the **Mobility specification** section. Locate the **Mobility Specification** section. From the **Specify using** list, choose **Lookup table**.

7 Click **Load from File**.

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

Surface Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>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 **Boundary Selection** section. From the **Selection** list, choose **Walls**.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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 **Boundary Selection** section. From the **Selection** list, choose **Walls**.

Wall 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

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

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

Ground 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

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

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

PLASMA (PLAS)

On the **Physics** toolbar, click **Electromagnetic Waves, Frequency Domain (emw)** and choose **Plasma (plas)**.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E14`.

Plasma Model 1

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

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

3 From the $\mathbf{B}$ list, choose **Magnetic flux density (mf)**.

4 In the T text field, type `300`.

5 In the p_A text field, type `1`.

6 Locate the **Electron Density and Energy** section. In the μ_e text field, type `1E25[1/(m*V*s)]/plas.Nn`.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EMW)

On the **Physics** toolbar, click **Plasma (plas)** and choose **Electromagnetic Waves, Frequency Domain (emw)**.

Port 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electromagnetic Waves, Frequency Domain (emw)** and choose **Port**.

2 Select Boundary 14 only.

3 In the **Settings** window for **Port**, locate the **Port Properties** section.

4 From the **Type of port** list, choose **Coaxial**.

5 From the **Wave excitation at this port** list, choose **On**.

6 Select the **Specify deposited power** check box.

7 In the P_{dep} text field, type `Psp`.

COMPONENT 1 (COMP1)

Mesh 2

On the **Mesh** toolbar, click **Add Mesh**.

MESH 2

Reference 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Meshes** right-click **Mesh 2** and choose **More Operations>Reference**.

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

3 From the **Mesh** list, choose **Level 1 Refined Mesh 1**.

Refine 1

1 In the **Model Builder** window, right-click **Mesh 2** and choose **More Operations>Refine**.

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

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

4 Select Domain 6 only.

5 Locate the **Refine Options** section. In the **Number of refinements** text field, type `2`.

Boundary Layers 1

1 Right-click **Mesh 2** and choose **Boundary Layers**.

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

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

4 Select Domain 2 only.

Boundary Layer Properties

1 In the **Model Builder** window, under **Component 1 (comp1)>Meshes>Mesh 2> Boundary Layers 1** click **Boundary Layer Properties**.

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

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

4 Locate the **Boundary Layer Properties** section. In the **Number of boundary layers** text field, type `4`.

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

6 Click **Build All**.

ADD STUDY

1 On 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 Multiphysics**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for the **Magnetic Fields (mf)** interface.

5 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Multiphysics>Frequency-Transient**.

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

STUDY 2

Step 1: Frequency-Transient

1 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

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

3 In the **Times** text field, type `0 10^{range(-8,6/10,-2)}`.

4 In the **Frequency** text field, type `2.45E9`.

5 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for the **Magnetic Fields (mf)** interface.

6 Click to expand the **Mesh selection** section. Locate the **Mesh Selection** section. In the table, enter the following settings:

Geometry	Mesh
Geometry 1	mesh2

7 Click to expand the **Mesh selection** section. Click to expand the **Values of dependent variables** section. In the **Settings** window for **Frequency-Transient**, locate 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 1, Stationary**.

11 From the **Solution** list, choose **Level 1 Refined Solution 2 (sol2)**.

Solution 3 (sol3)

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

2 In the **Model Builder** window, expand the **Study 2>Solver Configurations** node.

3 In the **Model Builder** window, expand the **Solution 3 (sol3)** node, then click **Dependent Variables 1**.

4 In the **Settings** window for **Dependent Variables**, locate the **General** section.

5 From the **Defined by study step** list, choose **User defined**.

6 Locate the **Values of Variables Not Solved For** section. From the **Method** list, choose **Solution**.

7 From the **Solution** list, choose **Level 1 Refined Solution 2 (sol2)**.

8 On the **Study** toolbar, click **Compute**.

RESULTS

Three new default plots show the electron density, electron temperature, and plasma potential respectively; compare with those in Figure 5, Figure 6, and Figure 7.

Electric Potential (plas)

Follow the instructions below to reproduce Figure 8 through Figure 15.

2D Plot Group 7

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

2 In the **Settings** window for **2D Plot Group**, type `Power Deposition` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Study 2/Solution 3 (sol3)**.

Surface 1

1 Right-click **Power Deposition** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain>Heating and losses>emw.Qrh - Resistive losses**.

3 On the **Power Deposition** toolbar, click **Plot**.

Compare with Figure 8.

Power Deposition 1

1 In the **Model Builder** window, under **Results** right-click **Power Deposition** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electron Source` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electron Source** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `plas.Re`.

4 On the **Electron Source** toolbar, click **Plot**.

Compare with Figure 9.

Electron Source 1

1 In the **Model Builder** window, under **Results** right-click **Electron Source** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electron Mobility, rr Component` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electron Mobility, *rr* Component** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Plasma (Drift Diffusion)> Electron transport properties>Electron mobility>plas.muerr - Electron mobility, *rr* component**.

3 On the **Electron Mobility, *rr* Component** toolbar, click **Plot**.

Compare with Figure 10.

Electron Mobility, rr Component 1

1 In the **Model Builder** window, under **Results** right-click **Electron Mobility, *rr* Component** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electron Mobility, zz Component` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electron Mobility, zz Component** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Plasma (Drift Diffusion)> Electron transport properties>Electron mobility>plas.muezz - Electron mobility, zz component**.

3 On the **Electron Mobility, zz Component** toolbar, click **Plot**.

Compare with Figure 11.

2D Plot Group 11

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

2 In the **Settings** window for **2D Plot Group**, type `Conduction Current Density, r-Component` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Study 2/Solution 3 (sol3)**.

Surface 1

1 Right-click **Conduction Current Density, r-Component** and choose **Surface**.

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

3 In the **Expression** text field, type `emw.Jr-emw.Jdr`.

4 On the **Conduction Current Density, r-Component** toolbar, click **Plot**.

Compare with Figure 12.

Conduction Current Density, r-Component 1

1 In the **Model Builder** window, under **Results** right-click **Conduction Current Density, r-Component** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Conduction Current Density, z-Component` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Conduction Current Density, z-Component** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `emw.Jz-emw.Jdz`.

4 On the **Conduction Current Density, z-Component** toolbar, click **Plot**.

Compare with Figure 13.

Conduction Current Density, z-Component 1

1 In the **Model Builder** window, under **Results** right-click **Conduction Current Density, z-Component** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Conduction Current Density, phi-Component` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Conduction Current Density, phi-Component** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `emw.Jphi-emw.Jdphi`.

4 On the **Conduction Current Density, phi-Component** toolbar, click **Plot**.

Compare with Figure 14.

Electron Mobility, rr Component 1

1 In the **Model Builder** window, under **Results** right-click **Electron Mobility, rr Component** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Mean Plasma Electrical Conductivity` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Mean Plasma Electrical Conductivity** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `(emw.sigmarr+emw.sigmaphiphi+emw.sigmazz)/3`.

4 On the **Mean Plasma Electrical Conductivity** toolbar, click **Plot**.

Compare with Figure 15.

Drift Diffusion Tutorial

Introduction

The foundation of the *COMSOL Multiphysics Plasma Module* is the Drift Diffusion interface which describes the transport of electrons in an electric field. The Drift Diffusion interface solves a pair of reaction/convection/diffusion equations, one for the electron density and the other for the electron energy density. The mean electron energy is computed by dividing the electron energy density by the electron number density.

Model Definition

This tutorial example computes the electron number density and mean electron energy in a drift tube. Electrons are released due to thermionic emission on the left boundary with an assumed mean electron energy. The electrons are then accelerated towards the right boundary due to an imposed external electric field which is oriented in the opposite direction from the electron drift velocity:

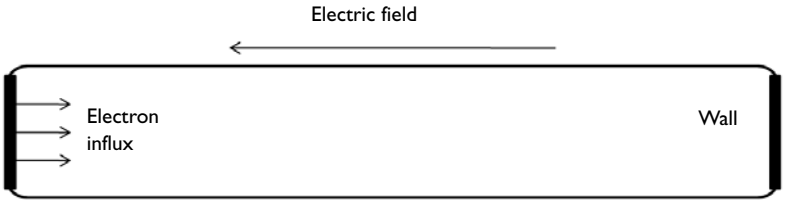

Figure 1: In the drift tube the electrons enter the left boundary and are accelerated by the electric field toward the wall.

MODEL EQUATIONS

A simple model is set up to test the Drift Diffusion interface. The equations solved are, for the electron number density:

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e \tag{1}$$

where

$$\boldsymbol{\Gamma}_e = -(\boldsymbol{\mu}_e \bullet \mathbf{E})n_e - \mathbf{D}_e \bullet \nabla n_e \tag{2}$$

and, n_e denotes the electron density $(1/\mathrm{m}^3)$, R_e is the electron rate expression $(1/(\mathrm{m}^3 \cdot \mathrm{s}))$, μ_e is the electron mobility which is either a scalar or tensor $(\mathrm{m}^2/(\mathrm{V} \cdot \mathrm{s}))$, $\mathbf{E}$ is the electric field (V/m), and D_e is the electron diffusivity, which is either a scalar or a tensor. The first term on the right side of Equation 2 represents migration of electrons due to an electric field. The seconds term on the right side of Equation 2 represents diffusion of electrons

from regions of high electron density to low electron density.

An equation for the electron energy density is solved in conjunction with Equation 1. The equation is:

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot \mathbf{\Gamma}_\varepsilon + \mathbf{E} \cdot \mathbf{\Gamma}_e = R_\varepsilon \tag{3}$$

where

$$\Gamma_\varepsilon = -(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) n_\varepsilon - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon$$

Here, n_ε is the electron energy density (V/m^3), R_ε is the energy loss/gain due to inelastic collisions ($V/(m^3 \cdot s)$), μ_ε is the electron energy mobility ($m^2/(V \cdot s)$), $\mathbf{E}$ is the electric field (V/m), and D_ε is the electron energy diffusivity (m^2/s). The subscript ε refers to electron energy. The third term on the left side of Equation 3 represents heating of the electrons due to an external electric field. Note that this term can either be a heat source or a heat sink depending on whether the electrons are drifting in the same direction as the electric field or not. For a Maxwellian electron energy distribution function, the following relationships hold:

$$D_e = \mu_e T_e, \mu_\varepsilon = \left(\frac{5}{3}\right)\mu_e, D_\varepsilon = \mu_\varepsilon T_e$$

where T_e is the electron "temperature". So, given the electron mobility, the other transport properties required can be computed. The electron "temperature" is a function of the mean electron energy, $\bar{\varepsilon}$ which is defined as:

$$\bar{\varepsilon} = \frac{n_\varepsilon}{n_e}$$

and then:

$$T_e = \left(\frac{2}{3}\right)\bar{\varepsilon}$$

SOURCE COEFFICIENTS

The electron source term, R_e is the sum of the electron impact reaction rates that make up the plasma chemistry. The electron energy loss due to inelastic collisions, R_ε is a function of the electron impact reaction rates multiplied by the energy loss corresponding to each reaction. Mathematically, the electron source is defined as:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (m^3/s), and N_n is the total neutral number density ($1/m^3$). The energy loss is defined as:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (V).

An influx of electron due to thermionic emission is specified on the left boundary. The electrons that are emitted from the surface are then accelerated toward the wall by the electric field. The acceleration leads to an increase in the mean electron energy and subsequently ionization occurs. This creates new electrons, which are ultimately lost into a wall opposite the emitting surface. The gain of electrons due to ionization is included in the model by assuming the drift tube contains argon. This example assumes that the mole fraction of electronically excited argon atoms and argon ions is very small. This means that you do not solve additional equations for the mole fractions of these two species. The following reactions are included in the model:

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\varepsilon$(eV)	A	B	E
1	e+Ar=>e+Ar	Elastic	0	1.99E-014	0.93	0.41
2	e+Ar=>e+Ars	Excitation	11.5	8.77E-015	0.62	18.16
3	e+Ar=>2e+Ar+	Ionization	15.8	2.15E-014	0.49	24.75

The rate constants for these reactions are given in Arrhenius form:

$$k_j = A T_e^B \exp(-E/T_e)$$

The rate constants are computed from cross-section data for each reaction assuming a Maxwellian electron energy distribution function.

The electron density is plotted in Figure 2. The peak electron density occurs close to the far wall. The peak electron density is five times higher than the electron density on the left wall due to new electrons being created through ionization.

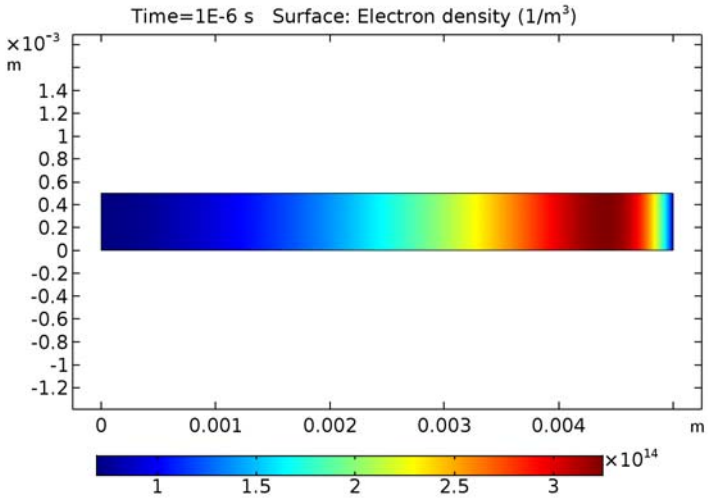

Figure 2: Plot of the electron density in the drift tube.

Because there are no variations in the solution in the y-direction it can be more convenient to create a 1D data set in the x-direction and plot various quantities v.s. the x-axis. Figure 3 plots the electron density as a function of the x-direction. The electron "temperature" is plotted in Figure 4. On the left wall the electron "temperature" is fixed to 2 eV. The temperature steadily increases over a narrow region. This is due to the fact that there is a strong drift velocity in the opposite direction to the electric field. As the electron temperature increases, so do the rate constants which are responsible for creating new electrons. The increase in electron temperature also has a significant on the number of inelastic collisions which occur in the tube. After the initial rise in electron temperature, the electron temperature remains constant until close to the far wall. In this region the joule heating caused by the electron drift velocity in the opposite direction to the electric field is balanced by the energy loss due to inelastic collisions.

The highly nonlinear behavior in such a simple example showcases the fact that very complicated dynamics occur in even the simplest of plasmas.

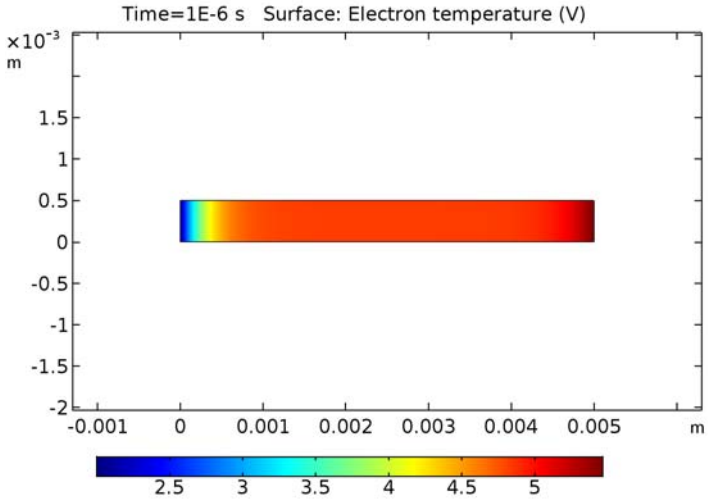

Figure 3: Plot of the electron "temperature" across the drift tube.

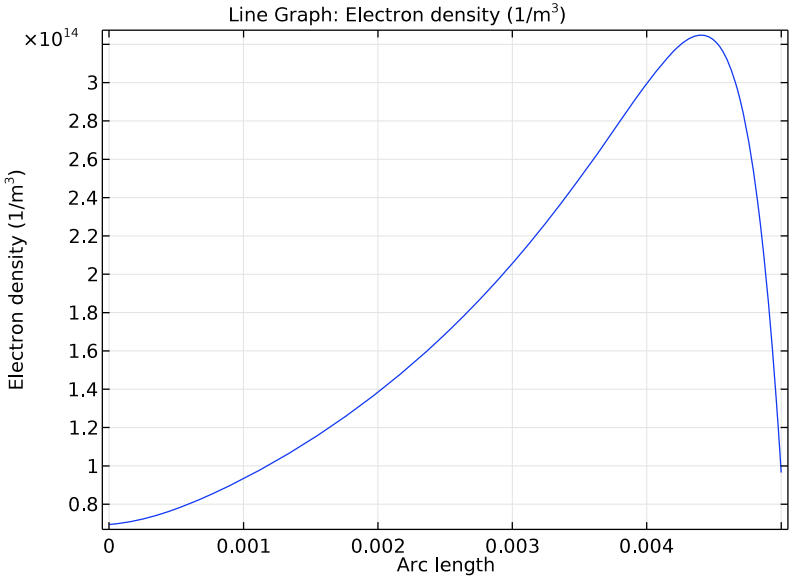

Figure 4: Cross section plot of electron density across the drift tube.

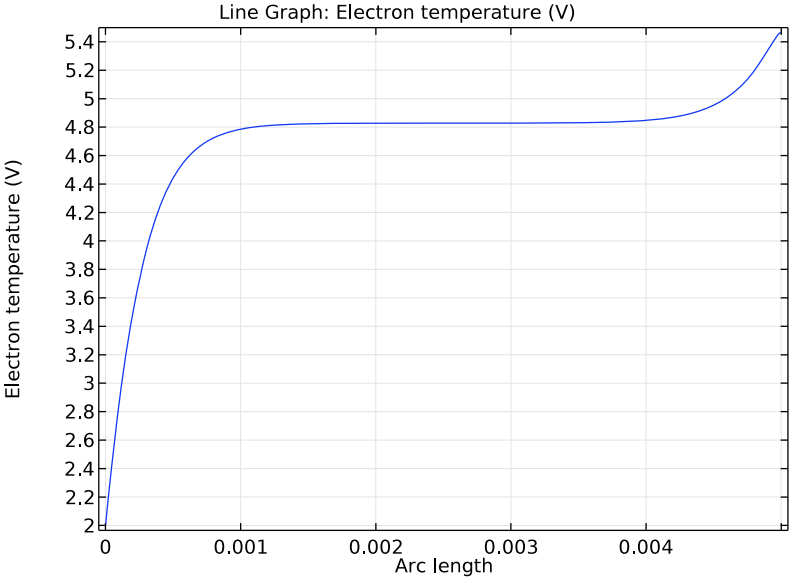

Figure 5: Cross plot of the electron temperature across the drift tube.

Reference

1. G.J.M. Hagelaar and L.C. Pitchford, "Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models," *Plasma Sources Sci. Technol*, vol. 14, pp. 722–733, 2005.

Application Library path: `Plasma_Module/Direct_Current_Discharges/drift_diffusion_tutorial`

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 **2D**.
2. In the **Select Physics** tree, select **Plasma>Drift Diffusion (dd)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies>Time Dependent**.
6. Click **Done**.

GEOMETRY 1

Rectangle 1 (r1)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `5E-3`.

4 In the **Height** text field, type `5E-4`.

Now add a table of expressions for the external electric field, temperature, pressure, and the electron impact reactions occurring in the drift tube. You also define the influx of electrons due to thermionic emission. The influx of electrons and the external electric field are both ramped up from an initial value of zero to aid convergence at early timesteps.

DEFINITIONS

Variables 1

1 On the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
ramp	tanh(1E7[1/s]*t)		Ramp function
T	300[K]	K	Gas temperature
p	10[torr]	Pa	Gas pressure
Nn0	p/k_B_const/T	1/m³	Neutral number density
k1	1.993039e-014*dd.Te^0.93* exp(-0.41/dd.Te)		Elastic rate coefficient
k2	8.773932e-015*dd.Te^0.62* exp(-18.16/dd.Te)		Excitation rate coefficient
k3	2.153106e-014*dd.Te^0.49* exp(-24.75/dd.Te)		Ionization rate coefficient
r1	k1*dd.Nn*dd.ne		Elastic collision reaction rate
r2	k2*dd.Nn*dd.ne		Electronic excitation reaction rate
r3	k3*dd.Nn*dd.ne		Ionization reaction rate
de1	0[V]	V	Energy loss, elastic collision
de2	11.56[V]	V	Energy loss, electronic excitation
de3	15.8[V]	V	Energy loss, ionization
Re	r3		Electron production rate

Name	Expression	Unit	Description
Sen	-e_const*(r1*de1+r2*de2+ r3*de3)		Collisional power loss
Ex	-d(V,x)	V/m	Electric field
V	-100[V]*ramp* (0.005[m]-x)/0.005[m]	V	Electric potential
Ain	0.5E-3^2[m^2]	m^2	Wall area
I	2E-6[A]	A	Thermal emission current
influx	I/Ain/e_const*ramp	$1/(m^2 \cdot s)$	Electron influx
mueN	4E24[1/(m*V*s)]	$1/(V \cdot m \cdot s)$	Reduced electron mobility

DRIFT DIFFUSION (DD)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Drift Diffusion (dd)**.

2 In the **Settings** window for **Drift Diffusion**, locate the **Electron Properties** section.

3 Select the **Use reduced electron transport properties** check box.

Drift Diffusion Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Drift Diffusion (dd)** click **Drift Diffusion Model 1**.

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

3 In the N_n text field, type `Nn0`.

4 In the V text field, type `V`.

5 In the S_{en} text field, type `Sen`.

6 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `mueN`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Drift Diffusion (dd)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E16`.

4 In the ε_0 text field, type `3`.

Electron Production Rate 1

1 In the **Model Builder** window, right-click **Drift Diffusion (dd)** and choose **Electron Production Rate**.

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

3 In the **Settings** window for **Electron Production Rate**, locate the **Electron Production Rate** section.

4 In the R_e text field, type `Re`.

Wall 1

1 Right-click **Drift Diffusion (dd)** and choose **Wall**.

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

3 Select the **Include migration effects** check box.

4 Select Boundary 4 only.

Electron Density and Energy 1

1 Right-click **Drift Diffusion (dd)** and choose **Electron Density and Energy**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Electron Density and Energy**, locate the **Electron Density and Energy** section.

4 Select the **Fix mean electron energy** check box.

Wall 2

1 Right-click **Drift Diffusion (dd)** and choose **Wall**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Wall**, locate the **Electron Density Wall Settings** section.

4 In the $\Gamma_t \cdot \mathbf{n}$ text field, type `influx`.

5 Locate the **Electron Energy Wall Settings** section. Clear the **Use wall for electron energy** check box.

The above boundary conditions applied to boundary 1 means that the mean electron energy will be fixed at 3 electron volts and there will be an influx of electrons resulting in a net current influx of 2E-6 amps.

When you create the mesh you want to use a finer mesh close to the walls so that the sharp gradients in the electron density and electron energy density are adequately resolved. You accomplish this by using a graded mapped mesh.

MESH 1

Distribution 1

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

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

3 Select Boundaries 2 and 3 only.

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

5 From the **Distribution properties** list, choose **Predefined distribution type**.

6 In the **Number of elements** text field, type 200.

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

8 From the **Distribution method** list, choose **Geometric sequence**.

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

Size

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

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

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

4 Click **Build All**.

The mean electron energy and electron density can change on a sub nanosecond timescale. The electron density and mean electron energy reach their steady state values very quickly so it is only necessary to solve the problem for 1 microsecond.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

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

3 In the **Times** text field, type 0.

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 -8.

7 In the **Stop** text field, type -6.

8 In the **Number of values** text field, type 100.

9 From the **Function to apply to all values** list, choose **exp10**.

10 Click **Add**.

11 On the **Home** toolbar, click **Compute**.

RESULTS

Electron Density (dd)

1. In the **Model Builder** window, under **Results** click **Electron Density (dd)**.
2. In the **Settings** window for **2D Plot Group**, click to expand the **Window settings** section.
3. Click to expand the **Color legend** section. Locate the **Color Legend** section. From the **Position** list, choose **Bottom**.
4. Click the **Zoom Extents** button on the **Graphics** toolbar.
5. On the **Electron Density (dd)** toolbar, click **Plot**.

Electron Temperature (dd)

1. In the **Model Builder** window, under **Results** click **Electron Temperature (dd)**.
2. In the **Settings** window for **2D Plot Group**, locate the **Color Legend** section.
3. From the **Position** list, choose **Bottom**.
4. Click the **Zoom Extents** button on the **Graphics** toolbar.
5. On the **Electron Temperature (dd)** toolbar, click **Plot**.

Cut Line 2D 1

1. On the **Results** toolbar, click **Cut Line 2D**.
2. Click the **Zoom Extents** button on the **Graphics** toolbar.
3. In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.
4. In row **Point 1**, set **Y** to `2.5e-4`.
5. In row **Point 2**, set **Y** to `2.5e-4` and **x** to `5-3`.
6. Click **Plot**.

1D Plot Group 3

1. On the **Results** toolbar, click **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, locate the **Data** section.
3. From the **Data set** list, choose **Cut Line 2D 1**.
4. From the **Time selection** list, choose **Last**.

Line Graph 1

1. Right-click **1D Plot Group 3** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Drift Diffusion> Electron density>dd.ne - Electron density**.

3 On the **1D Plot Group 3** toolbar, click **Plot**.

1D Plot Group 4

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

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Data set** list, choose **Cut Line 2D 1**.

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

Line Graph 1

1 Right-click **1D Plot Group 4** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Drift Diffusion> Electron energy density>dd.Te - Electron temperature**.

3 On the **1D Plot Group 4** toolbar, click **Plot**.

Electrodeless Lamp

Introduction

This model simulates an electrodeless lamp with argon/mercury chemistry. The low excitation threshold for mercury atoms means that even though the mercury is present in small concentrations, its interaction with electrons determines the overall discharge characteristics. here is strong UV emission from the plasma at 185 nm and 253 nm stemming from spontaneous decay of electronically excited mercury atoms. The UV emission can stimulate phosphors coated on the surface of the bulb resulting in visible light. From an electrical point of view, the lamp can be thought of as a transformer, where the coil acts as the primary and the plasma acts as the secondary. If the efficiency of discharge lamps could be increased by 1%, it would result in a saving of 10^9 kWh per year worldwide.

Note: This application requires the Plasma Module and the AC/DC Module.

Model Definition

A schematic of the geometry used to solve the problem is given in Figure 1. A sinusoidal current is applied to the copper coil (green) which creates a magnetic field in the ferrite core (gray). When the plasma ignites, a magnetic circuit is created between the ferrite core and the plasma. The free electrons in the plasma bulk are accelerated by the electric field. This leads to creation of new electrons through ionization which sustains the plasma. In

quasi steady-state, the creation of new electrons is balanced by the loss of electrons to the wall.

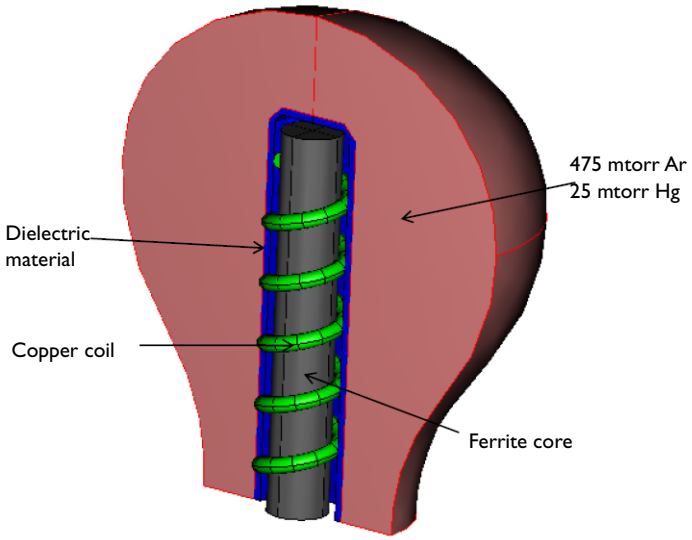

Figure 1: Diagram of electrodeless light source.

The presence of mercury leads to the formation of electronically excited mercury atoms. Certain excited states emit a photon at a given wavelength with a certain emission frequency. By solving for the number density of each of the excited species, you can determine the amount of energy channeled into creating the excited mercury atoms. You can then calculate the amount of energy emitted from the plasma as photons.

In order to simplify the analysis, the following assumptions are made:

- The model is assumed to be axially symmetric.
- The AC induction currents are solved in the frequency domain.
- The electron energy distribution function (EEDF) is assumed to be Maxwellian.
- Thermal quenching of excited atoms is not considered.
- Energy losses in the ferrite core are not considered.
- A trapping factor is used to specify an effective emission photon frequency for the excited mercury atoms. These trapping factors are based on published data.
- The electronically excited argon species are lumped into a single species.

PLASMA CHEMISTRY

The chemical mechanism comes from Ref. 1 and consists of 11 species and 96 reactions:

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon$(eV)
1	e+Ar=>e+Ar	Momentum	0
2	e+Ar=>e+Ar*	Excitation	11.56
3	e+Ar=>e+e+Ar^+	Ionization	15.80
4	e+Ar*=>e+Ar	Superelastic	-11.56
5	e+Ar*=>e+e+Ar^+	Ionization	4.24
6	e+Hg=>e+Hg	Momentum	0
7	e+Hg=>e+Hg(63P0)	Excitation	4.66
8	e+Hg=>e+Hg(63P1)	Excitation	4.87
9	e+Hg=>e+Hg(63P2)	Excitation	5.43
10	e+Hg=>e+Hg(61P1)	Excitation	6.70
11	e+Hg=>e+Hg(73S1)	Excitation	7.70
12	e+Hg=>e+Hg(63DJ)	Excitation	8.85
13	e+Hg=>e+e+Hg^+	Ionization	10.44
14	e+Hg(63P0)=>e+Hg(63P0)	Momentum	0
15	e+Hg(63P0)=>e+Hg	Superelastic	-4.66
16	e+Hg(63P0)=>e+Hg(63P1)	Excitation	0.21
17	e+Hg(63P0)=>e+Hg(63P2)	Excitation	0.77
18	e+Hg(63P0)=>e+Hg(61P1)	Excitation	2.04
19	e+Hg(63P0)=>e+Hg(73S1)	Excitation	3.04
20	e+Hg(63P0)=>e+Hg(63DJ)	Excitation	4.18
21	e+Hg(63P0)=>e+e+Hg^+	Ionization	5.78
22	e+Hg(63P1)=>e+Hg(63P1)	Momentum	0
23	e+Hg(63P1)=>e+Hg	Superelastic	-4.87
24	e+Hg(63P1)=>e+Hg(63P0)	Superelastic	-0.21
25	e+Hg(63P1)=>e+Hg(63P2)	Excitation	0.56
26	e+Hg(63P1)=>e+Hg(61P1)	Excitation	1.83
27	e+Hg(63P1)=>e+Hg(73S1)	Excitation	2.83
28	e+Hg(63P1)=>e+Hg(63DJ)	Excitation	3.98
29	e+Hg(63P1)=>e+e+Hg^+	Ionization	5.57

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon(\mathrm{eV})$
30	e+Hg(63P2)=>e+Hg(63P2)	Momentum	0
31	e+Hg(63P2)=>e+Hg	Superelastic	-5.43
32	e+Hg(63P2)=>e+Hg(63P0)	Superelastic	-0.77
33	e+Hg(63P2)=>e+Hg(63P1)	Superelastic	-0.56
34	e+Hg(63P2)=>e+Hg(61P1)	Excitation	1.27
35	e+Hg(63P2)=>e+Hg(73S1)	Excitation	2.27
36	e+Hg(63P2)=>e+Hg(63DJ)	Excitation	3.42
37	e+Hg(63P2)=>e+e+Hg^+	Ionization	5.01
38	e+Hg(61P1)=>e+Hg(61P1)	Momentum	0
39	e+Hg(61P1)=>e+Hg	Superelastic	-6.7
40	e+Hg(61P1)=>e+Hg(63P0)	Superelastic	-2.04
41	e+Hg(61P1)=>e+Hg(63P1)	Superelastic	-1.83
42	e+Hg(61P1)=>e+Hg(63P2)	Superelastic	-1.27
43	e+Hg(61P1)=>e+e+Hg^+	Ionization	3.74
44	e+Hg(73S1)=>e+Hg(73S1)	Momentum	0
45	e+Hg(73S1)=>e+Hg	Superelastic	-7.7
46	e+Hg(73S1)=>e+Hg(63P0)	Superelastic	-3.04
47	e+Hg(73S1)=>e+Hg(63P1)	Superelastic	-2.83
48	e+Hg(73S1)=>e+Hg(63P2)	Superelastic	-2.27
49	e+Hg(73S1)=>e+e+Hg^+	Ionization	2.74
50	e+Hg(63DJ)=>e+Hg(63DJ)	Momentum	0
51	e+Hg(63DJ)=>e+Hg	Superelastic	-8.85
52	e+Hg(63DJ)=>e+Hg(63P0)	Superelastic	-4.19
53	e+Hg(63DJ)=>e+Hg(63P1)	Superelastic	-3.98
54	e+Hg(63DJ)=>e+Hg(63P2)	Superelastic	-3.42
55	e+Hg(63DJ)=>e+e+Hg^+	Ionization	1.59
56	Ar*+Ar*=>e+Ar+Ar^+	Penning	0
57	Ar*+Hg=>e+Ar+Hg^+	Penning	0
58	Ar*+Hg(63P0)=>e+Ar+Hg^+	Penning	0
59	Ar*+Hg(63P1)=>e+Ar+Hg^+	Penning	0
60	Ar*+Hg(63P2)=>e+Ar+Hg^+	Penning	0

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon(\mathrm{eV})$
61	$Ar^*+Hg(61P1)\Rightarrow e+Ar+Hg^+$	Penning	0
62	$Ar^*+Hg(73S1)\Rightarrow e+Ar+Hg^+$	Penning	0
63	$Ar^*+Hg(63DJ)\Rightarrow e+Ar+Hg^+$	Penning	0
64	$Hg(63P2)+Hg(63P2)\Rightarrow e+Hg+Hg^+$	Penning	0
65	$Hg(63P2)+Hg(63P1)\Rightarrow e+Hg+Hg^+$	Penning	0
66	$Hg(63P2)+Hg(73S1)\Rightarrow e+Hg+Hg^+$	Penning	0
67	$Hg(63P2)+Hg(63DJ)\Rightarrow e+Hg+Hg^+$	Penning	0
68	$Hg(61P1)+Hg(63P0)\Rightarrow e+Hg+Hg^+$	Penning	0
69	$Hg(61P1)+Hg(63P1)\Rightarrow e+Hg+Hg^+$	Penning	0
70	$Hg(61P1)+Hg(63P2)\Rightarrow e+Hg+Hg^+$	Penning	0
71	$Hg(61P1)+Hg(61P1)\Rightarrow e+Hg+Hg^+$	Penning	0
72	$Hg(61P1)+Hg(73S1)\Rightarrow e+Hg+Hg^+$	Penning	0
73	$Hg(61P1)+Hg(63DJ)\Rightarrow e+Hg+Hg^+$	Penning	0
74	$Hg(73S1)+Hg(63P0)\Rightarrow e+Hg+Hg^+$	Penning	0
75	$Hg(73S1)+Hg(63P1)\Rightarrow e+Hg+Hg^+$	Penning	0
76	$Hg(73S1)+Hg(63P2)\Rightarrow e+Hg+Hg^+$	Penning	0
77	$Hg(73S1)+Hg(61P1)\Rightarrow e+Hg+Hg^+$	Penning	0
78	$Hg(73S1)+Hg(73S1)\Rightarrow e+Hg+Hg^+$	Penning	0
79	$Hg(73S1)+Hg(63DJ)\Rightarrow e+Hg+Hg^+$	Penning	0
80	$Hg(63DJ)+Hg(63P0)\Rightarrow e+Hg+Hg^+$	Penning	0
81	$Hg(63DJ)+Hg(63P1)\Rightarrow e+Hg+Hg^+$	Penning	0
82	$Hg(63DJ)+Hg(63P2)\Rightarrow e+Hg+Hg^+$	Penning	0
83	$Hg(63DJ)+Hg(61P1)\Rightarrow e+Hg+Hg^+$	Penning	0
84	$Hg(63DJ)+Hg(73S1)\Rightarrow e+Hg+Hg^+$	Penning	0
85	$Hg(63DJ)+Hg(63DJ)\Rightarrow e+Hg+Hg^+$	Penning	0
86	$Ar^++Hg\Rightarrow Hg^++Ar$	Charge exchange	0
87	$Ar^++Ar\Rightarrow Ar+Ar^+$	Charge exchange	0
88	$Hg^++Hg\Rightarrow Hg+Hg^+$	Charge exchange	0
89	$Hg(63P1)\Rightarrow Hg$	253nm	0
90	$Hg(61P1)\Rightarrow Hg$	185nm	0
91	$Hg(73S1)\Rightarrow Hg(63P0)$	405nm	0

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon$(eV)
92	Hg(73S1)=>Hg(63P1)	436nm	0
93	Hg(73S1)=>Hg(63P2)	546nm	0
94	Hg(63DJ)=>Hg(63P0)	297nm	0
95	Hg(63DJ)=>Hg(63P1)	-	0
96	Hg(63DJ)=>Hg(63P2)	365nm	0

The following surface reactions are considered:

TABLE 2: SURFACE REACTIONS.

REACTION	FORMULA
1	Ars=>Ar
2	Ar+=>Ar
3	Hg1=>Hg
4	Hg2=>Hg
5	Hg3=>Hg
6	Hg4=>Hg
7	Hg5=>Hg
8	Hg6=>Hg
9	Hg+=>Hg

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\mathrm{C}^{1/2}/\mathrm{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

For a nonmagnetized and nonpolarized plasma, the induction currents are computed in the frequency domain using the following equation:

$$(j\omega\sigma - \omega^2\varepsilon_0)\mathbf{A} + \nabla \times (\mu_0^{-1}\nabla \times \mathbf{A}) = \mathbf{J}^e$$

The plasma conductivity needs to be specified as a material property, usually from the cold plasma approximation:

$$\sigma = \frac{n_e q^2}{m_e(\nu_e + j\omega)}$$

where n_e is the electron density, q is the electron charge, m_e is the electron mass, ν_e is the collision frequency and ω is the angular frequency.

ELECTRICAL EXCITATION

The lamp is operated by a fixed power of 80 watts. This means that the total power dissipation in the system is 80 W. Some of the power is lost in the coil and the ferrite but the bulk of the power is channeled into the plasma.

The results are presented below.

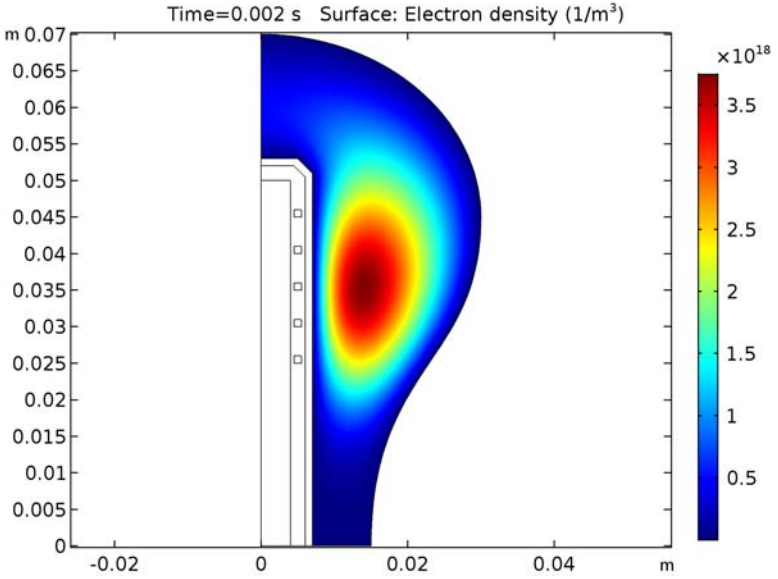

Figure 2: Surface plot of electron density inside the column.

The electron density is plotted in Figure 2. The electron density is high, as one would expect in an inductively coupled plasma. The peak value of the electron density at the driving frequency used in the model results in a peak plasma conductivity of around 180 S/m. The high value for the electron density and low excitation and ionization threshold for mercury results in a very low electron "temperature" which is plotted in Figure 3. The peak electron temperature is only 1.27 eV, which through Boltzmann's relation results in a low plasma potential. The plasma potential is plotted in Figure 4 and only peaks at 8 V.

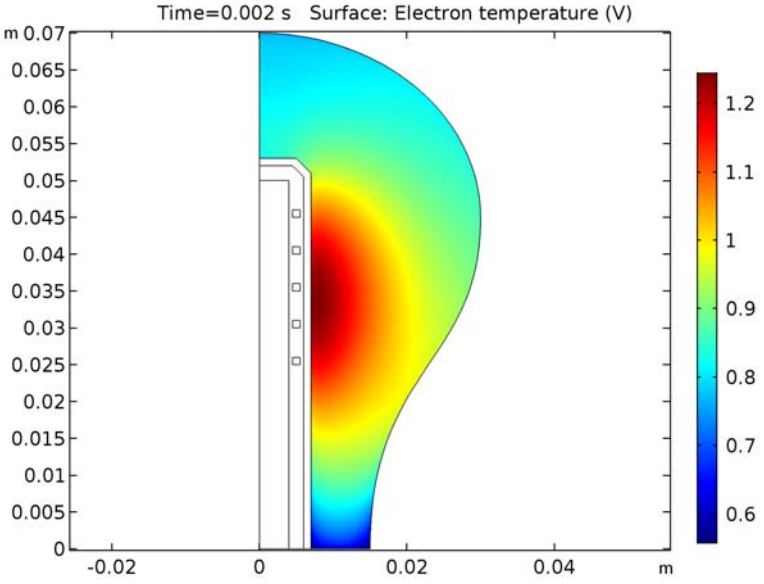

Figure 3: Plot of the electron "temperature".

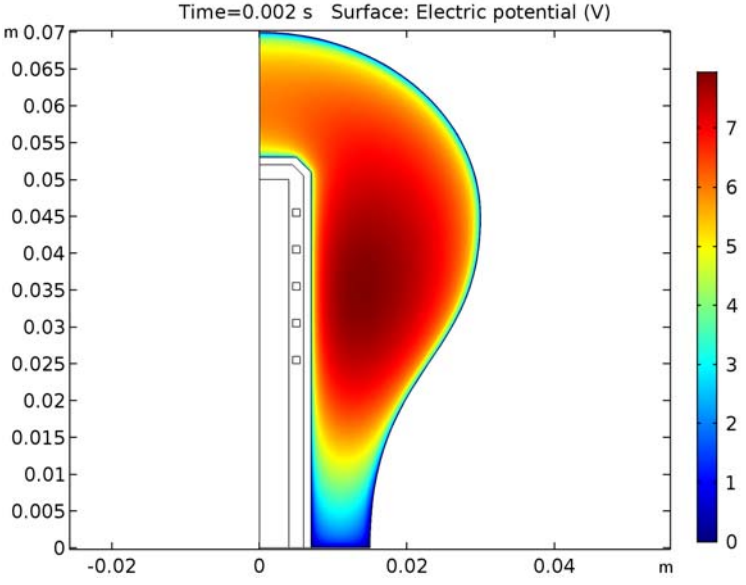

Figure 4: Plot of plasma potential.

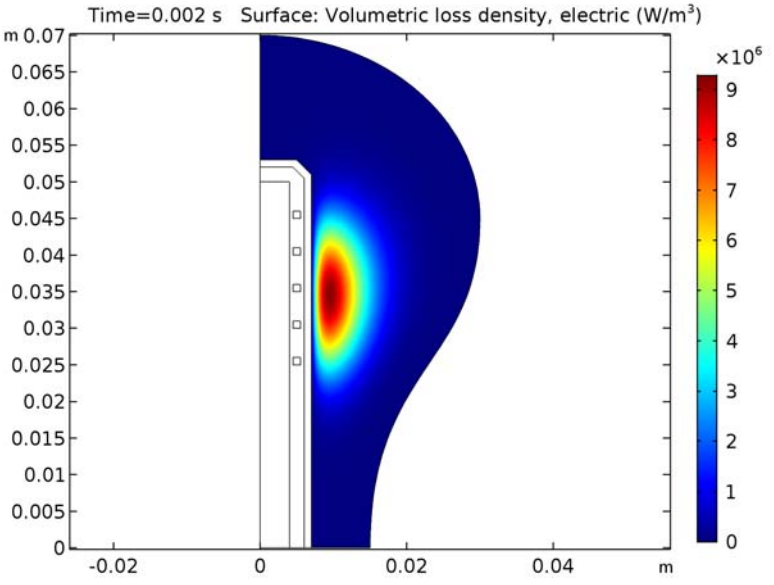

Figure 5: Plot of the resistive losses.

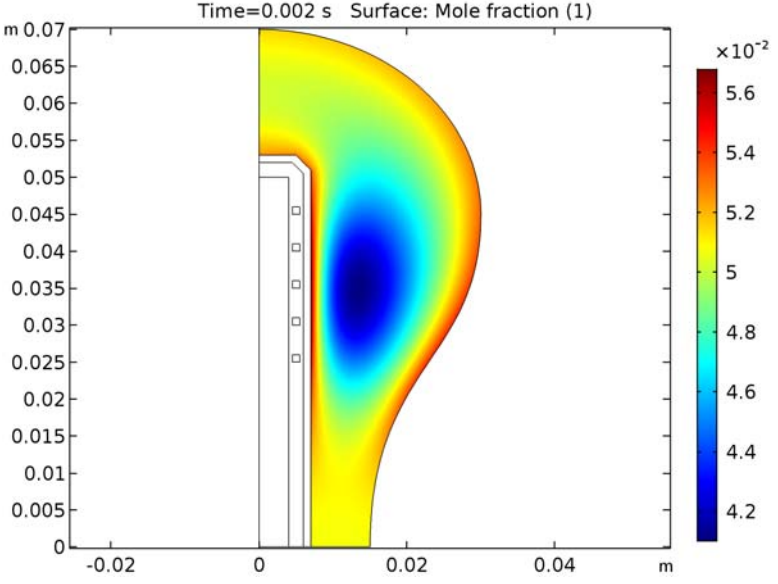

Figure 6: Plot of the mole fraction of ground state mercury.

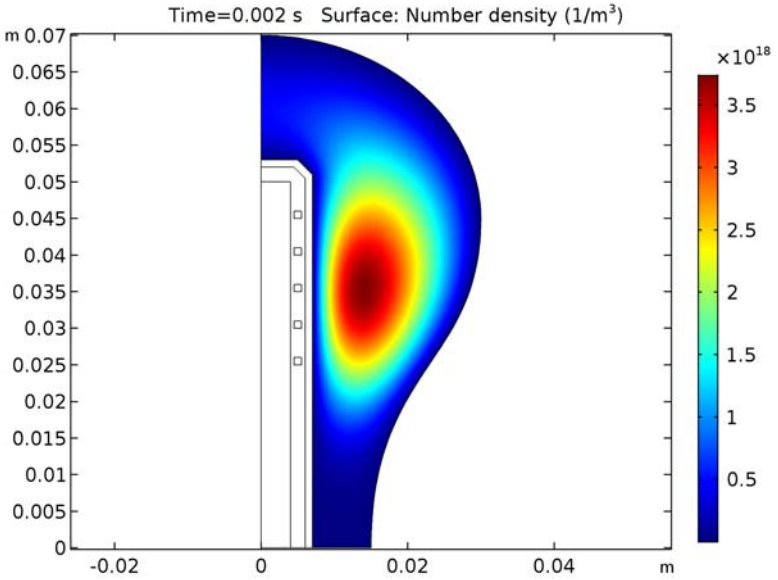

Figure 7: Plot of the number density of mercury ions.

The resistive losses in the plasma are plotted in Figure 5. The plasma skin depth is a few centimeters so there is no real shielding of the azimuthal electric field. The mole fraction of the ground state mercury is plotted in Figure 6. The mole fraction is low in the core of the plasma and higher on the walls. This is because the electrons consume the ground state mercury in the plasma core, converting it to electronically excited states. The electronically excited mercury atoms diffuse to the walls of the lamp where they de-excite back to the ground state. This continuous consumption of ground state mercury in the plasma bulk and release on the walls results in large gradients in mole fraction within the bulb.

There are two ion species present in the plasma, argon, and mercury. Despite the fact that the number density of ground state argon is 25 times higher than mercury, the density of mercury ions is several hundred times greater than the density of argon ions. This is because the ionization energy for mercury is only 10.44 eV compared to 15.7 eV for argon. Direct ionization of mercury is preferable to argon because the tail of the electron energy distribution function drops dramatically at higher electron energies. Additionally, any argon ions which encounter a ground state or electronically excited mercury atom donate their charge because it is energetically favorable.

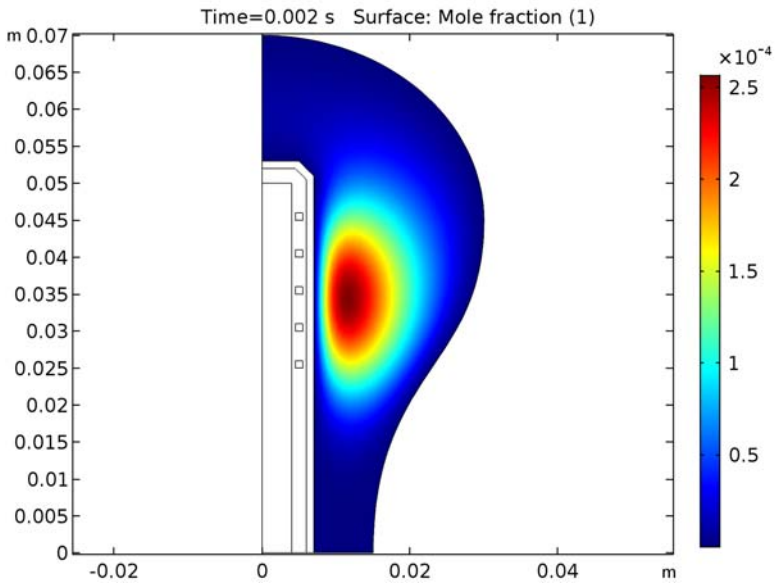

Figure 8: Plot of the mole fraction of Hg(63P1). Spontaneous decay of this species is responsible for the generation of 253nm radiation.

The mole fraction of Hg(63P1) is plotted in Figure 8. These atoms spontaneously emit photos at a frequency factor of $8 \cdot 10^6$ s^{-1}. On the way to the walls of the lamp, the photons continuously excite mercury atoms and then be released when spontaneous decay occurs. This resonant absorption and re-absorption of the photons means that the frequency factor appears to be much lower than it actually is. Since a self consistent model of the radiation imprisonment of the photons is computationally impractical, a trapping factor is used to approximate this effect. A trapping factor of 10 is used for the Hg(63P1) atoms which means that the frequency factor is lowered by a factor of 10. In Figure 9 the mole fraction of Hg(61P1) is plotted. A trapping factor of 1000 is used for the spontaneous decay back to ground state mercury.

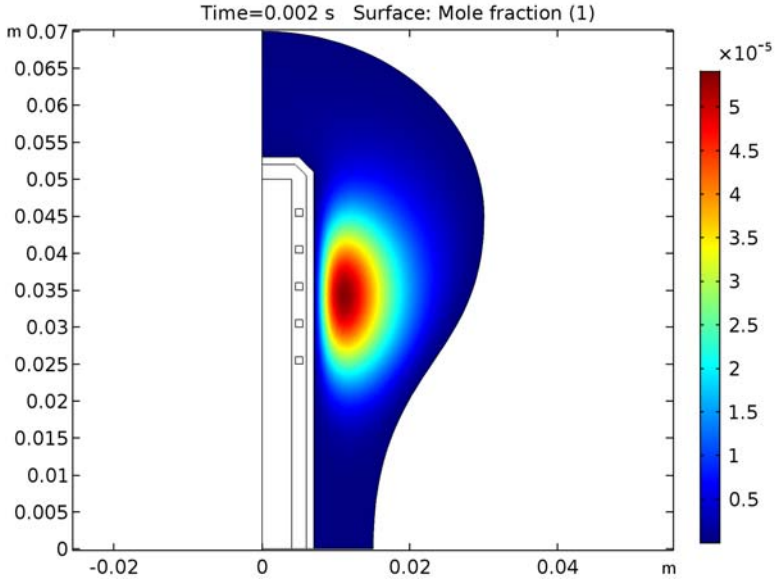

Figure 9: Plot of the mole fraction of Hg(61P1). Spontaneous decay of this species is responsible for the generation of 185nm radiation.

Reference

1. K. Rajaraman, *Radiation Transport in Low Pressure Plasmas: Lighting and Semiconductor Etching Plasmas*, Ph.D. thesis, Depart. of Physics, University of Illinois, 2005.

Application Library path: `Plasma_Module/Inductively_Coupled_Plasmas/electrodeless_lamp`

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 **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Plasma>Inductively Coupled Plasma**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Frequency-Transient**.

6 Click **Done**.

GEOMETRY 1

Bézier Polygon 1 (b1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Bézier Polygon**.

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

3 Find the **Added segments** subsection. Click **Add Linear**.

4 Find the **Control points** subsection. In row **2**, set **r** to `0.015`.

5 Find the **Added segments** subsection. Click **Add Cubic**.

6 Find the **Control points** subsection. In row **2**, set **z** to `0.025`.

7 In row **3**, set **r** to `0.03` and **z** to `0.025`.

8 In row **4**, set **r** to `0.03` and **z** to `0.045`.

9 Find the **Added segments** subsection. Click **Add Quadratic**.

10 Find the **Control points** subsection. In row **2**, set **z** to `0.07`.

11 In row **3**, set **r** to `0` and **z** to `0.07`.

12 Find the **Added segments** subsection. Click **Add Linear**.

13 Find the **Control points** subsection. In row **2**, set **z** to `0`.

14 Find the **Added segments** subsection. Click **Add Linear**.

15 Click **Build All Objects**.

Rectangle 1 (r1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.004`.

4 In the **Height** text field, type `0.05`.

Rectangle 2 (r2)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.006`.

4 In the **Height** text field, type `0.052`.

Rectangle 3 (r3)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.007`.

4 In the **Height** text field, type `0.053`.

Chamfer 1 (cha1)

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

2 Click the **Zoom In** button on the **Graphics** toolbar.

3 On the object **r2**, select Point 3 only.

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

5 In the **Distance from vertex** text field, type `1.5e-3`.

6 Click **Build All Objects**.

Chamfer 2 (cha2)

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

2 On the object **r3**, select Point 3 only.

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

4 In the **Distance from vertex** text field, type `2e-3`.

5 Click **Build All Objects**.

Square 1 (sq1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Square**.

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

3 In the **Side length** text field, type `0.001`.

4 Locate the **Position** section. In the **r** text field, type `0.0045`.

5 In the **z** text field, type `0.025`.

6 Click **Build All Objects**.

Array 1 (arr1)

1 On the **Geometry** toolbar, click **Transforms** and choose **Array**.

2 Select the object **sq1** only.

3 In the **Settings** window for **Array**, locate the **Size** section.

4 From the **Array type** list, choose **Linear**.

5 In the **Size** text field, type `5`.

6 Locate the **Displacement** section. In the **z** text field, type `5e-3`.

7 Click **Build All Objects**.

8 Click the **Zoom Extents** button on the **Graphics** toolbar.

DEFINITIONS

Variables 1

1 On the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`Tinit`	`350[K]`	K	`Gas temperature`
`pinit`	`101325*(500E-3/760)[Pa]`	Pa	`Initial total pressure`
`lamp_power`	`80[W]`	W	`Lamp power`
`tf1`	`10`		`Trapping factor`
`tf2`	`1000`		`Trapping factor`

Explicit 1

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

2 Select Domains 5–9 only.

3 In the **Settings** window for **Explicit**, locate the **Output Entities** section.

4 From the **Output entities** list, choose **Adjacent boundaries**.

5 In the **Label** text field, type `Coil boundaries`.

Explicit 2

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

2 Select Domains 5–9 only.

3 In the **Settings** window for **Explicit**, type `Coil domains` in the **Label** text field.

Explicit 3

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

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

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

4 Select Boundaries 8, 27, and 35–38 only.

5 In the **Label** text field, type `Boundary layers`.

Explicit 4

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

2 Select Domain 4 only.

3 In the **Settings** window for **Explicit**, type `Discharge` in the **Label** text field.

PLASMA (PLAS)

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

2 Select Domain 4 only.

Cross Section Import 1

1 Right-click **Component 1 (comp1)>Plasma (plas)** 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`.

Cross Section Import 2

1 In the **Model Builder** window, right-click **Plasma (plas)** 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 `Hg_xsecs.txt`.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

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

4 Locate the **Reaction Parameters** section. In the k^f text field, type `N_A_const*1.00E-15[m^3/s]`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> Reaction**.

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

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

4 Locate the **Reaction Parameters** section. In the k^f text field, type `N_A_const*9E-16[m^3/s]`.

58: Ars+Hg=>Hg++Ar+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>Reaction 2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars+Hg1=>Hg++Ar+e`.

59: Ars+Hg1=>Hg++Ar+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>58: Ars+Hg=>Hg++Ar+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars+Hg2=>Hg++Ar+e`.

60: Ars+Hg2=>Hg++Ar+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>59: Ars+Hg1=>Hg++Ar+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars+Hg3=>Hg++Ar+e`.

61: Ars+Hg3=>Hg++Ar+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>60: Ars+Hg2=>Hg++Ar+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars+Hg4=>Hg++Ar+e`.

62: Ars+Hg4=>Hg++Ar+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>61: Ars+Hg3=>Hg++Ar+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars+Hg5=>Hg++Ar+e`.

63: Ars+Hg5=>Hg++Ar+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>62: Ars+Hg4=>Hg++Ar+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Ars+Hg6=>Hg++Ar+e`.

64: Ars+Hg6=>Hg++Ar+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>63: Ars+Hg5=>Hg++Ar+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg3+Hg3=>Hg++Hg+e`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `N_A_const*3.50E-16[m^3/s]`.

65: Hg3+Hg3=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>64: Ars+Hg6=>Hg++Ar+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg3+Hg4=>Hg++Hg+e`.

66: Hg3+Hg4=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>65: Hg3+Hg3=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg3+Hg5=>Hg++Hg+e`.

67: Hg3+Hg5=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>66: Hg3+Hg4=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg3+Hg6=>Hg++Hg+e`.

68: Hg3+Hg6=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>67: Hg3+Hg5=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg4+Hg1=>Hg++Hg+e`.

69: Hg4+Hg1=>Hg++Hg+e

1. Right-click **Component 1 (comp1)>Plasma (plas)>68: Hg3+Hg6=>Hg++Hg+e** and choose **Duplicate**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Hg4+Hg2=>Hg++Hg+e`.

70: Hg4+Hg2=>Hg++Hg+e

1. Right-click **Component 1 (comp1)>Plasma (plas)>69: Hg4+Hg1=>Hg++Hg+e** and choose **Duplicate**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Hg4+Hg3=>Hg++Hg+e`.

71: Hg4+Hg3=>Hg++Hg+e

1. Right-click **Component 1 (comp1)>Plasma (plas)>70: Hg4+Hg2=>Hg++Hg+e** and choose **Duplicate**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Hg4+Hg4=>Hg++Hg+e`.

72: Hg4+Hg4=>Hg++Hg+e

1. Right-click **Component 1 (comp1)>Plasma (plas)>71: Hg4+Hg3=>Hg++Hg+e** and choose **Duplicate**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Hg4+Hg5=>Hg++Hg+e`.

73: Hg4+Hg5=>Hg++Hg+e

1. Right-click **Component 1 (comp1)>Plasma (plas)>72: Hg4+Hg4=>Hg++Hg+e** and choose **Duplicate**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Hg4+Hg6=>Hg++Hg+e`.

74: Hg4+Hg6=>Hg++Hg+e

1. Right-click **Component 1 (comp1)>Plasma (plas)>73: Hg4+Hg5=>Hg++Hg+e** and choose **Duplicate**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3. In the **Formula** text field, type `Hg5+Hg1=>Hg++Hg+e`.

75: Hg5+Hg1=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>74: Hg4+Hg6=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5+Hg2=>Hg++Hg+e`.

76: Hg5+Hg2=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>75: Hg5+Hg1=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5+Hg3=>Hg++Hg+e`.

77: Hg5+Hg3=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>76: Hg5+Hg2=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5+Hg4=>Hg++Hg+e`.

78: Hg5+Hg4=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>77: Hg5+Hg3=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5+Hg5=>Hg++Hg+e`.

79: Hg5+Hg5=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>78: Hg5+Hg4=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5+Hg6=>Hg++Hg+e`.

80: Hg5+Hg6=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>79: Hg5+Hg5=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6+Hg1=>Hg++Hg+e`.

81: Hg6+Hg1=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>80: Hg5+Hg6=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6+Hg2=>Hg++Hg+e`.

82: Hg6+Hg2=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>81: Hg6+Hg1=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6+Hg3=>Hg++Hg+e`.

83: Hg6+Hg3=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>82: Hg6+Hg2=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6+Hg4=>Hg++Hg+e`.

84: Hg6+Hg4=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>83: Hg6+Hg3=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6+Hg5=>Hg++Hg+e`.

85: Hg6+Hg5=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>84: Hg6+Hg4=>Hg++Hg+e** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6+Hg6=>Hg++Hg+e`.

86: Hg6+Hg6=>Hg++Hg+e

1 Right-click **Component 1 (comp1)>Plasma (plas)>85: Hg6+Hg5=>Hg++Hg+e** and choose **Duplicate**.

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

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

4 Locate the **Reaction Parameters** section. In the k^f text field, type `N_A_const*1.50E-17[m^3/s]`.

87: Ar++Hg=>Hg++Ar

1 Right-click **Component 1 (comp1)>Plasma (plas)>86: Hg6+Hg6=>Hg++Hg+e** and choose **Duplicate**.

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

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

4 Locate the **Reaction Parameters** section. In the k^f text field, type `N_A_const*4.60E-16[m^3/s]`.

88: Ar++Ar=>Ar++Ar

1 Right-click **Component 1 (comp1)>Plasma (plas)>87: Ar++Hg=>Hg++Ar** and choose **Duplicate**.

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

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

4 Locate the **Reaction Parameters** section. In the k^f text field, type `N_A_const*1.00E-15[m^3/s]`.

89: Hg++Hg=>Hg+Hg+

1 Right-click **Component 1 (comp1)>Plasma (plas)>88: Ar++Ar=>Ar++Ar** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg2=>Hg`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `8.00E6/tf1`.

90: Hg2=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>89: Hg++Hg=>Hg+Hg+** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg4=>Hg`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `7.50E8/tf2`.

91: Hg4=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>90: Hg2=>Hg** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5=>Hg1`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `2.2E7`.

92: Hg5=>Hg1

1 Right-click **Component 1 (comp1)>Plasma (plas)>91: Hg4=>Hg** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5=>Hg2`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `6.6E7`.

93: Hg5=>Hg2

1 Right-click **Component 1 (comp1)>Plasma (plas)>92: Hg5=>Hg1** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5=>Hg3`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `2E7`.

94: Hg5=>Hg3

1 Right-click **Component 1 (comp1)>Plasma (plas)>93: Hg5=>Hg2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6=>Hg1`.

95: Hg6=>Hg1

1 Right-click **Component 1 (comp1)>Plasma (plas)>94: Hg5=>Hg3** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6=>Hg2`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `6E7`.

96: Hg6=>Hg2

1 Right-click **Component 1 (comp1)>Plasma (plas)>95: Hg6=>Hg1** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6=>Hg3`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `5E7`.

Surface Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

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 **Boundary Selection** section. From the **Selection** list, choose **Boundary layers**.

2: Ars=>Ar

1 Right-click **Component 1 (comp1)>Plasma (plas)>Surface Reaction 1** and choose **Duplicate**.

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

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

3: Ar+=>Ar

1 Right-click **Component 1 (comp1)>Plasma (plas)>2: Ars=>Ar** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg1=>Hg`.

4: Hg1=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>3: 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 `Hg2=>Hg`.

5: Hg2=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>4: Hg1=>Hg** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg3=>Hg`.

6: Hg3=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>5: Hg2=>Hg** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg4=>Hg`.

7: Hg4=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>6: Hg3=>Hg** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg5=>Hg`.

8: Hg5=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>7: Hg4=>Hg** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Hg6=>Hg`.

9: Hg6=>Hg

1 Right-click **Component 1 (comp1)>Plasma (plas)>8: Hg5=>Hg** and choose **Duplicate**.

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

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

Species: Hg

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 In the x_0 text field, type `0.05`.

Species: Hg1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg1**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 In the x_0 text field, type `2E-6`.

Species: Hg2

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg2**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 In the x_0 text field, type `1E-6`.

Species: Hg3

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg3**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 In the x_0 text field, type `5E-6`.

Species: Hg4

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg4**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 In the x_0 text field, type `1E-6`.

Species: Hg5

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg5**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 In the x_0 text field, type `5E-6`.

Species: Hg6

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg6**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 In the x_0 text field, type `1E-6`.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar**.

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

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

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar+**.

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

3 In the n_0 text field, type `1E16`.

Species: Hg+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Hg+**.

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

3 In the M_w text field, type `0.2006`.

4 In the σ text field, type `2.969[angstrom]`.

5 In the ε/k_b text field, type `750`.

6 Locate the **Species Formula** section. Select the **Initial value from electroneutrality constraint** check box.

Plasma Model 1

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

2 In the **Settings** window for **Plasma Model**, locate the **Electron Density and Energy** section.

3 From the **Electron transport properties** list, choose **From electron impact reactions**.

4 Locate the **Model Inputs** section. In the T text field, type `Tinit`.

5 In the p_A text field, type `pinit`.

Ground 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

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

3 From the **Selection** list, choose **Boundary layers**.

Wall 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

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

3 From the **Selection** list, choose **Boundary layers**.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E17`.

4 In the ε_0 text field, type `2`.

5 Click the **Zoom Box** button on the **Graphics** toolbar.

MAGNETIC FIELDS (MF)

On the **Physics** toolbar, click **Plasma (plas)** and choose **Magnetic Fields (mf)**.

Coil 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Magnetic Fields (mf)** and choose the domain setting **Coil**.

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

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

4 Locate the **Coil** section. Select the **Coil group** check box.

5 From the **Coil excitation** list, choose **Power**.

6 In the P_{coil} text field, type `lamp_power`.

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

MATERIALS

Material 1 (mat1)

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

2 Select Domains 5–9 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Electrical conductivity	sigma	6e7	S/m	Basic
Relative permeability	mur	1	1	Basic
Relative permittivity	epsilonr	1	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 1 (mat1)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Coils` in the **New label** text field.

7 Click **OK**.

Material 2 (mat2)

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

2 Select Domain 1 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1e3	1	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	1	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 2 (mat2)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Ferrite` in the **New label** text field.

7 Click **OK**.

Material 3 (mat3)

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

2 Select Domain 2 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	1	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	1	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 3 (mat3)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Air` in the **New label** text field.

7 Click **OK**.

Material 4 (mat4)

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

2 Select Domain 3 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	1	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	4.2	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 4 (mat4)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Dielectric` in the **New label** text field.

7 Click **OK**.

MESH 1

1 In the **Settings** window for **Mesh**, locate the **Mesh Settings** section.

2 From the **Element size** list, choose **Extra fine**.

Edge 1

1 Right-click **Component 1 (comp1)>Mesh 1** and choose **More Operations>Edge**.

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

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

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Distribution**.

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

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

4 Locate the **Distribution** section. From the **Distribution properties** list, choose **Predefined distribution type**.

5 In the **Number of elements** text field, type 30.

6 In the **Element ratio** text field, type 6.

7 From the **Distribution method** list, choose **Geometric sequence**.

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

Mapped 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Mapped**.

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

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

4 From the **Selection** list, choose **Coil domains**.

Edge 2

1 Right-click **Mesh 1** and choose **More Operations>Edge**.

2 Select Boundaries 8, 27, and 35 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 2** and choose **Size**.

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

3 Click the **Custom** button.

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

5 In the associated text field, type `5e-4`.

Edge 3

1 In the **Model Builder** window, right-click **Mesh 1** and choose **More Operations>Edge**.

2 Select Boundaries 36–38 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 3** and choose **Size**.

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

3 Click the **Custom** button.

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

5 In the associated text field, type `1e-3`.

Boundary Layers 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Boundary Layers**.

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

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

4 Select Domain 4 only.

5 Click to expand the **Transition** section. Clear the **Smooth transition to interior mesh** check box.

Boundary Layer Properties

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Boundary Layers 1** click **Boundary Layer Properties**.

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

3 From the **Selection** list, choose **Boundary layers**.

4 Locate the **Boundary Layer Properties** section. In the **Boundary layer stretching factor** text field, type `1.1`.

5 In the **Thickness adjustment factor** text field, type `1`.

6 From the **Thickness of first layer** list, choose **Manual**.

7 In the **Thickness** text field, type `2E-5`.

Free Triangular 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

STUDY 1

Step 1: Frequency-Transient

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

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

3 In the **Times** text field, type `0`.

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 `-8`.

7 In the **Stop** text field, type `log10(2e-3)`.

8 In the **Number of values** text field, type `3`.

9 From the **Function to apply to all values** list, choose **exp10**.

10 Click **Add**.

11 On the **Home** toolbar, click **Compute**.

RESULTS

2D Plot Group 6

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

2 In the **Settings** window for **2D Plot Group**, type `Power Deposition` in the **Label** text field.

Surface 1

1 Right-click **Power Deposition** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Magnetic Fields> Heating and losses>mf.Qrh - Volumetric loss density, electric**.

Selection 1

1 In the **Model Builder** window, right-click **Surface 1** and choose **Selection**.

2 Select Domain 4 only.

3 On the **Power Deposition** toolbar, click **Plot**.

2D Plot Group 7

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

2 In the **Settings** window for **2D Plot Group**, type `Ground State Mercury Mole Fraction` in the **Label** text field.

Surface 1

1 Right-click **Ground State Mercury Mole Fraction** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Mole fractions>plas.x_wHg - Mole fraction**.

3 On the **Ground State Mercury Mole Fraction** toolbar, click **Plot**.

2D Plot Group 8

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

2 In the **Settings** window for **2D Plot Group**, type `Mercury Ion Number Density` in the **Label** text field.

Surface 1

1 Right-click **Mercury Ion Number Density** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Number densities>plas.n_wHg_1p - Number density**.

3 On the **Mercury Ion Number Density** toolbar, click **Plot**.

2D Plot Group 9

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

2 In the **Settings** window for **2D Plot Group**, type `Mole Fraction of Excited Mercury 2` in the **Label** text field.

Surface 1

1 Right-click **Mole Fraction of Excited Mercury 2** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Mole fractions>plas.x_wHg2 - Mole fraction**.

3 On the **Mole Fraction of Excited Mercury 2** toolbar, click **Plot**.

2D Plot Group 10

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

2 In the **Settings** window for **2D Plot Group**, type `Mole Fraction of Excited Mercury 4` in the **Label** text field.

Surface 1

1 Right-click **Mole Fraction of Excited Mercury 4** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Mole fractions>plas.x_wHg4 - Mole fraction**.

3 On the **Mole Fraction of Excited Mercury 4** toolbar, click **Plot**.

ICP Torch

Introduction

Thermal plasmas have nowadays a large range of industrial applications including: cutting, welding, spraying, waste destruction and surface treatment. Thermal plasmas are assumed to be under partial to complete local thermodynamic equilibrium (LTE) conditions. Under LTE, the plasma can be considered a conductive fluid mixture and therefore, be modeled using the magnetohydrodynamics (MHD) equations. This model shows how to use the Equilibrium Inductively Coupled Discharge interface to simulate the plasma generated in an inductively coupled plasma torch.

Figure 1 displays the geometry of the to-be-modeled inductive plasma torch.

Figure 1: Geometry of an inductively coupled plasma torch. The torch is composed of three concentric quartz tubes in which gas are injected from the bottom and exit from the top the torch. In this model, a fixed power of 11 kW is transfered to the plasma by a three turn coil operating at 3MHz.

Note: This application requires the Plasma Module and AC/DC Module.

Model Definition

This model is based on the work presented in Ref. 1 and uses the following assumptions:

- The plasma torch is modeled by a fully axisymmetric configuration.

2 The coil consists of parallel current carrying rings with a circle cross section, 6 mm in diameter. This implies neglecting the axial component of the coil current.

3 Steady state, laminar pure argon plasma flow at atmospheric pressure.

4 Optically thin plasma under local thermodynamic equilibrium (LTE) conditions.

5 Viscous dissipation and pressure work in the energy equation are neglected.

Figure 2 shows the geometry of the model.

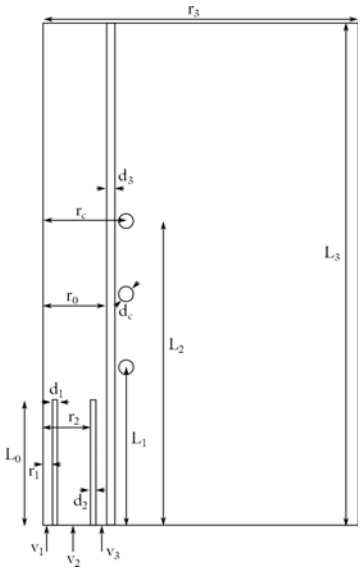

Figure 2: Schematic of the ICP torch. Flow enters from the base (v1, v2 and v3) and leaves out the top. The dimensions of the different part of the model are given in the Modeling Instructions section.

In this model excitation is provided to a three turns coil at 3 MHz. The gas flowing in the sheath tube (plasma confinement tube) is then ionized by Joule heating.

The model is solved using a frequency-transient study in combination with a single turn coil feature which set a fixed power to the system (11 kW). By fixing the power, the current and electric potential can vary in the coil as the plasma electrical conductivity builds up. Steady-state is reached when the coil current stabilized to it's nominal value.

In this model the three different gas stream velocities (v1 for the carrier tube, v2 for the central tube and v3 for the sheath tube) are composed of pure argon. The temperature dependent argon's physical properties are loaded from the material library under Equilibrium Discharge. Note that the temperature range of the physical properties span

from 500 K to 25 000K. Note also that a minimum electrical conductivity has been used to initiate the plasma. The latter has been set to 1 S/m.

Results and Discussion

Figure 3, and Figure 4 respectively shows the plasma temperature distribution, and velocity magnitude of the argon plasma after 0.1 s. Figure 5 shows the electrical conductivity of the plasma at the same time (0.1 s). Note that, for this figure, the electrical conductivity of the other constituents of the model has been set to 0 for sake of visualization.

Figure 6 displays the magnetic flux norm at steady state (0.1 s). Note that the electrical conductivity of the plasma screens the magnetic flux as a consequence of the skin effect.

Figure 7 shows the coil current as a function of the simulation time. The steady state is reached when the current stabilizes, i.e. around t=0.1 s.

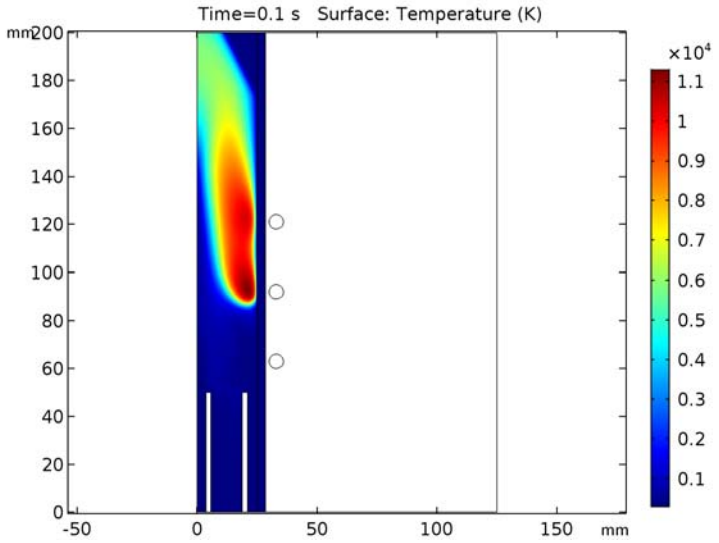

Figure 3: Surface plot of the LTE plasma temperature.

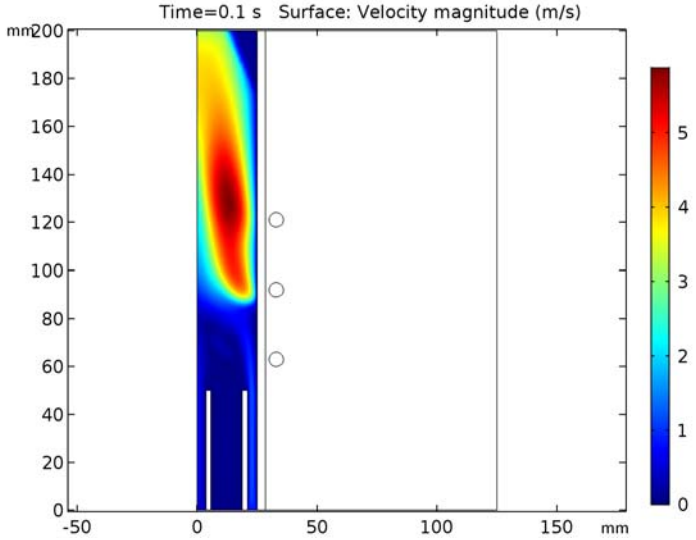

Figure 4: Plot of the velocity magnitude.

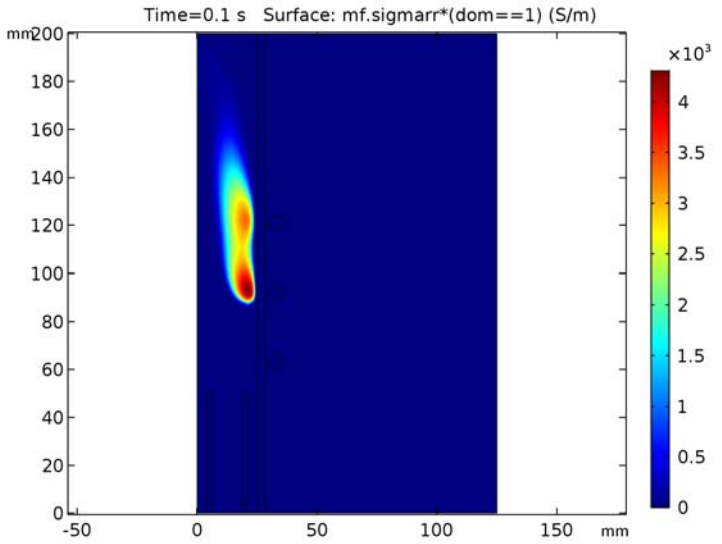

Figure 5: Plot of the plasma electrical conductivity.

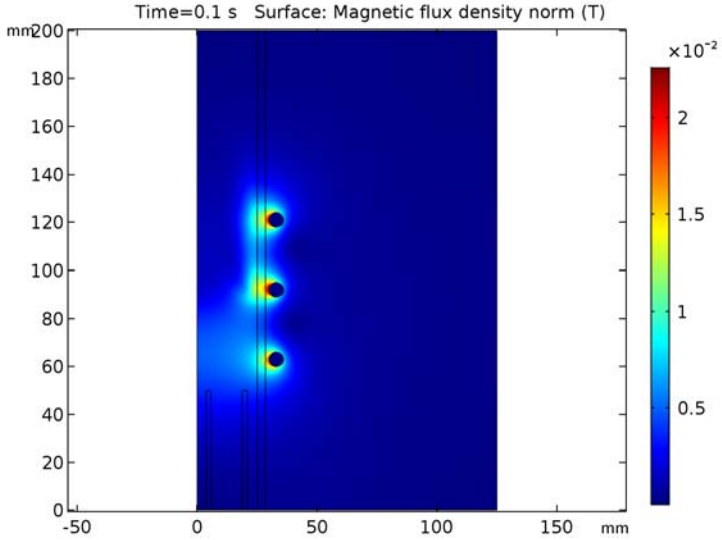

Figure 6: Norm of the magnetic flux. Note the effect of the resistivity on the penetration of the field (skin effect).

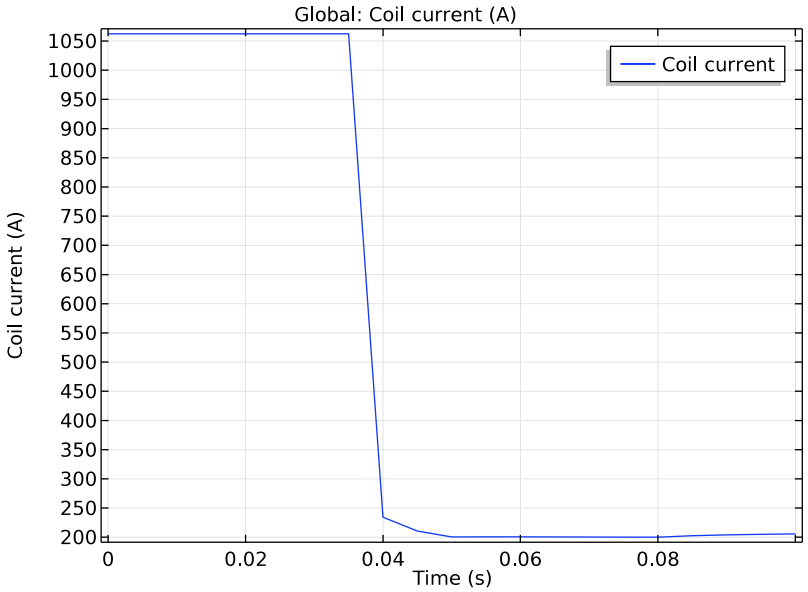

Figure 7: Coil current as a function of time for a fixed excitation power. Note the stabilization of the current density as the system reach the steady state.

Reference

1. S. Xue, P. Proulx and M.I. Boulos, "Extended-field electromagnetic model for inductively coupled plasma," *J. Phys. D.* 34, 1897, 2001

Application Library path: `Plasma_Module/Equilibrium_Discharges/icp_torch`

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 **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Plasma>Equilibrium Discharges> Equilibrium Inductively Coupled Plasma**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Frequency-Transient**.

6 Click **Done**.

ROOT

Select the mm units.

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**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
T0	300[K]	300 K	Ambient temperature
Pext	11[kW]	1.1E4 W	Coil excitation power
freq	3[MHz]	3E6 Hz	Coil excitation frequency
r_3	125[mm]	0.125 m	Axial length: Computational domain
L_3	200[mm]	0.2 m	Height: Computational domain and sheath tube
d_1	2[mm]	0.002 m	Thickness: Carrier tube
L_0	50[mm]	0.05 m	Height: Carrier tube and central tube
r_1	3.7[mm]	0.0037 m	Inner radius: Carrier tube
d_2	2.2[mm]	0.0022 m	Thickness: Central tube
r_2	18.8[mm]	0.0188 m	Inner radius: Central tube
d_3	3.5[mm]	0.0035 m	Thickness: Sheath tube
r_0	25[mm]	0.025 m	Inner radius: Sheath tube
d_c	6[mm]	0.006 m	Diameter: Coils
r_c	33[mm]	0.033 m	Axial length: Center of the coils
L_1	63[mm]	0.063 m	Height: Center of the lower coil
L_2	121[mm]	0.121 m	Height: Center of the upper coil
Q_1	1[l/min]	1.667E-5 m^3/s	Gas stream: Carrier tube
Q_2	3[l/min]	5E-5 m^3/s	Gas stream: Central tube
Q_3	31[l/min]	5.167E-4 m^3/s	Gas stream: Sheath tube
M	0.04[kg/mole]	0.04 kg/mol	Molar mass: Argon

Name	Expression	Value	Description
mv_stp	22.4[l/mole]	0.0224 m^3/mol	Molar volume at stp
mdot1	M*Q_1/mv_stp	2.976E-5 kg/s	Mass flow rate: Carrier tube
mdot2	M*Q_2/mv_stp	8.929E-5 kg/s	Mass flow rate: Central tube
mdot3	M*Q_3/mv_stp	9.226E-4 kg/s	Mass flow rate: Sheath tube
rho_stp	1.91[kg/m^3]	1.91 kg/m^3	Density of argon at stp
A1	pi*(r_1)^2	4.301E-5 m^2	Cross section: Carrier gas stream
A2	pi*(r_2^2-(r_1+d_1)^2)	0.001008 m^2	Cross section: Central gas stream
A3	pi*(r_0^2-(r_2+d_2)^2)	5.781E-4 m^2	Cross section: Sheath gas stream
v1	mdot1/rho_stp/A1	0.3623 m/s	Velocity: Carrier gas stream
v2	mdot2/rho_stp/A2	0.04636 m/s	Velocity: Central gas stream
v3	mdot3/rho_stp/A3	0.8356 m/s	Velocity: Sheath gas stream

Define the computational domain.

GEOMETRY 1

Rectangle 1 (r1)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `r_3`.
4. In the **Height** text field, type `L_3`.

Define the carrier tube.

Rectangle 2 (r2)

1. On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `d_1`.
4. In the **Height** text field, type `L_0`.

5 Locate the **Position** section. In the **r** text field, type `r_1`.

Define the central tube.

Rectangle 3 (r3)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `d_2`.

4 In the **Height** text field, type `L_0`.

5 Locate the **Position** section. In the **r** text field, type `r_2`.

Define the sheat tube.

Rectangle 4 (r4)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `d_3`.

4 In the **Height** text field, type `L_3`.

5 Locate the **Position** section. In the **r** text field, type `r_0`.

Define the coils.

Circle 1 (c1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Circle**.

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

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

4 Locate the **Position** section. In the **r** text field, type `r_c`.

5 In the **z** text field, type `L_1`.

Circle 2 (c2)

1 On the **Geometry** toolbar, click **Primitives** and choose **Circle**.

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

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

4 Locate the **Position** section. In the **r** text field, type `r_c`.

5 In the **z** text field, type `(L_1+L_2)/2`.

Circle 3 (c3)

1 On the **Geometry** toolbar, click **Primitives** and choose **Circle**.

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

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

4 Locate the **Position** section. In the **r** text field, type `r_c`.

5 In the **z** text field, type `L_2`.

6 Click **Build All Objects**.

Define a ramp function that will be used to bring the initial gas stream to their steady state values.

DEFINITIONS

Ramp 1 (rm1)

1 On the **Home** toolbar, click **Functions** and choose **Global>Ramp**.

Set the slope of the ramp function such that the steady state values are reached over a short interval of time, e.g. one excitation cycle. The steady state values are reached when the ramp function is equal to unity. Check the cutoff box and make sure the value of the cutoof is set to 1 in order to limit the value of the ramp function to one.

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

3 In the **Slope** text field, type `freq`.

4 Select the **Cutoff** check box.

Define the different domain type for easy selection.

Explicit 1

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

2 In the **Model Builder** window, right-click **Explicit 1** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Air` in the **New label** text field.

4 Click **OK**.

5 Select Domain 5 only.

Explicit 2

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

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

3 In the **Rename Explicit** dialog box, type `Plasma` in the **New label** text field.

4 Click **OK**.

5 Select Domain 1 only.

Explicit 3

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

2 In the **Model Builder** window, right-click **Explicit 3** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Quartz` in the **New label** text field.

4 Click **OK**.

5 Select Domains 2–4 only.

Explicit 4

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

2 In the **Model Builder** window, right-click **Explicit 4** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Coils` in the **New label** text field.

4 Click **OK**.

5 Select Domains 6–8 only.

Add the different materials used in the model using the material library.

ADD MATERIAL

1 On 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>Air**.

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

MATERIALS

Air (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Air (mat1)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

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

ADD MATERIAL

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

2 In the tree, select **AC/DC>Copper**.

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

MATERIALS

Copper (mat2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Copper (mat2)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

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

ADD MATERIAL

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

2 In the tree, select **AC/DC>Quartz**.

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

MATERIALS

Quartz (mat3)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Quartz (mat3)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

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

ADD MATERIAL

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

2 In the tree, select **Equilibrium Discharge>Argon**.

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

MATERIALS

Argon (mat4)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Argon (mat4)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

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

4 On the **Home** toolbar, click **Add Material** to close the **Add Material** window.

Adjust the selection and features of each physics composing the model.

The magnetic field interface is used over the whole computational domain. The Single-Turn Coil feature is used here to transfer the excitation power to the plasma.

MAGNETIC FIELDS (MF)

1 In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

2 In the **Model Builder** window, under **Component 1 (comp1)** click **Magnetic Fields (mf)**.

3 In the **Settings** window for **Magnetic Fields**, click to expand the **Discretization** section.

4 From the **Magnetic vector potential** list, choose **Linear**.

Coil 1

1 Right-click **Component 1 (comp1)>Magnetic Fields (mf)** and choose the domain setting **Coil**.

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

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

4 Locate the **Coil** section. Select the **Coil group** check box.

5 From the **Coil excitation** list, choose **Power**.

6 In the P_{coil} text field, type `Pext`.

The heat transfer in the air is neglected in this model.

HEAT TRANSFER IN FLUIDS (HT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heat Transfer in Fluids (ht)**.

2 Select Domains 1 and 4 only.

Solid 1

1 Right-click **Component 1 (comp1)>Heat Transfer in Fluids (ht)** and choose **Solid**.

2 Select Domain 4 only.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (ht)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, type `T0` in the T text field.

Add a heat transfer in solids feature for the solid part of the heat transfer model (tubes and coils).

Temperature 1

1 In the **Model Builder** window, right-click **Heat Transfer in Fluids (ht)** and choose **Temperature**.

2 Select Boundary 17 only.

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

4 In the T_0 text field, type `T0`.

The single phase flow is only applied to the plasma.

LAMINAR FLOW (SPF)

Since the density variation is not small, the flow cannot be regarded as incompressible. Therefore set the flow to be compressible. Add some isotropic diffusion which is initially bery high then ramps down to zero after the plasma has ignited.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.
2. In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.
3. From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.
4. Locate the **Domain Selection** section. From the **Selection** list, choose **Plasma**.
5. Click to expand the **Equation** section. From the **Equation form** list, choose **Stationary**.
6. In the **Model Builder** window's toolbar, click the **Show** button and select **Stabilization** in the menu.
7. Click to expand the **Consistent stabilization** section. Locate the **Consistent Stabilization** section. Find the **Navier-Stokes equations** subsection. Clear the **Crosswind diffusion** check box.
8. Click to expand the **Inconsistent stabilization** section. Locate the **Inconsistent Stabilization** section. Select the **Isotropic diffusion** check box.
9. In the δ_{id} text field, type `10-10*tanh(1000*(t-0.08))`.
10. Right-click **Component 1 (comp1)>Laminar Flow (spf)** and choose **Inlet**.

    Add the inlets with their proper velocities. Note the presence of the ramp function. The later is used to ramp the velocities from their initial values to the steady state.

Inlet 1

1. Select Boundary 2 only.
2. In the **Settings** window for **Inlet**, locate the **Velocity** section.
3. In the U_0 text field, type `v1*rm1(t[1/s])`.

Inlet 2

1. In the **Model Builder** window, right-click **Laminar Flow (spf)** and choose **Inlet**.
2. Select Boundary 8 only.
3. In the **Settings** window for **Inlet**, locate the **Velocity** section.
4. In the U_0 text field, type `v2*rm1(t[1/s])`.

Inlet 3

1. Right-click **Laminar Flow (spf)** and choose **Inlet**.
2. Select Boundary 13 only.

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

4 In the U_0 text field, type `v3*rm1(t[1/s])`.

Outlet 1

1 Right-click **Laminar Flow (spf)** and choose **Outlet**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.

4 Clear the **Suppress backflow** check box.

The Lorentz force can be neglected in this model. Neglecting this force also makes the model much easier to solve.

MULTIPHYSICS

In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** right-click **Lorentz Force 1 (lf1)** and choose **Disable**.

MESH 1

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edit Physics-Induced Sequence**.

Size 1

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

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

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

Size 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size 2**.

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

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

Boundary Layers 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Boundary Layers**.

2 Right-click **Boundary Layers 2** and choose **Move Up**.

3 In the **Settings** window for **Boundary Layers**, locate the **Domain Selection** section.

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

5 Select Domains 6–8 only.

Boundary Layer Properties

1 Click the **Select Box** button on the **Graphics** toolbar.

2 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Boundary Layers 2** click **Boundary Layer Properties**.

3 Select Boundaries 21–32 only.

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

5 In the **Number of boundary layers** text field, type `4`.

6 From the **Thickness of first layer** list, choose **Manual**.

7 In the **Thickness** text field, type `8[um]`.

8 Click **Build All**.

STUDY 1

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

2 Clear the **Generate default plots** check box.

Step 1: Frequency-Transient

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Frequency-Transient**.

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

3 In the **Times** text field, type `range(0,0.05,1)*0.1`.

4 In the **Frequency** text field, type `freq`.

Change some solver settings.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 Right-click **Time-Dependent Solver 1** and choose **Segregated**.

4 Right-click **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1>Segregated 1** and choose **Lower Limit**.

5 In the **Settings** window for **Lower Limit**, locate the **Lower Limit** section.

6 In the **Lower limits (field variables)** text field, type `comp1.T 300`.

7 Right-click **Segregated 1** and choose **Segregated Step**.

8 In the **Settings** window for **Segregated Step**, locate the **General** section.

9 Under **Variables**, click **Add**.

10 In the **Add** dialog box, In the **Variables** list, choose **Pressure (comp1.p)** and **Velocity field (comp1.u)**.

11 Click **OK**.

12 In the **Settings** window for **Segregated Step**, click to expand the **Method and termination** section.

13 Locate the **Method and Termination** section. From the **Jacobian update** list, choose **On every iteration**.

14 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)> Time-Dependent Solver 1>Segregated 1** click **Segregated Step**.

15 In the **Settings** window for **Segregated Step**, locate the **General** section.

16 In the **Variables** list, choose **Pressure (comp1.p)** and **Velocity field (comp1.u)**.

17 Under **Variables**, click **Delete**.

18 Locate the **Method and Termination** section. From the **Jacobian update** list, choose **On every iteration**.

19 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)** click **Time-Dependent Solver 1**.

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

21 Locate the **Time Stepping** section. From the **Steps taken by solver** list, choose **Intermediate**.

22 Select the **Nonlinear controller** check box.

23 On the **Study** toolbar, click **Compute**.

Create some relevant figures.

The temperature.

RESULTS

2D Plot Group 1

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

2 In the **Model Builder** window, right-click **2D Plot Group 1** and choose **Rename**.

3 In the **Rename 2D Plot Group** dialog box, type `Temperature` in the **New label** text field.

4 Click **OK**.

Surface 1

1 Right-click **Temperature** and choose **Surface**.

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

3 In the **Expression** text field, type `T`.

4 On the **Temperature** toolbar, click **Plot**.

Duplicate the figure to display the fluid velocity magnitude.

Temperature 1

1 In the **Model Builder** window, under **Results** right-click **Temperature** and choose **Duplicate**.

2 Right-click **Temperature 1** and choose **Rename**.

3 In the **Rename 2D Plot Group** dialog box, type `Velocity` in the **New label** text field.

4 Click **OK**.

Surface 1

1 In the **Model Builder** window, expand the **Results>Velocity** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `spf.U`.

4 On the **Velocity** toolbar, click **Plot**.

Duplicate the figure to display the electrical conductivity.

Velocity 1

1 In the **Model Builder** window, under **Results** right-click **Velocity** and choose **Duplicate**.

2 Right-click **Velocity 1** and choose **Rename**.

3 In the **Rename 2D Plot Group** dialog box, type `Electrical conductivity` in the **New label** text field.

4 Click **OK**.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electrical conductivity** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `mf.sigmarr*(dom==1)`.

4 On the **Electrical conductivity** toolbar, click **Plot**.

Duplicate the figure to display the norm of the magnetic flux. Note the effect of the plasma conductivity on the skin depth.

Electrical conductivity 1

1 In the **Model Builder** window, under **Results** right-click **Electrical conductivity** and choose **Duplicate**.

2 Right-click **Electrical conductivity 1** and choose **Rename**.

3 In the **Rename 2D Plot Group** dialog box, type `Magnetic flux` in the **New label** text field.

4 Click **OK**.

Surface 1

1 In the **Model Builder** window, expand the **Results>Magnetic flux** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `mf.normB`.

4 On the **Magnetic flux** toolbar, click **Plot**.

Display the coil current as a function of time. Note the time it takes to get the steady state (constant current in the coils).

1D Plot Group 5

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

2 In the **Model Builder** window, right-click **1D Plot Group 5** and choose **Rename**.

3 In the **Rename 1D Plot Group** dialog box, type `Coil current` in the **New label** text field.

4 Click **OK**.

Global 1

1 Right-click **Coil current** 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
`mf.ICoil_1`	`A`	`Coil current`

4 On the **Coil current** toolbar, click **Plot**.

Create a nice 3D plot for the model thumbnail.

Create first a revolution data set.

Revolution 2D 1

1 On the **Results** toolbar, click **More Data Sets** and choose **Revolution 2D**.

2 In the **Settings** window for **Revolution 2D**, click to expand the **Revolution layers** section.

3 Locate the **Revolution Layers** section. In the **Start angle** text field, type `-90`.

4 In the **Revolution angle** text field, type `225`.

Then create the 3D plot.

3D Plot Group 6

1 On the **Results** toolbar, click **3D Plot Group**.

2 In the **Model Builder** window, right-click **3D Plot Group 6** and choose **Rename**.

3 In the **Rename 3D Plot Group** dialog box, type `Temperature 3D` in the **New label** text field.

4 Click **OK**.

Volume 1

1 Right-click **Temperature 3D** and choose **Volume**.

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

3 In the **Expression** text field, type `T`.

4 On the **Temperature 3D** toolbar, click **Plot**.

5 Click **Go to Default View**.

Set the figure as a model thumbnail by clicking on the root folder in the model builder than expand the model thumbnail section and click on set model thumbnail.

In-Plane Microwave Plasma

Introduction

Wave-heated discharges can be very simple, such as when a plane wave is guided into a reactor using a waveguide, or very complicated, such as in the case with ECR (electron cyclotron resonance) reactors. In this simple example, a wave is launched down a waveguide where it intersects a flowing gas at low pressure, resulting in formation of an argon plasma. Microwave plasmas typically have high number density without requiring significant power absorption. The plasma potential is also quite low compared to capacitive or DC discharges. Therefore, microwave plasmas share many of the characteristics of inductive discharges.

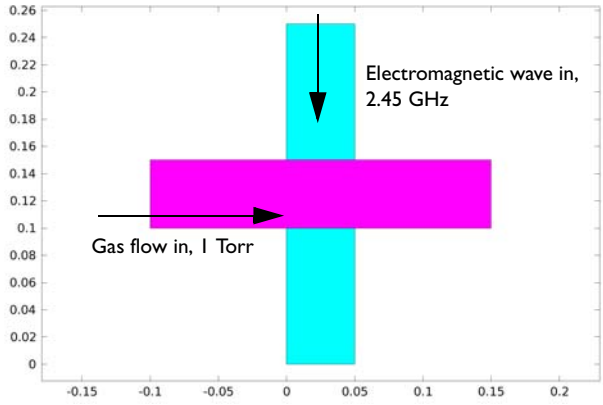

Figure 1: Diagram of geometry modeled. A TE or TM mode wave enters from the top port and intersects the gas flow leading to the formation of a plasma.

Note: The model requires the Plasma Module and RF Module.

Model Definition

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\mathrm{C}^{1/2}/\mathrm{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

In a microwave reactor the high frequency electric field is computed in the frequency domain using the following equation:

$$\nabla\times(\mu_r^{-1}\nabla\times\mathbf{E}) - k_0^2\left(\varepsilon_r - \frac{j\boldsymbol{\sigma}}{\omega\varepsilon_0}\right)\mathbf{E} = 0$$

The relationship between the plasma current density and the electric field becomes more complicated in the presence of a DC magnetic field. The following equation defines this relationship:

$$\boldsymbol{\sigma}^{-1} \bullet \mathbf{J} = \mathbf{E}$$

Here, σ is the plasma conductivity tensor, which is a function of the electron density, collision frequency, and magnetic flux density. Using the definitions:

$$\alpha = \frac{q}{m_e(\nu_e + j\omega)}, \beta = n_e q \alpha$$

where q is the electron charge, m_e is the electron mass, n_e is the collision frequency, and ω is the angular frequency of the electromagnetic field. In this example, the inverse of the plasma conductivity is diagonal because there is no external DC magnetic field:

$$\boldsymbol{\sigma}^{-1} = \begin{bmatrix} \frac{1}{\beta} & 0 & 0 \\ 0 & \frac{1}{\beta} & 0 \\ 0 & 0 & \frac{1}{\beta} \end{bmatrix}$$

The gas flow is modeled assuming a constant velocity in the x-direction.

PLASMA CHEMISTRY

The chemical mechanism for the plasma consists of only 3 species and 7 reactions:

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	-

Stepwise ionization (reaction 5) can play an important role in sustaining low pressure argon discharges. Excited argon atoms are consumed via superelastic collisions with electrons, quenching with neutral argon atoms, ionization or Penning ionization where two metastable argon atoms react to form a neutral argon atom, an argon ion and an electron. Reaction number 7 is responsible for heating of the gas. The 11.5 eV of energy which was consumed in creating the electronically excited argon atom is returns to the gas as thermal energy when the excited metastable quenches. In addition to volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When a metastable argon atom makes contact with the wall, it reverts to the ground state argon atom with some probability (the sticking coefficient).

ELECTRICAL EXCITATION

The plasma is sustained through absorption of electromagnetic waves. The Port boundary condition is used to excite the plasma. A total absorbed power of 30 W is fed into the port.

In a second study, the electrical excitation is changed to the TM mode, where the electric field has only an in-plane component. The total absorbed power is the same as the TE mode case.

Results and Discussion

The electron density is plotted in Figure 2 and peaks slightly downstream of the crossing point. The electron density is also slightly asymmetric in the y-plane due to the fact that the electromagnetic waves are absorbed asymmetrically. The electron "temperature" is plotted in Figure 3. The electron temperature is relatively low everywhere, in part due to the high operating pressure (1 Torr). The electron "temperature" peaks directly underneath the waveguide where the wave is absorbed. The norm of the electric field can be seen in Figure 5. The electric field is high inside the waveguide and there are no losses. Once the wave is exposed to the plasma, the energy is absorbed by the electrons, raising the electron temperature enough to generate new electrons through ionization. The ionization rate is high enough to sustain the plasma. The contour of the critical plasma density is also plotted in Figure 5. The electromagnetic wave cannot penetrate into regions exceeding the critical plasma density. Since the electron "temperature" is relatively low, one would expect the plasma potential to be low. The plasma potential is plotted in Figure 4 and is only around 10 volts.

In the TE mode, electrons do not experience any change in the high-frequency electric field during the microwave time scale. This means that the phase coherence between the electrons and electromagnetic waves is only destroyed through collisions with the background gas. The loss of phase coherence between the electrons and high-frequency fields is what results in energy gain for the electrons. Therefore, the momentum collision frequency is simply given by:

$$\nu_m = \nu_e$$

where ν_e is the collision frequency between the electrons and neutrals.

When switching to the TM mode, the electron density, electron "temperature" and plasma potential are quite similar to the TE mode case. This can be seen in Figure 7, Figure 8 and Figure 9. The electric field is very different however, Figure 9. The electric field cannot penetrate past the contour of critical electron density, and has its greatest magnitude in this location. The power deposition, Figure 10 is also highly localized to the contour of critical electron density. The TM mode causes in-plane motion of the electrons on the microwave time scale, so in regions where the high-frequency electric field is significant (the contour where the electron density is equal to the critical density), the time-averaged electric field experienced by the electrons may be non-zero. This destroys the phase coherence between the electrons and the fields, causing the electrons to gain energy. This is an example of a non-local kinetic effect, which is difficult to approximate with a fluid model. However, since this effect is similar to collisions with a background gas, the non-local effects can be

approximated by adding an effective collision frequency to the momentum collision frequency:

$$\nu_m = \upsilon_e + \nu_{\text{eff}}$$

where ν_{eff} is the effective collision frequency to account for non-local effects. In this example, since the Doppler broadening parameter is set to 20, this corresponds to an effective collision frequency of:

$$\nu_{\text{eff}} = \frac{\omega}{20}$$

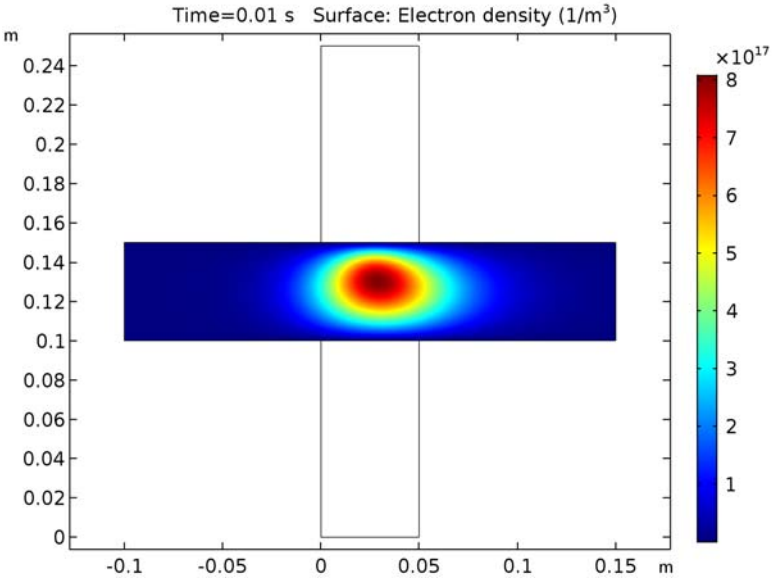

Figure 2: Plot of the electron density.

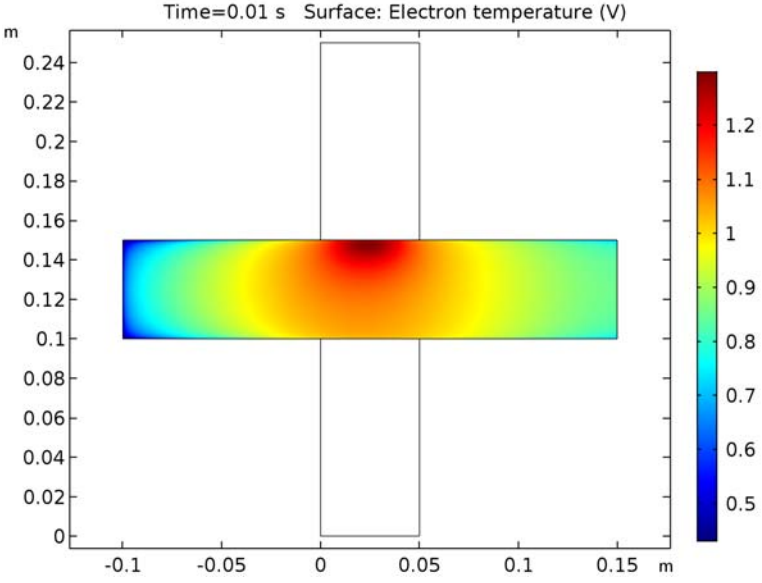

Figure 3: Plot of the electron temperature in the reactor.

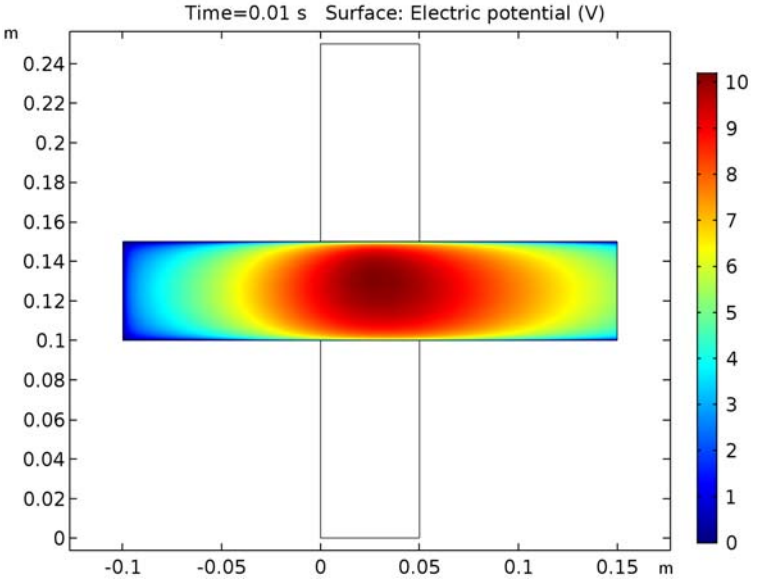

Figure 4: Plot of the plasma potential in the reactor.

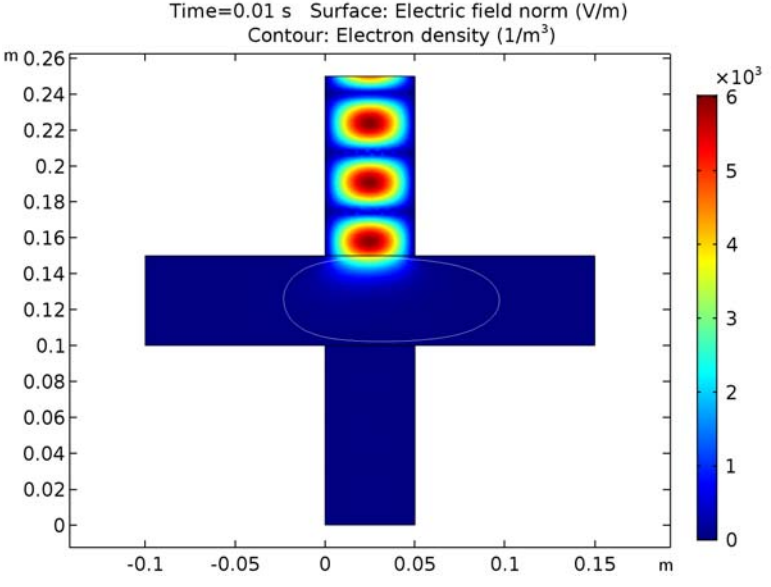

Figure 5: Plot of the electric field norm. The white contour represents the critical plasma

density, where the electron density is equal to 7.6E16[1/m^3].

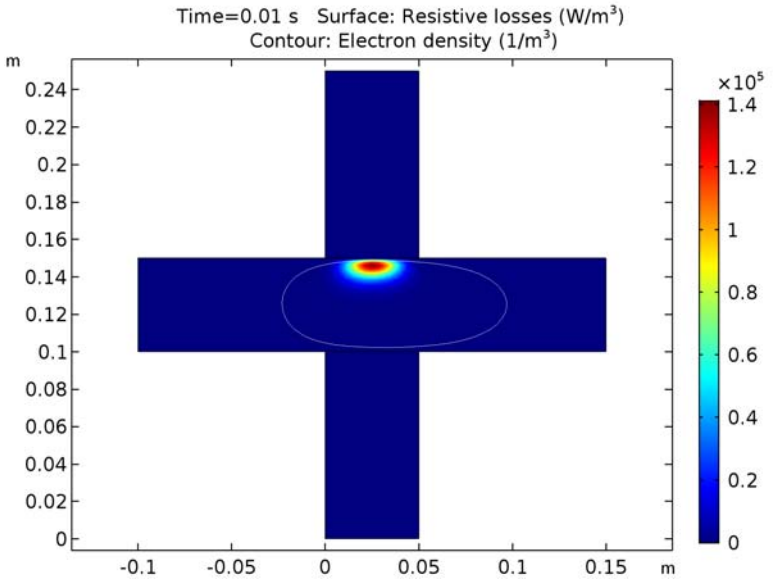

Figure 6: Plot of the power deposition into the plasma. The white contour represents the critical plasma density, where the electron density is equal to 7.6E16[1/m^3].

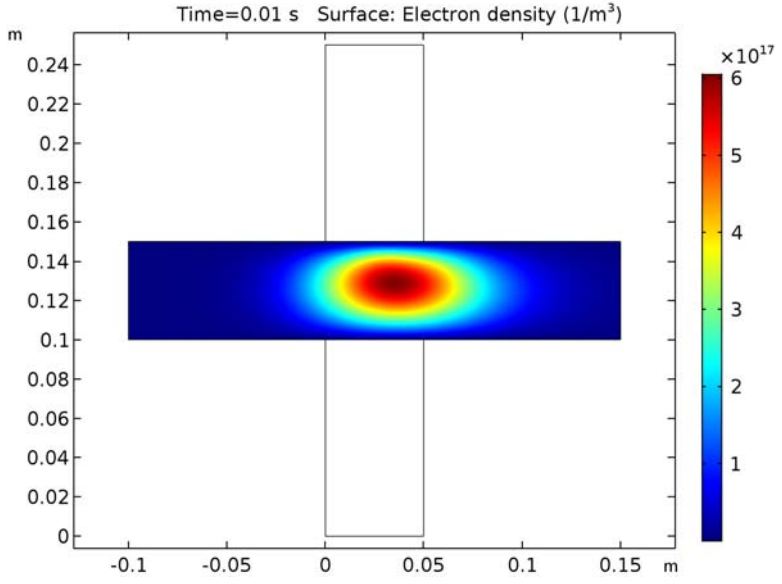

Figure 7: Electron density for the TM mode case.

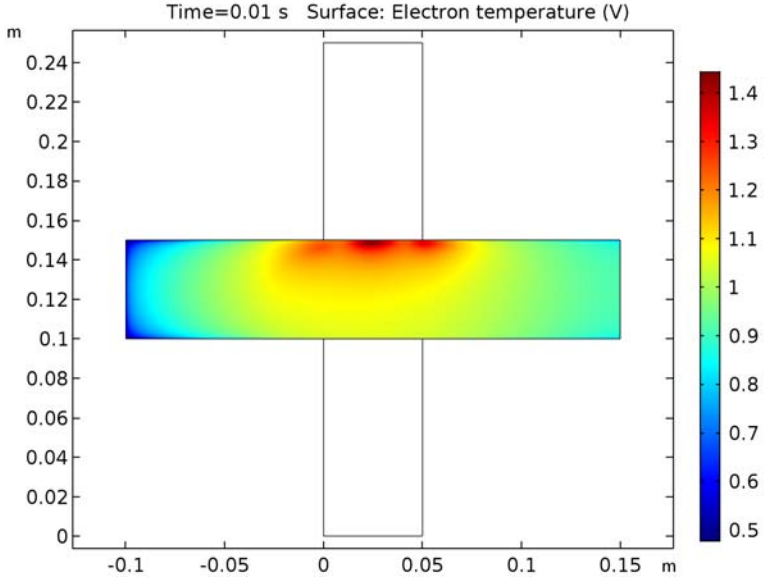

Figure 8: Plot of the electron temperature for the TM mode case.

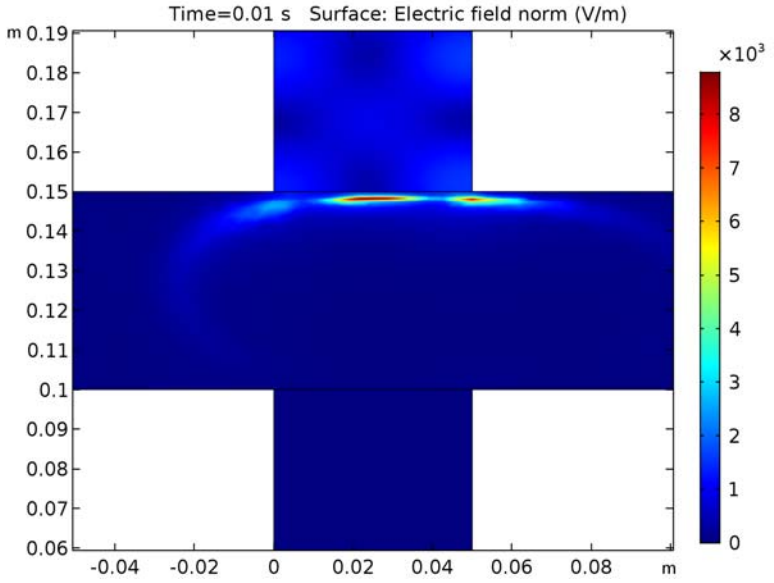

Figure 9: Close up of the high frequency electric field norm for the TM mode case.

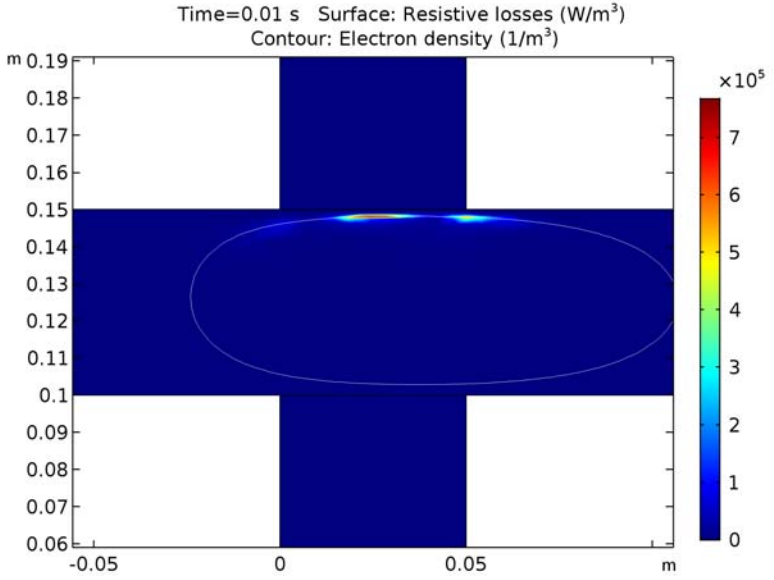

Figure 10: Close up of the power deposition into the plasma for the TM mode case.

Reference

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

Application Library path: `Plasma_Module/Wave-Heated_Discharges/inplane_microwave_plasma`

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 **2D**.

2 In the **Select Physics** tree, select **Plasma>Microwave Plasma**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Frequency-Transient**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
P0	30[W]	30 W	Absorbed power

GEOMETRY 1

Rectangle 1 (r1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.05`.

4 In the **Height** text field, type `0.1`.

5 Click **Build All Objects**.

Rectangle 2 (r2)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.25`.

4 In the **Height** text field, type `0.05`.

5 Locate the **Position** section. In the **x** text field, type `-0.1`.

6 In the **y** text field, type `0.1`.

Rectangle 3 (r3)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.05`.

4 In the **Height** text field, type `0.1`.

5 Locate the **Position** section. In the **y** text field, type `0.15`.

6 Click **Build All Objects**.

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

DEFINITIONS

Explicit 1

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

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

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

4 Select Boundaries 1–3, 6, 8, 11, and 13 only.

5 Right-click **Explicit 1** and choose **Rename**.

6 In the **Rename Explicit** dialog box, type `Walls` in the **New label** text field.

7 Click **OK**.

PLASMA (PLAS)

1 In the **Settings** window for **Plasma**, locate the **Domain Selection** section.

2 Click **Clear Selection**.

3 Select Domain 1 only.

Cross Section Import 1

1 In the **Model Builder** window, right-click **Plasma (plas)** 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`.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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 `3.734E8`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar**.

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

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

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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.

Surface Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

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 **Boundary Selection** section. From the **Selection** list, choose **Walls**.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> 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 **Boundary Selection** section. From the **Selection** list, choose **Walls**.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Transport Settings** section.

7 Select the **Convection** check box.

8 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** check box.

Plasma Model 1

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

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

3 Specify the $\mathbf{u}$ vector as

10	x
0	y

4 In the T text field, type `350`.

5 In the p_A text field, type `1[torr]`.

6 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `4E24`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E17`.

Wall 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

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

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

Ground 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

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

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

Electron Outlet 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion> Electron Outlet**.

2 Select Boundary 14 only.

Outflow 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** right-click **Species: Ars** and choose **Outflow**.

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

3 Click **Clear Selection**.

4 Select Boundary 14 only.

Outflow 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** right-click **Species: Ar+** and choose **Outflow**.

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

3 Click **Clear Selection**.

4 Select Boundary 14 only.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EMW)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain (emw)**.

2 In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, locate the **Components** section.

3 From the **Electric field components solved for** list, choose **Out-of-plane vector**.

Port 1

1 In the **Model Builder** window, right-click **Electromagnetic Waves, Frequency Domain (emw)** and choose **Port**.

2 Select Boundary 9 only.

3 In the **Settings** window for **Port**, locate the **Port Properties** section.

4 From the **Type of port** list, choose **Rectangular**.

5 From the **Wave excitation at this port** list, choose **On**.

6 Select the **Specify deposited power** check box.

7 In the P_{dep} text field, type `P0`.

MATERIALS

Material 1 (mat1)

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

2 Select Domains 2 and 3 only.

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

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Electrical conductivity	epsilonr	5	1	Basic
Relative permeability	mur	1	1	Basic
Relative permittivity	sigma	0	S/m	Basic

MESH 1

Boundary Layers 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Boundary Layers**.

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

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

4 Select Domain 1 only.

Boundary Layer Properties

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Boundary Layers 1** click **Boundary Layer Properties**.

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

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

Size

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

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

3 From the **Calibrate for** list, choose **Plasma**.

4 From the **Predefined** list, choose **Fine**.

5 Click **Build All**.

STUDY 1

Step 1: Frequency-Transient

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

2 In the **Times** text field, type `0`.

3 Click **Range**.

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

5 In the **Start** text field, type `-8`.

6 In the **Stop** text field, type `-2`.

7 In the **Number of values** text field, type `31`.

8 From the **Function to apply to all values** list, choose **exp10**.

9 Click **Add**.

10 In the **Settings** window for **Frequency-Transient**, locate the **Study Settings** section.

11 In the **Frequency** text field, type `2.45[GHz]`.

12 On the **Home** toolbar, click **Compute**.

RESULTS

Contour 1

1 In the **Model Builder** window, under **Results** right-click **Electric Field (emw)** and choose **Contour**.

2 In the **Settings** window for **Contour**, locate the **Levels** section.

3 From the **Entry method** list, choose **Levels**.

4 In the **Levels** text field, type `7.6E16`.

5 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

6 From the **Coloring** list, choose **Uniform**.

7 From the **Color** list, choose **White**.

8 On the **Electric Field (emw)** toolbar, click **Plot**.

Electric Field (emw) 1

1 Right-click **Electric Field (emw)** and choose **Duplicate**.

2 In the **Model Builder** window, expand the **Electric Field (emw) 1** node.

3 Right-click **Results>Electric Field (emw) 1** and choose **Rename**.

4 In the **Rename 2D Plot Group** dialog box, type `Resistive Heating` in the **New label** text field.

5 Click **OK**.

Surface 1

1 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain>Heating and losses>emw.Qrh - Resistive losses**.

2 On the **Resistive Heating** toolbar, click **Plot**.

Now change to the in-plane electric field, which makes the problem much more difficult to solve. This is because all the power will be absorbed on the contour of critical electron density. Setting a **Doppler broadening parameter** of 20 smooths out the region over which power is deposited to help with convergence.

MULTIPHYSICS

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Plasma Conductivity Coupling 1 (pcc1)**.

2 In the **Settings** window for **Plasma Conductivity Coupling**, locate the **Compute Tensor Plasma Conductivity** section.

3 Select the **Compute tensor plasma conductivity** check box.

4 In the δ text field, type `20`.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EMW)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain (emw)**.

2 In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, locate the **Components** section.

3 From the **Electric field components solved for** list, choose **In-plane vector**.

Port 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Electromagnetic Waves, Frequency Domain (emw)** click **Port 1**.

2 In the **Settings** window for **Port**, locate the **Port Mode Settings** section.

3 From the **Mode type** list, choose **Transverse magnetic (TM)**.

ADD STUDY

1 On 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 Multiphysics>Frequency-Transient**.

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

STUDY 2

Step 1: Frequency-Transient

1 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

2 In the **Model Builder** window, under **Study 2** click **Step 1: Frequency-Transient**.

3 In the **Settings** window for **Frequency-Transient**, locate the **Study Settings** section.

4 In the **Times** text field, type `0`.

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 `-8`.

8 In the **Stop** text field, type `-2`.

9 In the **Number of values** text field, type `31`.

10 From the **Function to apply to all values** list, choose **exp10**.

11 Click **Add**.

12 In the **Settings** window for **Frequency-Transient**, locate the **Study Settings** section.

13 In the **Frequency** text field, type `2.45[GHz]`.

14 On the **Home** toolbar, click **Compute**.

RESULTS

Electric Field (emw) 1

1. In the **Model Builder** window, under **Results** click **Electric Field (emw) 1**.
2. In the **Settings** window for **2D Plot Group**, locate the **Data** section.
3. From the **Data set** list, choose **Study 2/Solution 2 (sol2)**.
4. On the **Electric Field (emw) 1** toolbar, click **Plot**.
5. Click the **Zoom In** button on the **Graphics** toolbar.

Resistive Heating 1

1. In the **Model Builder** window, under **Results** right-click **Resistive Heating** and choose **Duplicate**.
2. In the **Settings** window for **2D Plot Group**, locate the **Data** section.
3. From the **Data set** list, choose **Study 2/Solution 2 (sol2)**.
4. On the **Resistive Heating 1** toolbar, click **Plot**.

1D Plot Group 11

1. On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Port Power` in the **Label** text field.

Global 1

1. Right-click **Port Power** and choose **Global**.
2. In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain>Global>emw.Pin - Port input power**.
3. On the **Port Power** toolbar, click **Plot**.
4. Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
5. In the table, enter the following settings:

Legends
TE Mode

6. Click the **x-Axis Log Scale** button on the **Graphics** toolbar.

Port Power

1. In the **Model Builder** window, under **Results** click **Port Power**.
2. In the **Settings** window for **1D Plot Group**, click to expand the **Legend** section.
3. From the **Position** list, choose **Upper left**.

Global 2

1 In the **Model Builder** window, under **Results>Port Power** right-click **Global 1** and choose **Duplicate**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Data set** list, choose **Study 2/Solution 2 (sol2)**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
TM Mode

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

6 On the **Port Power** toolbar, click **Plot**.

Ion Energy Distribution Function

Introduction

One of the most useful quantities of interest after solving a self-consistent plasma model is the ion energy distribution function (IEDF). The magnitude and shape of the IEDF depends on many of the discharge parameters; pressure, plasma potential, sheath width and so forth. At very low pressures the plasma sheath is said to be collisionless, meaning that the ion energy is not retarded by collisions with the background gas. At higher pressures the ions collide with the background gas molecules in the sheath and their energy at the moment of impact with a surface is reduced.

Note: This application requires the Plasma Module, Particle Tracing Module, and AC/DC Module.

Model Definition

The equations of motion for ions in an electric field and background gas are

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

where m is the ion mass (SI unit: kg), $\mathbf{v}$ is the particle velocity (SI unit: m/s), q is unit charge (SI unit: C), Z is the ion charge number (SI unit: dimensionless).

When an ion undergoes a collision with the background gas, its velocity vector changes. The probability of a collision event occurring depends in the ion-neutral collision frequency, ν (SI unit: 1/s) which is defined as:

$$\nu = N_d \sigma |\mathbf{v}_p - \mathbf{v}_g|$$

where N_d is the background number density (SI unit: $1/\mathrm{m}^3$), σ is the ion-neutral charge exchange collision cross section (SI unit: m^2) and $\mathbf{v}_p$ is the particle velocity and $\mathbf{v}_g$ is the velocity of the background gas atoms or molecules. In this example the collision cross section is assumed to be constant, $6\mathrm{x}10^{-19}\mathrm{m}^2$, as given in Ref. 2.

The collision probability defined as:

$$P = 1 - \exp(-\nu \Delta t)$$

If P is greater than a random number between 0 and 1 then the particle velocity is reinitialized to the following expression:

$$\mathbf{v}_p' = (m_p\mathbf{v}_p + m_g\mathbf{v}_g - m_g|\mathbf{v}_g - \mathbf{v}_p|\mathbf{R})/(m_p + m_g)$$

where $\mathbf{v}_p$ is the precollision particle velocity, m_g is the mass of the background gas atoms or molecules, $\mathbf{R}$ is a uniformly distributed random unit vector, and $\mathbf{v}_g$ is the velocity of the background gas atoms or molecules, which is sampled from a Maxwellian distribution function:

$$f(\mathbf{v}_g) = \frac{1}{2\pi k_B T/m_g{}^{3/2}} \exp\left[\frac{-(\mathbf{v}_g - \mathbf{u})^2}{(2k_B T)/m_g}\right]$$

where T is the temperature of the background gas.

The particles are released 5 mm away from the wafer surface and 20 mm radially inwards from the center of the reactor. There are 22,500 ions modeled. They all start at the same point in space and have an initial Maxwellian distribution function, which is for each velocity direction

$$f(v_i) = \sqrt{\frac{m}{2\pi kT}} \exp\left(-\frac{mv_i^2}{2kT}\right)$$

where T is the initial temperature of the ions, in this case 400K. This results in a distribution function of

$$\mathbf{f}(\mathbf{v}) = \prod_{i=1}^{\text{nsdim}} f(v_i)$$

When the ions strike the wafer their velocity is frozen for all subsequent timesteps. This allows the velocity and energy distribution function to be recovered once all the ions have made contact with the wall.

The angle at which the ions strike the wafer is also of interest. This can be recovered by plotting a histogram of the inverse tangent of the radial and axial particle velocities.

The electric potential for an argon plasma at an operating pressure of 20mtorr is plotted in Figure 1. The initial starting position for the ions is also shown:

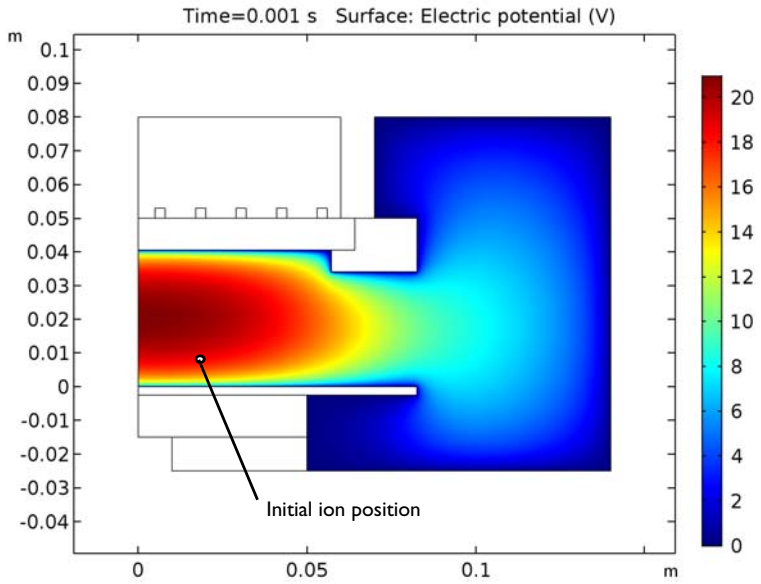

Figure 1: Plot of the plasma potential used to compute the IEDF.

The IEDF is plotted in Figure 2. Most of the ions have kinetic energy between around 20 and 22 eV. At the initial starting coordinate, the plasma potential is 20.98V , so it is expected that the kinetic energy of the ions at the wall is of similar order. As the pressure decreases the collision frequency between ions and neutrals is reduced, so the IEDF should shift to the right, towards the maximum value given by the plasma potential. As the pressure increases the sheath becomes more collisional which inhibits the ions from reaching higher energies. Of course, changing the pressure results in a change in the

discharge characteristics which may alter the shape and magnitude of the IEDF in a nonlinear way.

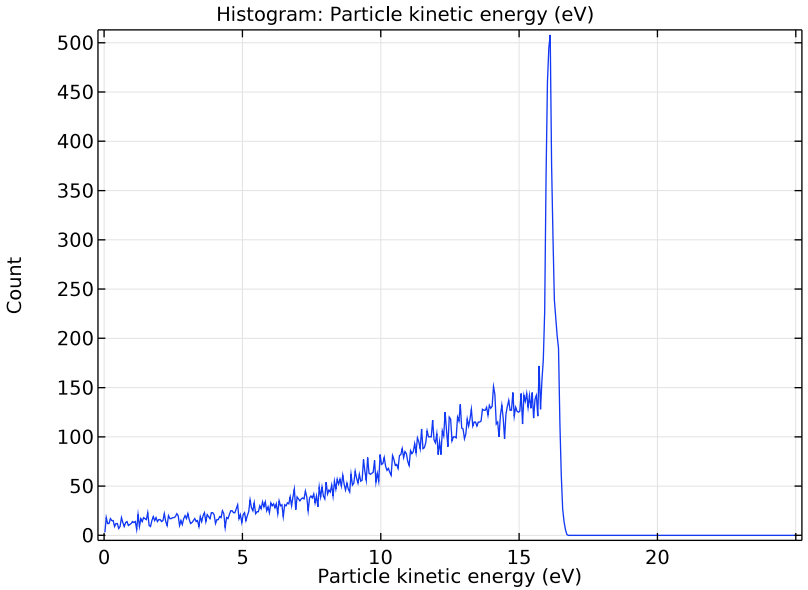

Figure 2: Plot of the ion energy distribution function (IEDF) in an inductively coupled plasma.

The angle at which the ions are striking the wafer surface are plotted in Figure 3. Due to the fact that the ions are released relatively close to the wafer surface, the range of angles is small, typically between -20 and 20 degrees. The plot is not quite symmetric due to the presence of a small outward component of the ambipolar electric field.

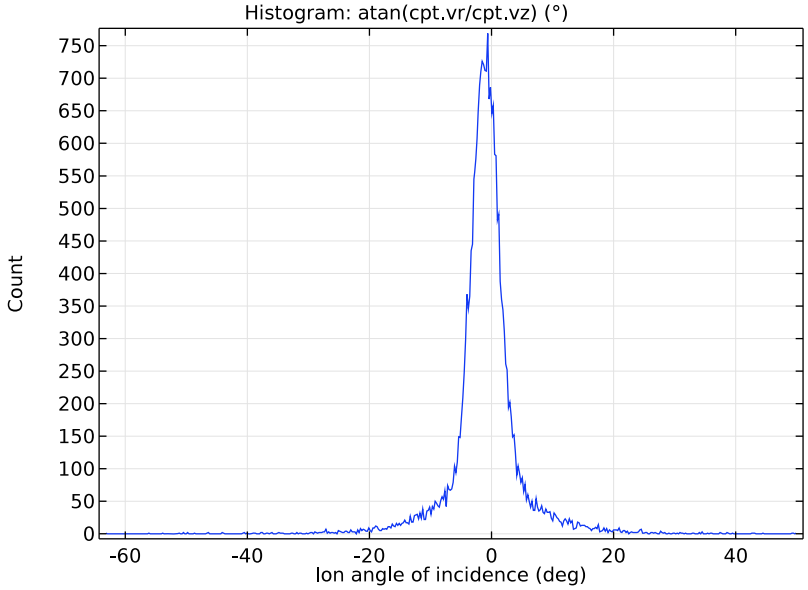

Figure 3: Plot of the angle at which the ions strike the surface of the wafer.

The ion angular energy distribution function is plotted in Figure 4. The angle is not quite symmetric about zero due to the profile of the electric field at the release point.

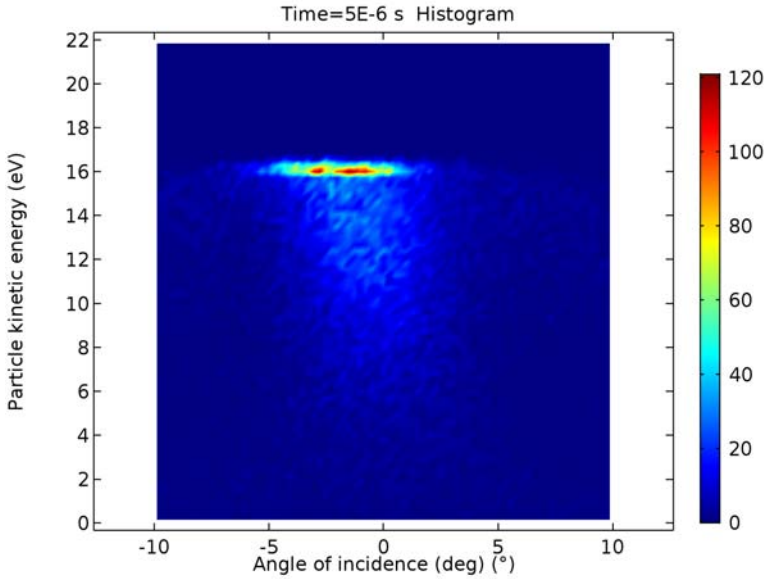

Figure 4: Plot of the ion angular energy distribution function.

Notes About the COMSOL Implementation

This model is most conveniently solved by opening an existing model in the Plasma Module Application Library, then computing the ion trajectories.

References

1. O.V. Vozniy, G.Y. Yeom, and A. Yu. Kropotov, "Plasma Potential Influence on Ion Energy Distribution Function in ICP Source," PSE, vol 5, no 1-2, pp. 28–33, http://www.pse.scpt.org.ua/en/jornal/1-2_07/3.pdf.

2. M. Surendra, "Radiofrequency Discharge Benchmark Model Comparison," *Plasma Sources Sci. Technol*, vol. 4, pp 56–73, 1995.

3. A. V. Phelps, "The application of scattering cross sections to ion flux models in discharge sheaths," *J. Appl. Phys.* vol. 76, pp. 747-753, 1994.

Application Library path: `Plasma_Module/Inductively_Coupled_Plasmas/ion_energy_distribution_function`

Modeling Instructions

Start by opening the model of the inductively coupled GEC reference cell from the **Plasma Module** Application Library.

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

Browse to the model's Application Libraries folder and double-click the file `argon_gec_icp.mph`.

COMPONENT 1 (COMP1)

Now add a **Charged Particle Tracing** interface to compute the ion energy distribution function.

ADD PHYSICS

1. On 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. Click **Add to Component** in the window toolbar.
5. On the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ADD STUDY

1. On 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**.
4. Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Plasma (plas)** and **Magnetic Fields (mf)**.
5. Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies> Time Dependent**.
6. Click **Add Study** in the window toolbar.

STUDY 2

Step 1: Time Dependent

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

CHARGED PARTICLE TRACING (CPT)

1. In the **Model Builder** window, expand the **Component 1 (comp1)** node, then click **Charged Particle Tracing (cpt)**.
2. In the **Settings** window for **Charged Particle Tracing**, locate the **Domain Selection** section.
3. Click **Clear Selection**.
4. Select Domain 3 only.

GLOBAL DEFINITIONS

Parameters

1. On the **Home** toolbar, click **Parameters**.
2. In the **Settings** window for **Parameters**, locate the **Parameters** section.
3. In the table, enter the following settings:

Name	Expression	Value	Description
Mw	0.04[kg/mol]	0.04 kg/mol	Ion molecular weight
mi	Mw/N_A_const	6.642E-26 kg	Ion mass

DEFINITIONS

Analytic 1 (an1)

1. On the **Home** toolbar, click **Functions** and choose **Global>Analytic**.

   Enter the analytic approximation for momentum cross section for elastic scattering between Ar+ ions and neutral Ar atoms, which which depends on the kinetic energy of the particles.
2. In the **Settings** window for **Analytic**, type `Qm` in the **Function name** text field.
3. Locate the **Definition** section. In the **Expression** text field, type `1.15e-18*x^(-0.1)*(1+0.015/x)^0.6`.
4. Locate the **Units** section. In the **Arguments** text field, type `eV`.
5. In the **Function** text field, type `m^2`.

Analytic 2 (an2)

1 On the **Home** toolbar, click **Functions** and choose **Global>Analytic**.

Enter the analytic approximation for isotropic elastic collision between Ar+ ions and neutral Ar atoms from, which which depends on the kinetic energy of the particles.

2 In the **Settings** window for **Analytic**, type `Qi` in the **Function name** text field.

3 Locate the **Definition** section. 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`.

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`.

Now add an **Electric Force** feature. The electric potential comes from the solved plasma model. Specify that piecewise polynomial recovery should be used when computing the electric force. This results in a more accurate reconstruction of the electric field.

Electric Force 1

1 In the **Model Builder** window, right-click **Charged Particle Tracing (cpt)** and choose **Electric Force**.

2 Select Domain 3 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 (plas/pes1)**.

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

Now you add the collisional force between the ions and background gas. The collision frequency is a function of the neutral number density (`plas.Nn`), the elastic and charge exchange cross section and the particle velocity (`cpt.V`).

Collisions 1

1 Right-click **Charged Particle Tracing (cpt)** and choose **Collisions**.

2 Select Domain 3 only.

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

4 In the N_d text field, type `plas.Nn`.

5 In the M_g text field, type `Mw`.

6 In the T text field, type `plas.T`.

Elastic 1

1 Right-click **Component 1 (comp1)>Charged Particle Tracing (cpt)>Collisions 1** and choose **Elastic**.

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

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

Resonant Charge Exchange 1

1 Right-click **Collisions 1** 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 `(Qm(cpt.Ep)-Qi(cpt.Ep))/2`.

Release from Grid 1

1 In the **Model Builder** window, right-click **Charged Particle Tracing (cpt)** and choose **Release from Grid**.

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

3 In the $q_{r,\,0}$ text field, type `0.02`.

4 In the $q_{z,\,0}$ text field, type `0.005`.

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

6 In the $N_{\mathbf{v}}$ text field, type `150`.

7 In the T_0 text field, type `400`.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

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

3 In the **Times** text field, type `range(0,5.0e-6/30,5.0e-6)`.

4 Click to expand the **Values of dependent variables** section. Locate 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 **Study 1, Frequency-Transient**.

7 On the **Home** toolbar, click **Compute**.

RESULTS

1D Plot Group 13

1 On 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 **Data set** 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> Charged Particle Tracing>Velocity and energy>cpt.Ep - Particle kinetic energy**.

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

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

5 In the **Limits** text field, type `range(0,25/500,25)`.

6 On the **Ion Energy Distribution Function** toolbar, click **Plot**.

1D Plot Group 14

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

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

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

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

Histogram 1

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

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

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

4 Locate the **Bins** section. In the **Number** text field, type `500`.

5 Locate the **Expression** section. From the **Unit** list, choose **°**.

6 On the **Ion Angular Distribution Function** toolbar, click **Plot**.

Ion Angular Distribution Function

1 In the **Model Builder** window, under **Results** click **Ion Angular Distribution Function**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Ion angle of incidence (deg)`.

5 On the **Ion Angular Distribution Function** toolbar, click **Plot**.

2D Plot Group 15

1 On 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` in the **Label** text field.

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

4 From the **Time (s)** list, choose **5E-6**.

Histogram 1

1 On the **Ion Angular Energy Distribution Function** 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 of incidence (deg)`.

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 In the **Limits** text field, type `range(-10,20/79,10)`.

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

12 In the **Limits** text field, type `range(0,22/79,22)`.

Ion Angular Energy Distribution Function

1. In the **Model Builder** window, under **Results** click **Ion Angular Energy Distribution Function**.
2. In the **Settings** window for **2D Plot Group**, locate the **Plot Settings** section.
3. Clear the **Plot data set edges** check box.
4. On the **Ion Angular Energy Distribution Function** toolbar, click **Plot**.
5. Click the **Zoom Extents** button on the **Graphics** toolbar.

Microwave Microplasma

Introduction

Plasmas sustained in micro-scale discharge gaps are able to operate at high pressure (1 atm) with high electron number density (10^{20} m^{-3}) and power density (10^{9} $W.m^{-3}$) while maintaining a relatively cool heavy-particle temperature.

Microplasmas can be thought as dimensional scaled down versions of their low-pressure macroscopic counterparts where the product of the gas pressure (p) and the discharge characteristic dimension (d) is kept constant at atmospheric pressure by reducing the discharge dimensions below the millimeter. However the pd scaling is often useful to conceive a first image, it should be noticed that some aspects of the plasma physics scale differently. One of them is the increase in importance of three-body-reactions with gas pressure, which lead to the formation of dimmers in noble gases plasmas.

This model simulates an atmospheric pressure Argon plasma sustained by a time-varying electric excitation in the microwave range. The model is 1-dimensional in the direction of the applied field and describes the space and temporal evolution of several macroscopic properties of the plasma.

The reader can found more information about microplasmas and plasmas excited with microwaves in Ref. 1 and Ref. 2 and in the references therein.

Model Definition

The model here described adopts the electrostatic approximation since the discharge dimension is much smaller than the wavelength. Neglecting wave effects in the plasma considerable simplifies the model. The operating principle of this microwave microplasma is similar to a capacitively coupled plasma (CCP) reactor. The plasma is sustained by applying a sinusoidal electrostatic potential across a small gap (200 µm in this case) filled with a high pressure (760 Torr in this case) gas. The model equations are solved in time domain allowing for the expression of nonlinear behaviors of the discharge (e.g. harmonic content in the measured current). The model is transient, with the system allowed to reach a periodic steady state solution. This condition is reached after a suitable number of cycles.

The model here presented is based on the one reported in Ref. 1 and Ref. 2. Perhaps the most important difference is that in the present model inertia terms are not included in the momentum equation, which reduces the validity of the model to conditions where the electron collision frequency for momentum transfer is larger than the angular excitation frequency. A detailed description of the model follows.

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $C^{1/2}/kg^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho\frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u}\cdot\nabla)w_k = \nabla\cdot\mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla\cdot\varepsilon_0\varepsilon_r\nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

BOUNDARY CONDITIONS

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the following boundary condition for the electron flux:

$$\mathbf{n}\cdot\Gamma_e = \left(\frac{1}{2}\nu_{e,\,\mathrm{th}} n_e\right) - \sum_p \gamma_p(\Gamma_p\cdot\mathbf{n}) \tag{1}$$

and the electron energy flux:

$$\mathbf{n}\cdot\Gamma_\varepsilon = \left(\frac{5}{6}\nu_{e,\,\mathrm{th}} n_\varepsilon\right) - \sum_p \varepsilon_p\gamma_p(\Gamma_p\cdot\mathbf{n}) \tag{2}$$

The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the

secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

The discharge is driven by a sinusoidal electric potential applied to the left boundary of the dielectric plate:

$$V = V_0 \cos(\omega t)$$

where the applied peak voltage, V_0 is 150 V and the angular frequency being 0.5 GHz. The right boundary is grounded.

PLASMA CHEMISTRY

Argon plasmas have one of the simplest reactions schemes. The electronically excited states can be lumped into single states. At atmospheric pressure and low gas temperature three-body reactions are important and lead to the creation of dimmers. We use a plasma chemistry similar to the one in Ref. 2 that comprises 17 volume reactions involving electrons, atomic and molecular ions, lumped levels representing the Argon 4s levels, and an excited dimmer.

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	e+Ar2s=>2e+Ar2+	Ionization	3.55
7	e+Ar2s=>e+2Ar	Excitation	-10.95
8	e+Ar2+=>Ars+Ar	Excitation	-3
9	e+Ar2+=>e+Ar+Ar+	Excitation	1.26
10	Ars+Ars =>e+Ar+Ar+	Penning ionization	-
11	Ars+Ar=>Ar+Ar	Metastable quenching	-
12	Ar2s+Ar2s=>2Ar+e+Ar2+	Penning ionization	-
13	2Ar+Ar+=>Ar+Ar2+	3-body Ar2+ creation	-
14	2Ar+Ars=>Ar2s+Ar	3-body Ar2s creation	-
15	Ar+Ar2+=>2A+Ar+	Ion conversion	-

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\varepsilon(eV)$
16	Ars => Ar	Spontaneous emission	-
17	Ar2s => Ar + Ar	Spontaneous emission	-

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	0
2	Ar2s=>2Ar	1	0	0
3	Ar+=>Ar	1	0.07	4
4	Ar2+=>2Ar	1	0.07	4

When an excited states make contact with the wall, they revert to the ground state argon atom with some probability (the sticking coefficient). The ions use their internal energy to extract one electron from the wall with a probability of 0.07 and a mean energy of 4 V.

Results and Discussion

In this section we present and discuss the main features of this microdischarge. In the set of simulations shown below a periodic steady state was not attained. However, the results are close to the ones in steady state and allows us to illustrate the behavior of the microwave microplasma. Further discussion can be found in Ref. 1 and Ref. 2. We reinforce the idea that to obtain a steady state it is need to solve considerable more cycles.

Figure 1shows the spatial distribution of the charged species in the 200 µm gap. As it was advanced 3-body reactions that create molecular ions are important at high pressure. For the present conditions Ar2+ accounts for approximately 30% of the positive charges in the center of the discharge. At this high excitation frequencies the ions density remain static in time and due to the model symmetry the spatial profiles are symmetric to the center of the discharge. The electron density is also symmetric and almost static in time in a central region from 50 to 150 µm. However, in the regions near the wall the electron density evolves in time driven by the applied time-varying electric field. In these regions near the wall (often called plasma sheaths) there is an important charge separation (clearly seen in Figure 1at the right boundary) and an consequent intense electric field. In contrast, the central part of the discharge remains quasi-neutral and shielded from the external field.

The temporal evolution of the one dimensional electron density is conveniently represented by extruding the solution into two dimensions. The extra dimension

represents time. In COMSOL Multiphysics this is accomplished by adding a *Parametric Extrusion 1D* data set.

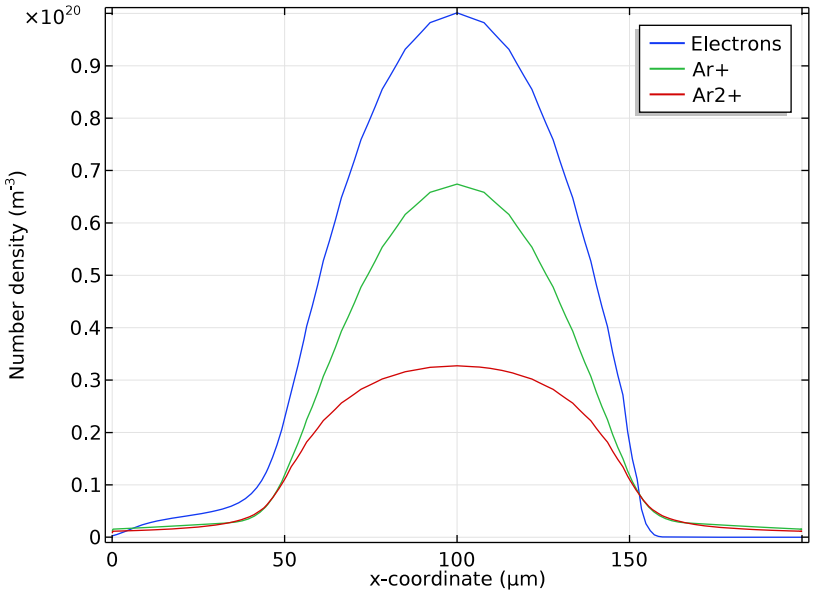

Figure 1: Charge species number density as a function of space for a time instant.

Figure 2 presents the spatial distribution of the electron number density (along the horizontal axis) extruded in time for one cycle of the external excitation along the vertical axis (cycle 500: phase 0 at 500 and phase 2π at 501). The periodic electron motion near the wall is clearly seen. At the instant when the applied potential on the left boundary is at its minimum ($-V_0$ at phase π) the plasma sheath is at its largest expansion near the same wall (and at the minimum expansion in the opposite wall).

The electron temperature near the wall is also strongly time modulated as seen in Figure 3. The electrons are accelerated towards the center of the discharge during the sheath expansion. At the powered electrode the electron temperature attains a maximum at phase π when the potential is at its minimum $-V_0$. In the plasma bulk the electron temperature is much cooler than near the walls and remains constant in time and space since the electric field is much less intense than in the sheaths.

The main current contributions to the total current density in the discharge gap are shown in Figure 4 and Figure 5. For the present conditions the current on the discharge bulk is

dominated by the electron conduction current whereas in the plasma sheath region it is the displacement current that contributes the most to the total current. Ion current is negligible over all discharge length.

In this one dimensional model the total current density is constant across the discharge gap. From Figure 4 and Figure 5 it is possible to observe that the maxima and minima of the currents coincide in time. The current minima occur at 0 and π when the applied potential is (almost) at V_0 and $-V_0$, respectively. This means that the applied voltage and the total current are almost 90° out of phase.

Most of the microwave power is absorbed by electrons in the spatial transition between the bulk and the temporal modulated sheath. This behavior is represented in Figure 6 with the time-average of the power density absorbed by electrons (time-averaged over one cycle of the internal product of the electric field by the electron current density).

Power densities of the order of 10^9 W.m^{-3} are uncommon in continuously excited cold plasmas. In fact, the ability to sustain a stable discharge with this high power densities is one of the special features of microplasmas that stimulated the development of new technologies and applications.

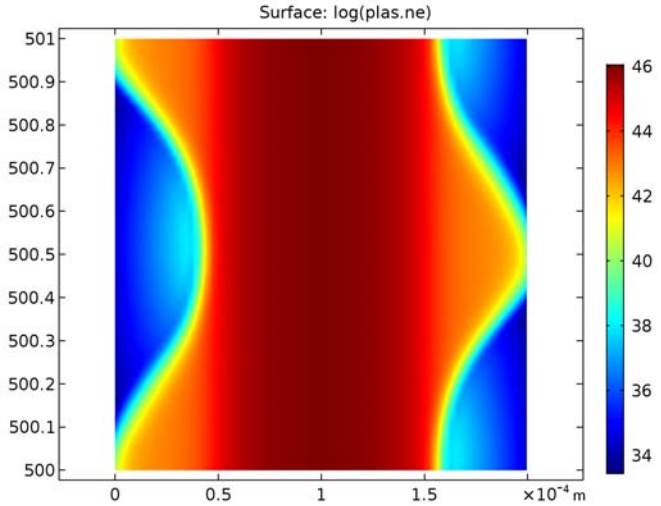

Figure 2: Electron number density spatial distribution (horizontal axis) for one cycle of the external excitation (vertical axis). The scale is in logarithm scale to allow for a clear visualization of the plasma sheath excursion.

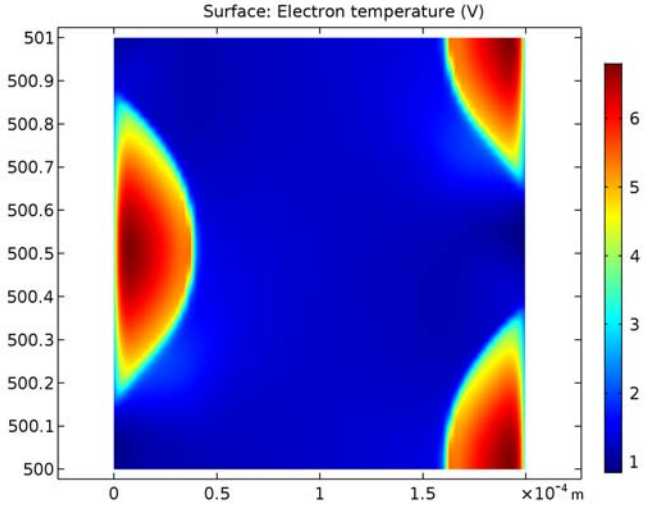

Figure 3: Electron temperature spatial distribution (horizontal axis) for one cycle of the external excitation (vertical axis).

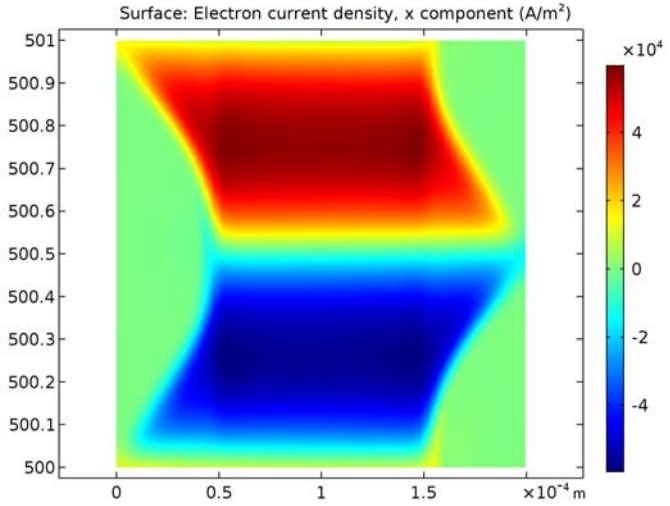

Figure 4: Electron current density spatial distribution (horizontal axis) for one cycle of the external excitation (vertical axis).

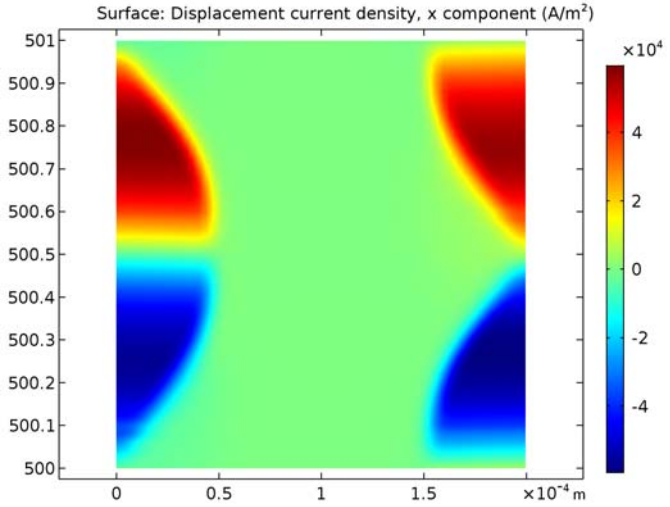

Figure 5: Displacement current density spatial distribution (horizontal axis) for one cycle of the external excitation (vertical axis).

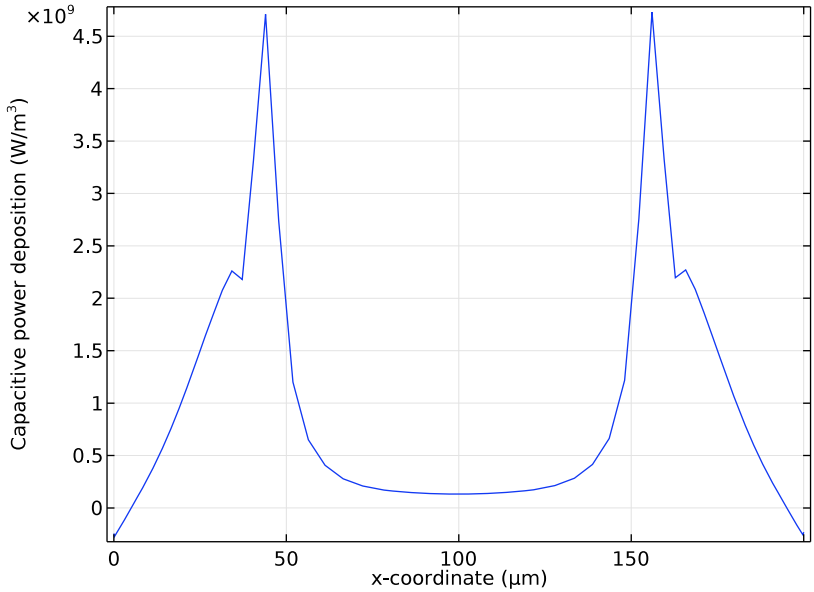

Figure 6: Time-averaged power absorbed by the electrons during one cycle of the excitation.

Reference

1. J. Gregorio, A. R. Hoskinson, and J. Hopwood, "Modeling od microplasmas from GHz to THz," *J. Appl. Phys.*, vol. 118, p. 083305 (9pp), 2015.

2. A. R . Hoskinson, J. Gregorio, S. Parsons, and J. Hopwood, "Electron confinement and heating in microwave-sustained argon microplasmas," *J. Appl. Phys.*, vol. 117, p. 163301 (10pp), 2015.

Application Library path: `Plasma_Module/Capacitively_Coupled_Plasmas/microwave_microplasma`

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 **1D**.

2 In the **Select Physics** tree, select **Plasma>Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Add parameters to be used in this simulation.

Parameters

1 On the **Home** toolbar, click **Parameters**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
freq	0.5[GHz]	5E8 Hz	Excitation frequency
omega	2*pi*freq	3.142E9 Hz	Angular frequency
P0	760[torr]	1.013E5 Pa	Gas pressure
T0	800[K]	800 K	Gas temperature
Vapp	150[V]	150 V	Applied voltage
Cross_x	4e-6[m^2]	4E-6 m²	Plasma cross section
Gap	200e-6[m]	2E-4 m	Discharge gap

GEOMETRY 1

Define the geometry for the problem. This model has a simple 1D geometry with the plasma formed in a gap between two metal boundaries.

Interval 1 (i1)

1 On the **Geometry** toolbar, click **Interval**.

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

3 In the **Right endpoint** text field, type `Gap`.

Import argon electron scattering cross sections. The cross sections are used to compute different rate coefficients describing electron impact reactions that appear in the source terms of continuity equations. Moreover, in this model the effective collision frequency for electron momentum transfer is deduced from the cross sections and used to compute the electron transport parameters (mobility and diffusivity).

PLASMA (PLAS)

Cross Section Import 1

1 On 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 electron impact reactions for which you wish to use a rate constant.

Electron Impact Reaction 6

1 On the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e + Ar2s => e + e + Ar2+`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the $\Delta\varepsilon$ text field, type `3.55`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `5.4e10*plas.Te^0.7`.

Electron Impact Reaction 7

1 On the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e + Ar2s => Ar + Ar +e`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the $\Delta\varepsilon$ text field, type `-10.95`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `6.022e11`.

Electron Impact Reaction 8

1 On the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e + Ar2+ => Ars + Ar`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `-3`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `6.263e11*(0.026/plas.Te)^0.67*( (1-exp(-418/T0)) / (1-0.31*exp(-418/T0)))`.

Electron Impact Reaction 9

1 On the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

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

3 In the **Formula** text field, type `e +Ar2+ => e + Ar + Ar+`.

4 Locate the **Collision Type** section. From the list, choose **Excitation**.

5 In the Δε text field, type `1.26`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `6.685e11 * exp( (-2.94+3*(T0/11600-0.026)) / plas.Te )`.

Add other reactions relevant for the plasma chemistry under study.

Reaction 1

1 On 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 `9.785e7*T0^0.5`.

Reaction 2

1 On 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`.

Reaction 3

1 On 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 `Ar2s + Ar2s => Ar + Ar + e + Ar2+`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `9.785e7*T0^0.5`.

Reaction 4

1 On 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 `Ar + Ar + Ar+  => Ar + Ar2+`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `2.72e7/T0`.

Reaction 5

1 On 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 `Ar + Ar + Ars => Ar2s + Ar`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `1.197e4`.

Reaction 6

1 On 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 `Ar + Ar2+ => Ar + Ar + Ar+`.

4 Locate the **Reaction Parameters** section. Select the **Use Arrhenius expressions** check box.

5 In the A^{f} text field, type `3.649e12`.

6 In the n^{f} text field, type `-1`.

7 In the E^{f} text field, type `1.258e5`.

Reaction 7

1 On 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`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `3.145e5`.

Reaction 8

1 On 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 `Ar2s => Ar + Ar`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `6e7`.

Specify the properties of the Argon ground state, excited states and ions.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ars**.

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

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

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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**.

Species: Ar2s

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar2s**.

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

3 In the M_w text field, type `2*0.04[kg/mol]`.

Species: Ar2+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ar2+**.

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

3 In the M_w text field, type `2*0.04[kg/mol]`.

4 In the n_0 text field, type `1E15[1/m^3]`.

Specify model inputs (background gas temperature and pressure) and select how do you want to compute or set electron trasnport parameters. In this model we deduce electron trasnport properties from electron impact reactions.

Plasma Model 1

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

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

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

4 In the p_A text field, type `P0`.

5 Locate the **Electron Density and Energy** section. From the **Electron transport properties** list, choose **From electron impact reactions**.

Specify the initial electron density. The value used is quite high since we are only interested in the steady sate and we are not interest in study any transient regime like discharge breakdown.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E17 [1/m^3]`.

Specify surface reactions to tell what should hapen when a specie reached the wall. Note that Argon ground state does not have a surface reaction since its density is computed from mass constraint.

Surface Reaction 1

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

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

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

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ar+=>Ar`.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0.07`.

6 In the ε_i text field, type `4`.

Surface Reaction 2

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

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

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

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ars=>Ar`.

Surface Reaction 3

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

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

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

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ar2+ => Ar +Ar`.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0.07`.

6 In the ε_i text field, type `4`.

Surface Reaction 4

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

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

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

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ar2s => Ar +Ar`.

Specify the boundary conditions for the plasma in contact with the metal and set the rigth boundary to be grounded and the left boundary to be driven by a volatge source with a sinusoidal wave form.

Wall 1

1 On 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**.

Ground 1

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

2 Select Boundary 2 only.

Metal Contact 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 In the V_0 text field, type `Vapp*cos(omega*t)`.

Define a mesh that is fine enough near the boundaries where the electric field is most intense and the ions can be acelerated to important velocities.

MESH 1

Distribution 1

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

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

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

4 From the **Distribution properties** list, choose **Predefined distribution type**.

5 In the **Number of elements** text field, type `100`.

6 In the **Element ratio** text field, type `50`.

7 From the **Distribution method** list, choose **Geometric sequence**.

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

9 Click **Build All**.

STUDY 1

The model can solve faster by deactivating the convergence plots. Also, the default plots are unnecessary since custom plots will be used during results processing.

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

2 Clear the **Generate default plots** check box.

3 Clear the **Generate convergence plots** check box.

Set up a simulation to run for 501 periods of the excitation frequency and to save 50 samples of the last period. Note that the simulation should run longer if it is wished to attain a steady state.

Step 1: Time Dependent

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

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

3 Click **Range**.

4 In the **Times** text field, type `0`.

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

6 In the **Start** text field, type `500/freq`.

7 In the **Stop** text field, type `501/freq`.

8 In the **Number of values** text field, type `51`.

9 Click **Add**.

10 On the **Home** toolbar, click **Compute**.

RESULTS

In the **Model Builder** window, expand the **Results** node.

Parametric Extrusion 1D 1

1 On the **Results** toolbar, click **More Data Sets** and choose **Parametric Extrusion 1D**.

2 In the **Settings** window for **Parametric Extrusion 1D**, locate the **Data** section.

3 From the **Time selection** list, choose **From list**. In the **Times (s)** list, choose **1E-6** through **1.0002E-6**.

4 Locate the **Settings** section. In the **Level scale factor** text field, type `0.5e9`.

Time Average 1

1 On the **Results** toolbar, click **More Data Sets** and choose **Evaluation>Time Average**.

2 In the **Settings** window for **Time Average**, locate the **Data** section.

3 From the **Time selection** list, choose **From list**. In the **Times (s)** list, choose **1E-6** through **1.0002E-6**.

1D Plot Group 1

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

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

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **y-axis label** check box.

5 In the associated text field, type `Number density (m<sup>-3</sup>)`.

Line Graph 1

1 Right-click **Charged species** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Electrons` in the **Label** text field.

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

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 From the **Unit** list, choose **µm**.

8 Click to expand the **Legends** section. Select the **Show legends** check box.

9 From the **Legends** list, choose **Manual**.

10 In the table, enter the following settings:

Legends
Electrons

11 On the **Charged species** toolbar, click **Plot**.

12 Click **Plot**.

Line Graph 2

1 In the **Model Builder** window, under **Results** right-click **Charged species** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Ar+` in the **Label** text field.

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

4 Locate the **Title** section. From the **Title type** list, choose **None**.

5 Click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Plasma (Heavy Species Transport)>Number densities> plas.n_wAr_1p - Number density**.

6 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

7 In the **Expression** text field, type `x`.

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

9 Locate the **Legends** section. Select the **Show legends** check box.

10 From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
Ar+

12 On the **Charged species** toolbar, click **Plot**.

Line Graph 3

1 Right-click **Charged species** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Ar2+` in the **Label** text field.

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

4 Locate the **Title** section. From the **Title type** list, choose **None**.

5 Click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>Plasma (Heavy Species Transport)>Number densities> plas.n_wAr2_1p - Number density**.

6 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

7 In the **Expression** text field, type `x`.

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

9 Locate the **Legends** section. Select the **Show legends** check box.

10 From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
Ar2+

12 On the **Charged species** toolbar, click **Plot**.

1D Plot Group 2

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

2 In the **Settings** window for **1D Plot Group**, type `Time averaged power absorbed by electrons` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Time Average 1**.

Line Graph 1

1 Right-click **Time averaged power absorbed by electrons** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Drift Diffusion)>Power and collisions>plas.Pcap - Capacitive power deposition**.

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `x`.

6 From the **Unit** list, choose **µm**.

7 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

8 On the **Time averaged power absorbed by electrons** toolbar, click **Plot**.

9 Click the **Zoom Extents** button on the **Graphics** toolbar.

2D Plot Group 3

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

2 In the **Settings** window for **2D Plot Group**, type `Electron density vs. time` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot data set edges** check box.

Surface 1

1 Right-click **Electron density vs. time** and choose **Surface**.

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

3 In the **Expression** text field, type `log(plas.ne)`.

4 On the **Electron density vs. time** toolbar, click **Plot**.

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

Electron density vs. time 1

1 In the **Model Builder** window, under **Results** right-click **Electron density vs. time** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electron Temperature vs. time` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electron Temperature vs. time** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Plasma (Drift Diffusion)> Electron energy density>plas.Te - Electron temperature**.

3 On the **Electron Temperature vs. time** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Electron Temperature vs. time 1

1 In the **Model Builder** window, under **Results** right-click **Electron Temperature vs. time** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Electron current density vs. time` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Electron current density vs. time** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Plasma (Drift Diffusion)> Current>Electron current density>plas.Jelx - Electron current density, x component**.

3 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

4 On the **Electron current density vs. time** toolbar, click **Plot**.

5 Click **Plot**.

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

Electron current density vs. time 1

1 In the **Model Builder** window, under **Results** right-click **Electron current density vs. time** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Displacement current density vs. time` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Results>Displacement current density vs. time** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Plasma (Electrostatics)> Currents and charge>Displacement current density>plas.Jdx - Displacement current density, x component**.

3 On the **Displacement current density vs. time** toolbar, click **Plot**.

4 Click **Plot**.

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

DC Glow Discharge, 1D

Introduction

DC glow discharges in the low pressure regime have long been used for gas lasers and fluorescent lamps. DC discharges are attractive to study because the solution is time independent. This model shows how to use the **Plasma** interface to set up an analysis of a positive column. The discharge is sustained by emission of secondary electrons at the cathode.

Model Definition

The DC discharge consists of two electrodes, one powered (the anode) and one grounded (the cathode):

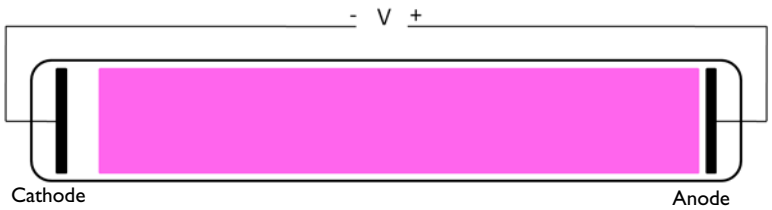

Figure 1: Schematic of the DC discharge. The voltage applied across the electrodes leads to formation of a plasma.

DOMAIN EQUATIONS

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

where:

$$\boldsymbol{\Gamma}_e = -(\boldsymbol{\mu}_e \bullet \mathbf{E})n_e - \mathbf{D}_e \bullet \nabla n_e$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions which contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (m^3/s), and N_n is the total neutral number density ($1/m^3$). For DC discharges it is better practice to use Townsend coefficients instead of rate coefficients to define reaction rates. Townsend coefficients provide a better description of what happens in the cathode fall region Ref 1. When Townsend coefficients are used, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j \alpha_j N_n |\Gamma_e|$$

where α_j is the Townsend coefficient for reaction j (m^2) and Γ_e is the electron flux as defined above ($1/(m^2 \cdot s)$). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges. The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (V). The rate coefficients may be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ ($C^{1/2}/kg^{1/2}$), m_e is the electron mass (kg), ε is energy (V), σ_k is the collision cross section (m^2) and f is the electron energy distribution function. In this

case a Maxwellian EEDF is assumed. When Townsend coefficients are used, the electron energy loss is taken as:

$$R_\varepsilon = \sum_{j=1}^{P} x_j \alpha_j N_n |\Gamma_e| \Delta\varepsilon_j$$

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

BOUNDARY CONDITIONS

Unlike RF discharges, the mechanism for sustaining the discharge is emission of secondary electrons from the cathode. An electron is emitted from the cathode surface with a specified probability when struck by an ion. These electrons are then accelerated by the strong electric field close to the cathode where they acquire enough energy to initiate ionization. The net result is a rapid increase in the electron density close to the cathode in a region often known as the *cathode fall* or *Crookes dark space*.

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the following boundary condition for the electron flux:

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} \nu_{e,\,\mathrm{th}} n_e\right) - \sum_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \qquad (1)$$

and the electron energy flux:

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6}\nu_{e,\,\mathrm{th}} n_\varepsilon\right) - \sum_p \varepsilon_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{2}$$

The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

PLASMA CHEMISTRY

Argon is one of the simplest mechanisms to implement at low pressures. The electronically excited states can be lumped into a single species which results in a chemical mechanism consisting of only 3 species and 7 reactions:

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 this discharge, the electron density and density of excited species is relatively low so stepwise ionization is not as important as in high density discharges. In addition to volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When a metastable argon atom makes contact with the wall, it reverts to the ground state argon atom with some probability (the sticking coefficient).

Results and Discussion

The electric potential, electron density, and mean electron energy are all quantities of interest. Most of the variation in each of these quantities occurs along the axial length of the column. Figure 2 plots the electron density in the column. The electron density peaks in the region between the cathode fall and positive column. This region is sometimes referred to as Faraday dark space. The electron density obtained in this 1D model is different than that obtained in the 2D model due to the fact that the diffusive loss of electrons to the outer walls and the accumulation of surface charge on the walls is not modeled.

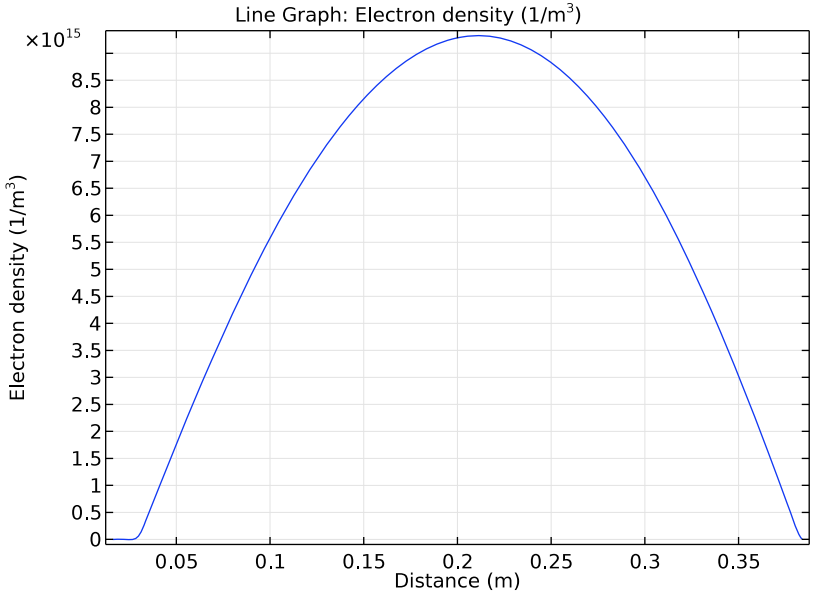

Figure 2: Plot of electron density inside the column.

In Figure 3 the electric potential is plotted along the axial length of the column. Notice that the potential profile is markedly different from the linear drop in potential which results in the absence of the plasma. The strong electric field in the cathode region can lead to high energy ion bombardment of the cathode. Heating of the cathode surface occurs which may in turn lead to thermal electron emission where additional electrons are emitted from the cathode surface.

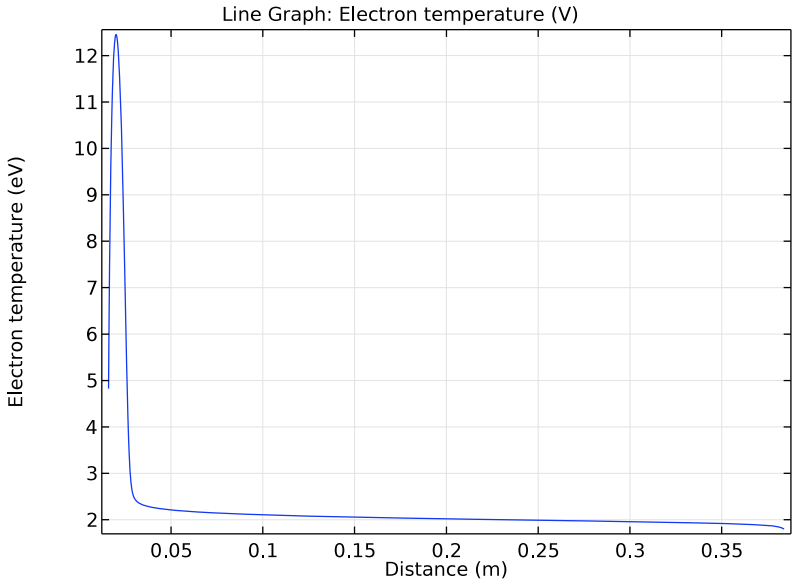

Figure 3: Plot of the electron temperature along the axial length of the positive column.

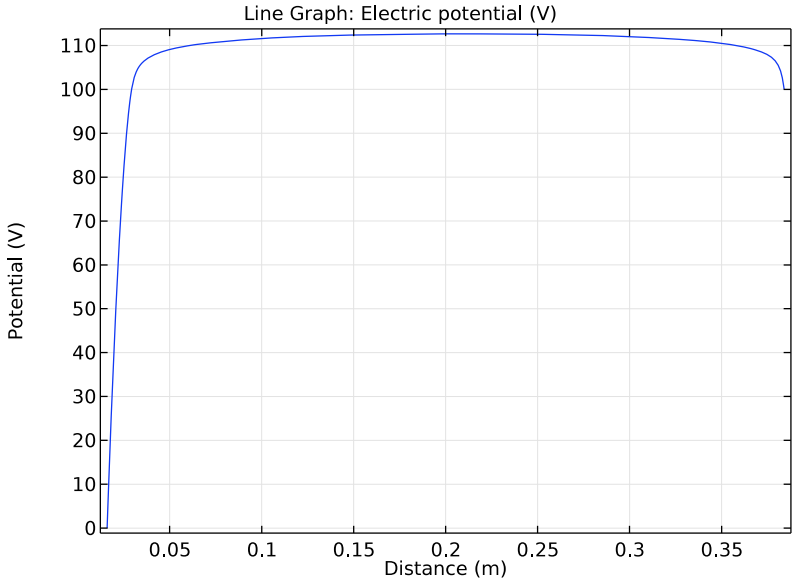

Figure 4: Plot of electron "temperature" along the axial length of the positive column.

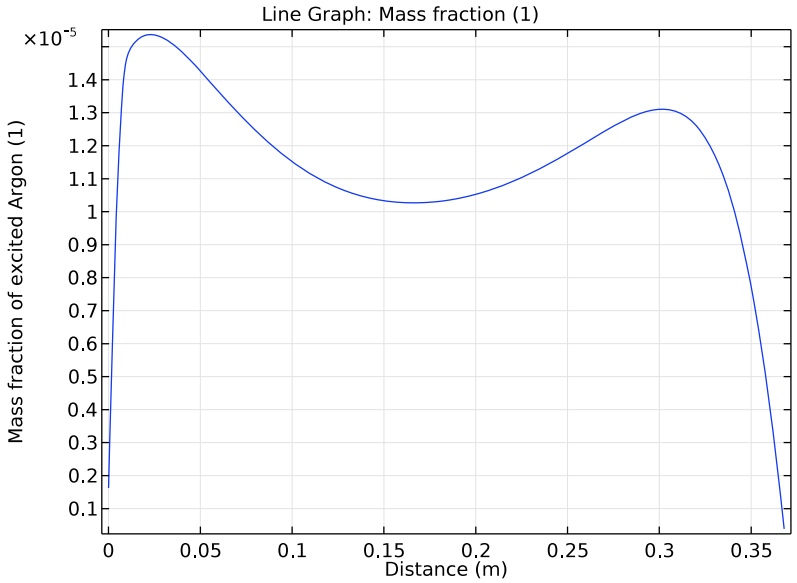

Figure 5: Plot of the mass fraction of excited argon atoms.

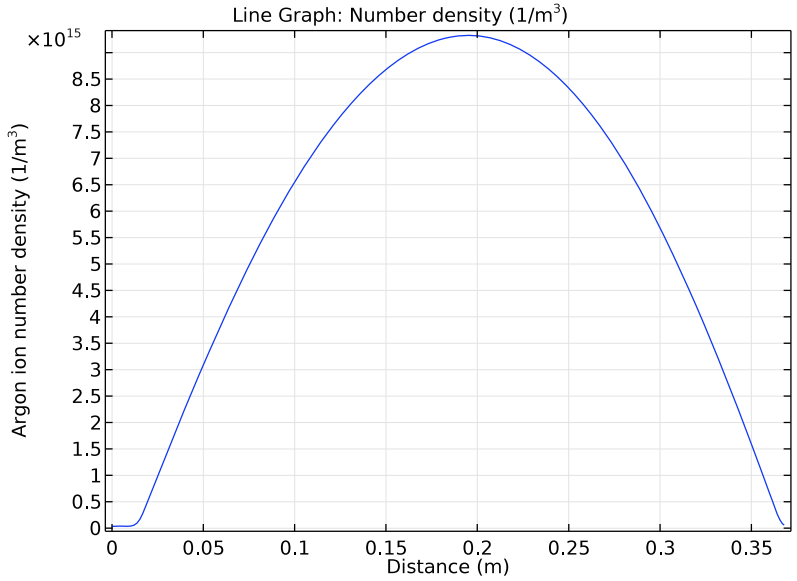

Figure 6: Plot of the number density of argon ions.

The plasma current due to electrons, ions and their sum is plotted in Figure 7. As expected, the ion current is highest at the cathode and increases sharply in the cathode fall region. The ion bombardment of the cathode results in an electron current released from the electrode. The electron current increases sharply in the cathode fall region because the high electron temperature results in production of new electrons which then contribute to the total electron current. Once the electrons pass the cathode fall region the electron current density further increases due to further production of new electrons through electron impact ionization with the background gas.

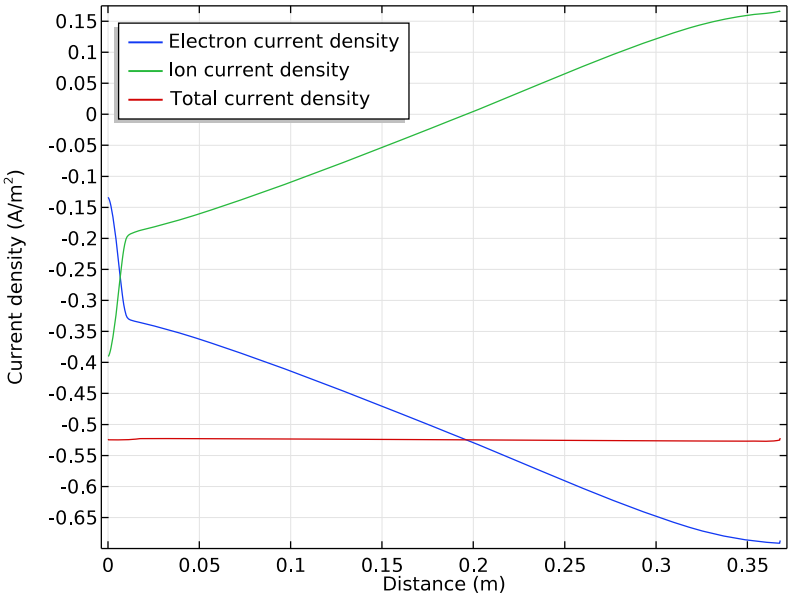

Figure 7: Plot of the electron current density (blue), the ion current density (green) and the total current density (red) in the positive column.

Reference

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

Application Library path: `Plasma_Module/Direct_Current_Discharges/positive_column_1d`

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

NEW

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

MODEL WIZARD

1. In the **Model Wizard** window, click **1D**.
2. In the **Select Physics** tree, select **Plasma>Plasma (plas)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies>Time Dependent**.
6. Click **Done**.
7. In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

GEOMETRY 1

The geometry interval is defined to be consistent with the 2D version of the model, which is available in the **Application Library**.

Interval 1 (i1)

1. On the **Geometry** toolbar, click **Interval**.
2. In the **Settings** window for **Interval**, locate the **Interval** section.
3. In the **Left endpoint** text field, type `0.016`.
4. In the **Right endpoint** text field, type `0.384`.

DEFINITIONS

Variables 1

1. On the **Home** toolbar, click **Variables** and choose **Local Variables**.
2. In the **Settings** window for **Variables**, locate the **Variables** section.
3. In the table, enter the following settings:

Name	Expression	Unit	Description
`ramp`	`tanh(1E7[1/s]*t)`		`Ramp function for the applied voltage`
`mueN`	`1E25[1/(m*V*s)]`	1/(V·m·s)	`Electron mobility`

Name	Expression	Unit	Description
V0	100[V]*ramp	V	Applied voltage
Wf	5		Surface work function
p0	0.1[torr]	Pa	Gas pressure

PLASMA (PLAS)

Cross Section Import 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Plasma (plas)** 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`.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Plasma Properties** section.

7 Select the **Use reduced electron transport properties** check box.

Because you will examine the electron, ion, and net currents flowing in the plasma, raise the element order to 2. The current density is computed from space derivatives of the charge carrying degrees of freedom, so using 2nd order shape functions gives a more accurate value for the current density.

8 Click to expand the **Discretization** section. From the **Formulation** list, choose **Finite element, log formulation (quadratic shape function)**.

Plasma Model 1

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

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

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

4 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `mueN`.

Now change the way the source coefficients for electronic excitation and ionization are specified. By default, COMSOL Multiphysics computes rate coefficients based on the cross section data you supplied. For DC discharges, Townsend coefficients provide a more accurate description of the cathode fall region so they should be used. The Townsend coefficients are typically computed using the **Boltzmann Equation, Two-Term Approximation** interface.

2: e+Ar=>e+Ars

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **2: e+Ar=> e+Ars**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Collision** section.

3 From the **Specify reaction using** list, choose **Use lookup table**.

4 Locate the **Reaction Parameters** section. From the **Rate constant form** list, choose **Townsend coefficient**.

5 Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `town2.txt`.

4: e+Ar=>2e+Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **4: e+Ar=> 2e+Ar+**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Collision** section.

3 From the **Specify reaction using** list, choose **Use lookup table**.

4 Locate the **Reaction Parameters** section. From the **Rate constant form** list, choose **Townsend coefficient**.

5 Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `town4.txt`.

Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport>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 `3.734E8`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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, under **Component 1 (comp1)>Plasma (plas)** 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**.

When solving a reacting flow problem there always needs to be one species which is selected to fullfill the mass constraint. This should be taken as the species with the largest mass fraction.

Species: Ars

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ars**.

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

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

When solving a plasma problem the plasma must be initially charge neutral. COMSOL automatically computes the initial concentration of a selected ionic species such that the electroneutrality constraint is satisfied.

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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**.

Now add a surface reaction which describes the neutralization of argon ions on the electrode. Secondary emission of electrons is required to sustain the discharge, so enter the emission coefficient and an estimate of the mean energy of the secondary electrons based on the ionization energy threshold and the work function of the surface.

Surface Reaction 1

1 In the **Model Builder** window, right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport>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 Select Boundary 1 only.

Make the secondary emission coefficient 0.35 and set the mean energy of the secondary electrons to be the ionization energy (given by the expression `plas.de_4`) minus twice the work function of the electrode.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0.35`.

6 In the ε_i text field, type `plas.de_4-2*Wf`.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> 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 Select Boundary 2 only.

Surface Reaction 3

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

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

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

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

Wall 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

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

Ground 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

2 Select Boundary 1 only.

Metal Contact 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics> Metal Contact**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 In the V_0 text field, type `V0`.

MESH 1

Distribution 1

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

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

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

4 From the **Distribution properties** list, choose **Predefined distribution type**.

5 In the **Number of elements** text field, type `350`.

6 In the **Element ratio** text field, type `8`.

7 From the **Distribution method** list, choose **Geometric sequence**.

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

9 Click **Build All**.

STUDY 1

Step 1: Time Dependent

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

2 In the **Times** text field, type `0`.

3 Click **Range**.

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

5 In the **Start** text field, type `-8`.

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

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

8 From the **Function to apply to all values** list, choose **exp10**.

9 Click **Add**.

10 On the **Home** toolbar, click **Compute**.

RESULTS

Electron Density (plas)

1 In the **Model Builder** window, under **Results** click **Electron Density (plas)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Electron density (1/m<sup>3</sup>)`.

8 Click the **Zoom Extents** button on the **Graphics** toolbar.

Electron Temperature (plas)

1 In the **Model Builder** window, under **Results** click **Electron Temperature (plas)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Electron temperature (eV)`.

8 Click the **Zoom Extents** button on the **Graphics** toolbar.

Electric Potential (plas)

1 In the **Model Builder** window, under **Results** click **Electric Potential (plas)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

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

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Potential (V)`.

8 Click the **Zoom Extents** button on the **Graphics** toolbar.

1D Plot Group 4

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

2 In the **Settings** window for **1D Plot Group**, type `Excited Argon Mass Fraction` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Mass fraction of excited Argon (1)`.

Line Graph 1

1 Right-click **Excited Argon Mass Fraction** and choose **Line Graph**.

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

3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Mass fractions>plas.wArs - Mass fraction**.

4 On the **Excited Argon Mass Fraction** toolbar, click **Plot**.

1D Plot Group 5

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

2 In the **Settings** window for **1D Plot Group**, type `Argon Ion Number Density` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Argon ion number density (1/m<sup>3</sup>)`.

Line Graph 1

1 Right-click **Argon Ion Number Density** and choose **Line Graph**.

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

3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Number densities>plas.n_wAr_1p - Number density**.

4 On the **Argon Ion Number Density** toolbar, click **Plot**.

Argon Ion Number Density 1

1 In the **Model Builder** window, under **Results** right-click **Argon Ion Number Density** and choose **Duplicate**.

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

3 Click to expand the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Current density (A/m<sup>2</sup>)`.

5 Click to expand the **Legend** section. From the **Position** list, choose **Upper left**.

Line Graph 1

1 In the **Model Builder** window, expand the **Results>Current Density** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1>**

Plasma (Drift Diffusion)>Current>Electron current density>plas.Jelx - Electron current density, x component.

3 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

4 From the **Recover** list, choose **Within domains**.

5 Click to expand the **Legends** section. Select the **Show legends** check box.

6 From the **Legends** list, choose **Manual**.

7 On the **Current Density** toolbar, click **Plot**.

8 In the table, enter the following settings:

Legends
Electron current density

Line Graph 2

1 Right-click **Results>Current Density>Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Species>Species wAr_1p>Ion current density> plas.Jix_wAr_1p - Ion current density, x component**.

3 On the **Current Density** toolbar, click **Plot**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Ion current density

Line Graph 3

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `plas.Jix_wAr_1p+plas.Jelx`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Total current density

5 On the **Current Density** toolbar, click **Plot**.

DC Glow Discharge

Introduction

DC glow discharges in the low pressure regime have long been used for gas lasers and fluorescent lamps. DC discharges are attractive to study because the solution is time independent. This model shows how to use the **Plasma** interface to set up an analysis of a positive column. The discharge is sustained by emission of secondary electrons at the cathode.

Model Definition

The DC discharge consists of two electrodes, one powered (the anode) and one grounded (the cathode). The positive column is coupled to an external circuit:

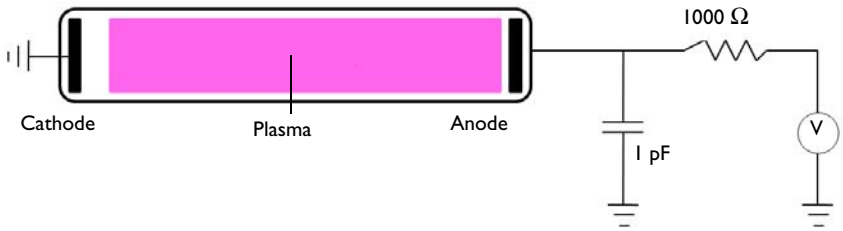

Figure 1: Schematic of the DC discharge and external circuit.

DOMAIN EQUATIONS

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

where:

$$\boldsymbol{\Gamma}_e = -(\boldsymbol{\mu}_e \bullet \mathbf{E})n_e - \mathbf{D}_e \bullet \nabla n_e$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions which contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (m^3/s), and N_n is the total neutral number density ($1/m^3$). For DC discharges it is better practice to use Townsend coefficients instead of rate coefficients to define reaction rates. Townsend coefficients provide a better description of what happens in the cathode fall region Ref 1. When Townsend coefficients are used, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j \alpha_j N_n |\boldsymbol{\Gamma}_e|$$

where α_j is the Townsend coefficient for reaction j (m^2) and Γ_e is the electron flux as defined above ($1/(m^2 \cdot s)$). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges. The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (V). The rate coefficients may be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ ($C^{1/2}/kg^{1/2}$), m_e is the electron mass (kg), ε is energy (V), σ_k is the collision cross section (m^2) and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed. When Townsend coefficients are used, the electron energy loss is taken as:

$$R_\varepsilon = \sum_{j=1}^{P} x_j \alpha_j N_n |\Gamma_e| \Delta\varepsilon_j$$

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

BOUNDARY CONDITIONS

Unlike RF discharges, the mechanism for sustaining the discharge is emission of secondary electrons from the cathode. An electron is emitted from the cathode surface with a specified probability when struck by an ion. These electrons are then accelerated by the strong electric field close to the cathode where they acquire enough energy to initiate ionization. The net result is a rapid increase in the electron density close to the cathode in a region often known as the *cathode fall* or *Crookes dark space*.

Electrons are lost to the wall due to random motion within a few mean free paths of the wall and gained due to secondary emission effects, resulting in the following boundary condition for the electron flux:

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} \nu_{e,\,\mathrm{th}} n_e\right) - \sum_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{1}$$

and the electron energy flux:

$$\mathbf{n} \cdot \Gamma_\varepsilon = \left(\frac{5}{6} \nu_{e,\,\mathrm{th}} n_\varepsilon\right) - \sum_p \varepsilon_p \gamma_p (\Gamma_p \cdot \mathbf{n}) \tag{2}$$

The second term on the right-hand side of Equation 1 is the gain of electrons due to secondary emission effects, γ_p being the secondary emission coefficient. The second term in Equation 2 is the secondary emission energy flux, ε_p being the mean energy of the secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n}) [Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0]$$

PLASMA CHEMISTRY

Argon is one of the simplest mechanisms to implement at low pressures. The electronically excited states can be lumped into a single species which results in a chemical mechanism consisting of only 3 species and 7 reactions:

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 this discharge, the electron density and density of excited species is relatively low so stepwise ionization is not as important as in high density discharges. In addition to volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When a metastable argon atom makes contact with the wall, it reverts to the ground state argon atom with some probability (the sticking coefficient).

Results and Discussion

The electric potential, electron density and mean electron energy are all quantities of interest. Most of the variation in each of these quantities occurs along the axial length of the column. Figure 2 plots the electron density in the column. The electron density peaks in the region between the cathode fall and positive column. This region is sometimes referred to as Faraday dark space. The electron density also decreases rapidly in the radial direction. The is caused by diffusive loss of electrons to the outer walls of the column where they accumulate a surface charge. The build up of negative charge leads to a positive potential in the center of the column with respect to the walls.

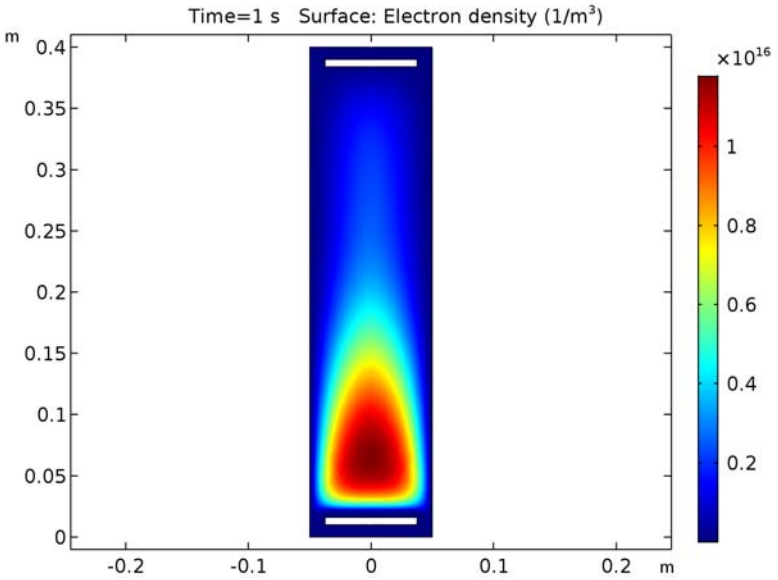

Figure 2: Surface plot of electron density inside the column.

In Figure 4 the electric potential is plotted along the axial length of the column. Notice that the potential profile is markedly different from the linear drop in potential which results in the absence of the plasma. The strong electric field in the cathode region can lead to high energy ion bombardment of the cathode. Heating of the cathode surface occurs

which may in turn lead to thermal electron emission where additional electrons are emitted from the cathode surface.

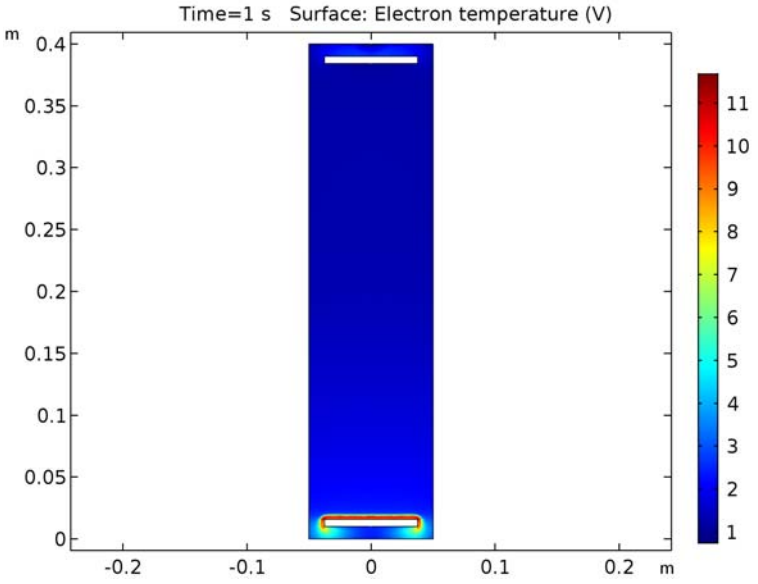

Figure 3: Plot of electron "temperature" along the axial length of the positive column.

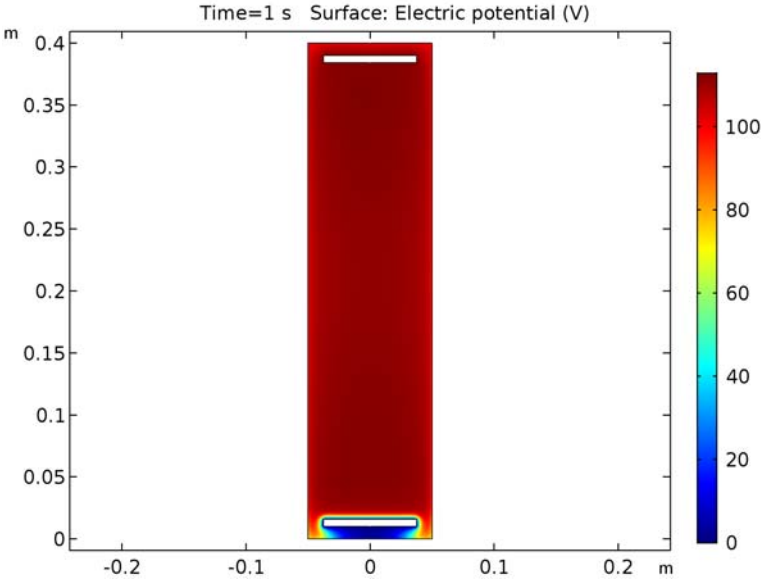

Figure 4: Plot of the electric potential along the axial length of the positive column.

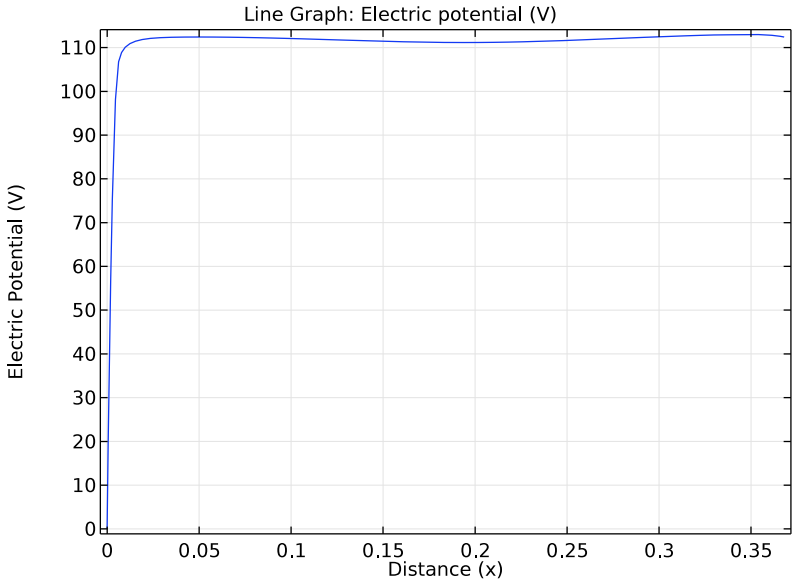

Figure 5: Plot of electric potential along the axial length of the positive column.

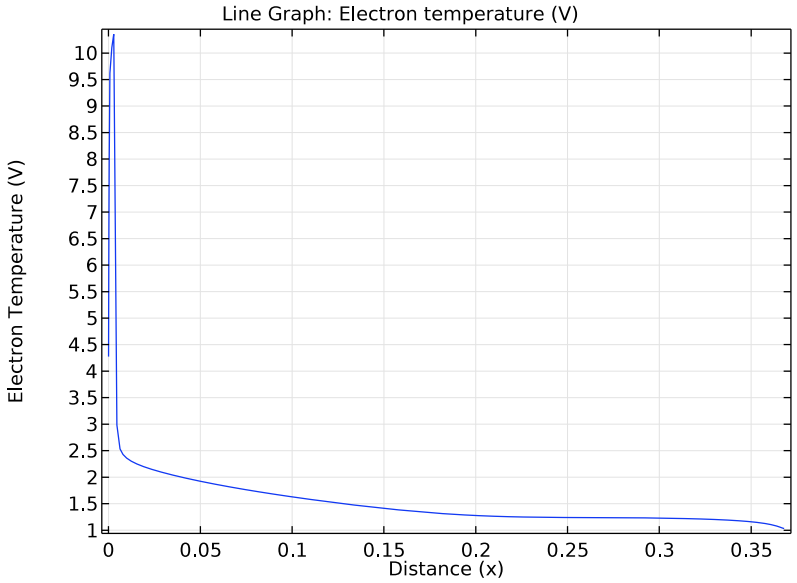

Figure 6: Plot of the electron temperature along the axial length of the positive column.

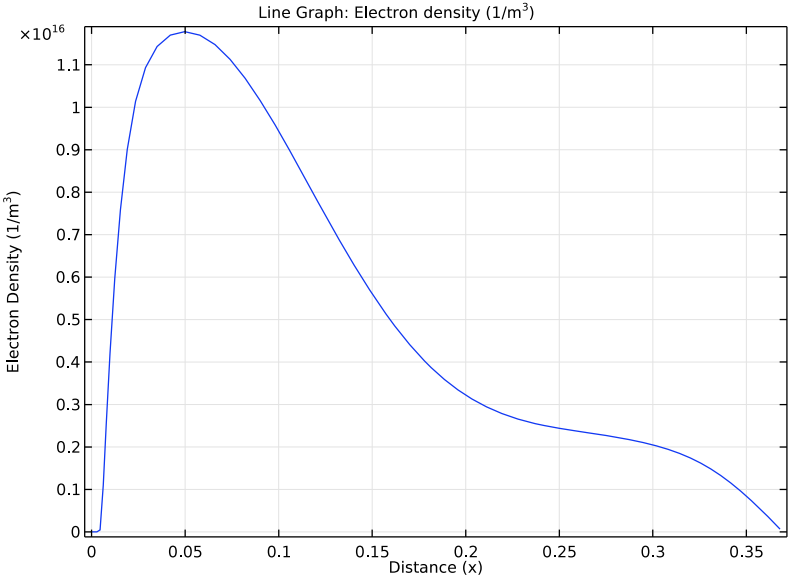

Figure 7: Plot of the electron density along the axial length of the positive column.

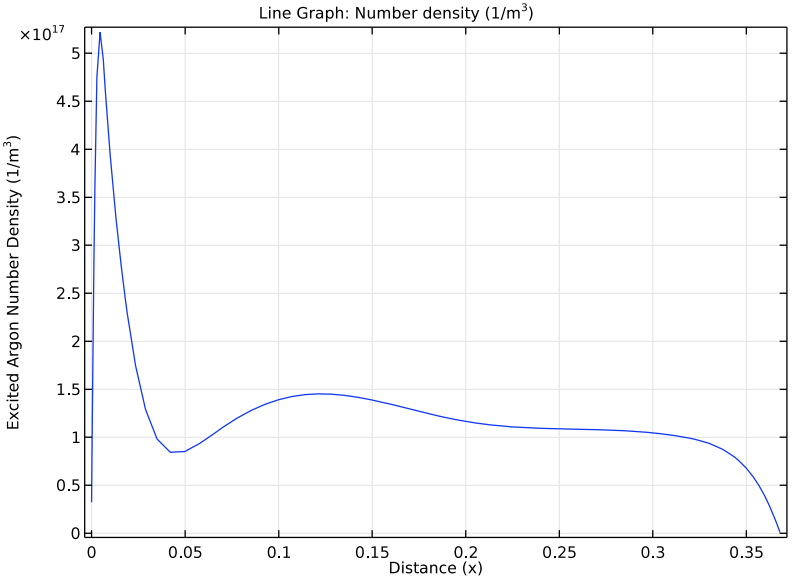

Figure 8: Plot of the number density of excited argon atoms.

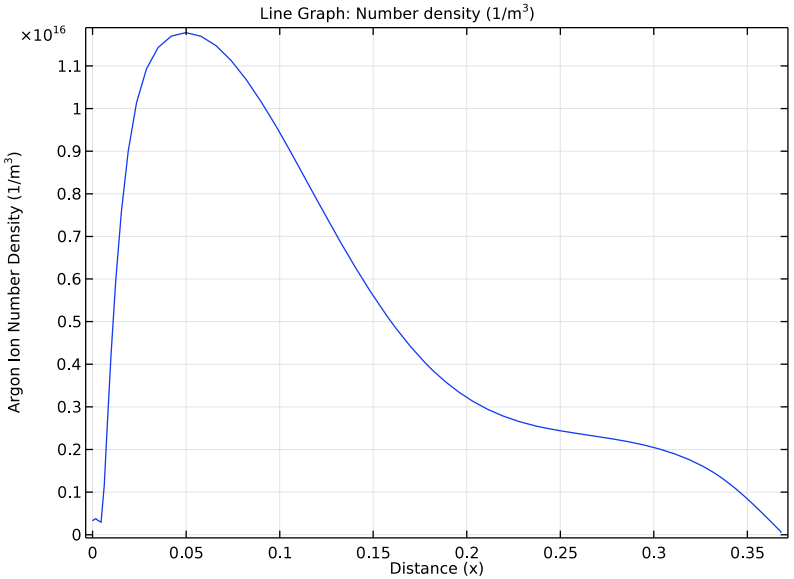

Figure 9: Plot of the number density of argon ions.

Reference

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

Application Library path: `Plasma_Module/Direct_Current_Discharges/positive_column_2d`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Plasma>Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GEOMETRY 1

Rectangle 1 (r1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.05`.

4 In the **Height** text field, type `0.4`.

Rectangle 2 (r2)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.0375`.

4 In the **Height** text field, type `6e-3`.

5 Locate the **Position** section. In the **z** text field, type `0.01`.

Rectangle 3 (r3)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

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

3 In the **Width** text field, type `0.0375`.

4 In the **Height** text field, type `6e-3`.

5 Locate the **Position** section. In the **z** text field, type `0.384`.

Compose 1 (co1)

1 On the **Geometry** toolbar, click **Booleans and Partitions** and choose **Compose**.

2 Select the object **r1** only.

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

4 In the **Set formula** text field, type `r1-r2-r3`.

Bézier Polygon 1 (b1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Bézier Polygon**.

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

3 Find the **Added segments** subsection. Click **Add Linear**.

4 Find the **Control points** subsection. In row **1**, set **z** to `0.02`.

5 In row **2**, set ***r*** to `0.0375` and **z** to `0.02`.

6 Click **Build All Objects**.

Mesh Control Edges 1 (mce1)

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

2 On the object **fin**, select Boundary 7 only.

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

DEFINITIONS

Variables 1

1 On the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`mueN`	`1E25[1/(m*V*s)]`	1/(V·m·s)	`Reduced electron mobility`
`V0`	`125[V]`	V	`Applied voltage`
`Wf`	`5`		`Work function`
`p0`	`0.5[torr]`	Pa	`Gas pressure`

Explicit 1

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

2 In the **Model Builder** window, right-click **Explicit 1** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Cathode` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundaries 3, 5, and 10 only.

Explicit 2

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

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

3 In the **Rename Explicit** dialog box, type `Anode` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundaries 6, 8, and 11 only.

Explicit 3

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

2 In the **Model Builder** window, right-click **Explicit 3** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Walls` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundaries 2, 9, and 12 only.

Explicit 4

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

2 In the **Model Builder** window, right-click **Explicit 4** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `All Walls` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundaries 2, 3, 5, 6, and 8–12 only.

Explicit 5

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

2 In the **Model Builder** window, right-click **Explicit 5** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Non Cathode Walls` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundaries 2, 6, 8, 9, 11, and 12 only.

PLASMA (PLAS)

Cross Section Import 1

1 On 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`.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Plasma Properties** section.

7 Select the **Use reduced electron transport properties** check box.

Plasma Model 1

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

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

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

4 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `mueN`.

You change the way the source coefficients for electronic excitation and ionization are specified. By default, COMSOL computes rate coefficients based on the cross section data you supplied. For DC discharges, Townsend coefficients provide a more accurate description of the cathode fall region so they should be used. The Townsend coefficients are typically computed using the **Boltzmann Equation, Two-Term Approximation** interface.

2: e+Ar=>e+Ars

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **2: e+Ar=> e+Ars**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Collision** section.

3 From the **Specify reaction using** list, choose **Use lookup table**.

4 Locate the **Reaction Parameters** section. From the **Rate constant form** list, choose **Townsend coefficient**.

5 Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `town2.txt`.

4: e+Ar=>2e+Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **4: e+Ar=> 2e+Ar+**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Collision** section.

3 From the **Specify reaction using** list, choose **Use lookup table**.

4 Locate the **Reaction Parameters** section. From the **Rate constant form** list, choose **Townsend coefficient**.

5 Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `town4.txt`.

Reaction 1

1 On 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 `3.734E8`.

Reaction 2

1 On 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`.

When solving a reacting flow problem there always needs to be one species which is selected to fullfill the mass constraint. This should be taken as the species with the largest mass fraction.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ars**.

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

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

When solving a plasma problem the plasma must be initially charge neutral. COMSOL automatically computes the initial concentration of a selected ionic species such that the electroneutrality constraint is satisfied.

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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**.

Wall 1

1 On 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 Walls**.

Ground 1

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

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

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

Metal Contact 1

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

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

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

4 Locate the **Terminal** section. In the V_0 text field, type `V0`.

5 Locate the **Quick Circuit Settings** section. From the **Quick circuit type** list, choose **Series RC circuit**.

Dielectric Contact 1

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

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

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

Now you add a surface reaction which describes the neutralization of Argon ions on the electrode. Secondary emission of electrons is required to sustain the discharge, so you enter the emission coefficient and an estimate of the mean energy of the secondary electrons based on the ionization energy threshold and the work function of the surface.

Surface Reaction 1

1 On 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 **Boundary Selection** section. From the **Selection** list, choose **Cathode**.

Make the secondary emission coefficient 0.25 and set the mean energy of the secondary electrons to be the ionization energy (given by the expression `plas.de_4`) minus twice the work function of the electrode.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0.25`.

6 In the ε_i text field, type `plas.de_4-2*Wf`.

Surface Reaction 2

1 On 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 **Boundary Selection** section. From the **Selection** list, choose **Non Cathode Walls**.

Surface Reaction 3

1 On 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 `Ars=>Ar`.

4 Locate the **Boundary Selection** section. From the **Selection** list, choose **All Walls**.

MESH 1

Edge 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **More Operations>Edge**.

2 Select Boundaries 3, 5, 6, 8, 10, 11, and 14 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Size**.

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

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

4 Click the **Custom** button.

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

6 In the associated text field, type `0.001`.

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

Size 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

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

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

4 From the **Predefined** list, choose **Extra fine**.

Boundary Layer Properties

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Boundary Layers**.

2 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All Walls**.

4 Locate the **Boundary Layer Properties** section. In the **Number of boundary layers** text field, type `4`.

5 Click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `0`.

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 `-8`.

7 In the **Stop** text field, type `0`.

8 In the **Number of values** text field, type 21.

9 From the **Function to apply to all values** list, choose **exp10**.

10 Click **Add**.

11 On the **Home** toolbar, click **Compute**.

RESULTS

Study 1/Solution 1 (sol1)

In the **Model Builder** window, expand the **Data Sets** node, then click **Study 1/ Solution 1 (sol1)**.

Selection

1 On the **Results** toolbar, click **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 Walls**.

Cut Line 2D 1

1 On the **Results** toolbar, click **Cut Line 2D**.

2 In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.

3 In row **Point 1**, set **Z** to `0.016`.

4 In row **Point 2**, set **R** to 0 and **z** to `0.384`.

Electron Density (plas)

1 On the **Results** toolbar, click **More Data Sets** and choose **Mirror 2D**.

2 In the **Model Builder** window, under **Results** click **Electron Density (plas)**.

3 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

4 From the **Data set** list, choose **Mirror 2D 1**.

5 On the **Electron Density (plas)** toolbar, click **Plot**.

6 Click the **Zoom Extents** button on the **Graphics** toolbar.

Electron Temperature (plas)

1 In the **Model Builder** window, under **Results** click **Electron Temperature (plas)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Data set** list, choose **Mirror 2D 1**.

4 On the **Electron Temperature (plas)** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

Electric Potential (plas)

1 In the **Model Builder** window, under **Results** click **Electric Potential (plas)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Data set** list, choose **Mirror 2D 1**.

4 On the **Electric Potential (plas)** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

1D Plot Group 4

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Electric Potential on Axis` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (x)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Electric Potential (V)`.

8 Locate the **Data** section. From the **Data set** list, choose **Cut Line 2D 1**.

Line Graph 1

1 Right-click **Electric Potential on Axis** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1> Plasma (Electrostatics)>Electric>V - Electric potential**.

Electric Potential on Axis

1 In the **Model Builder** window, under **Results** click **Electric Potential on Axis**.

2 On the **Electric Potential on Axis** toolbar, click **Plot**.

3 Click the **Zoom Extents** button on the **Graphics** toolbar.

1D Plot Group 5

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Electron Temperature on Axis` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (x)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Electron Temperature (V)`.

8 Locate the **Data** section. From the **Data set** list, choose **Cut Line 2D 1**.

Line Graph 1

1 Right-click **Electron Temperature on Axis** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1> Plasma (Drift Diffusion)>Electron energy density>plas.Te - Electron temperature**.

3 On the **Electron Temperature on Axis** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

1D Plot Group 6

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Electron Density on Axis` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (x)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Electron Density (1/m<sup>3</sup>)`.

8 Locate the **Data** section. From the **Data set** list, choose **Cut Line 2D 1**.

Line Graph 1

1 Right-click **Electron Density on Axis** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1> Plasma (Drift Diffusion)>Electron density>plas.ne - Electron density**.

3 On the **Electron Density on Axis** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

1D Plot Group 7

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Excited Argon Number Density on Axis` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (x)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Excited Argon Number Density (1/m<sup>3</sup>)`.

8 Locate the **Data** section. From the **Data set** list, choose **Cut Line 2D 1**.

Line Graph 1

1 Right-click **Excited Argon Number Density on Axis** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1> Plasma (Heavy Species Transport)>Number densities>plas.n_wArs - Number density**.

3 On the **Excited Argon Number Density on Axis** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

1D Plot Group 8

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Argon Ion Number Density on Axis` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Distance (x)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Argon Ion Number Density (1/m<sup>3</sup>)`.

8 Locate the **Data** section. From the **Data set** list, choose **Cut Line 2D 1**.

Line Graph 1

1 Right-click **Argon Ion Number Density on Axis** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Model>Component 1> Plasma (Heavy Species Transport)>Number densities>plas.n_wAr_1p - Number density**.

3 On the **Argon Ion Number Density on Axis** toolbar, click **Plot**.

4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Negative Streamer in Nitrogen

Introduction

Streamers are transient filamentary electric discharges that can develop in a non-conducting background in the presence of an intense electric field. These discharges can attain high electron number density and consequently, a high concentration of chemical active species that are relevant for numerous applications. Industrial applications include: ozone production, pollution control, and surface processing.

The propagation of streamers is driven by very non-linear dynamics that involve very steep density gradients and high space-charge density distributed in very thin layers. The charge separation at the front (or head) of the streamer generates intense electric fields that are responsible for sharp ionization fronts propagating into the neutral medium.

In negative (anode directed) streamers, ionizing electrons are accelerated outwards by the space-charge (the streamer extends towards the anode). These high energy electrons may have been transported by drift or diffusion, or created by another mechanism that provides pre-ionization ahead of the streamer such as photoionization or ionization from runway electrons. In positive (or cathode directed) streamers the space-charge field in the streamer head accelerates the electrons inwards. Consequently, the ionizing electrons must be produced by a pre-ionization mechanism. The pre-ionization of the streamer is a complex subject that is believed to be critical for both negative and positive streamers propagation and is still under intense investigation. This document is an introduction to streamer modeling with focus on basic concepts of streamer propagation. With that in mind it is followed a simplified approach where all pre-ionization is neglected and only negative streamers are discussed.

This example presents a study of a negative streamer in atmospheric pressure nitrogen. The streamer propagates with a constant electric field of 100 kV/cm in front of the streamer. The model here presented is similar to the fluid model used in Ref. 1 and gives similar results. Furthermore, in Ref. 1, results from a fluid and particle-in-cell model are compared to agree very well for fields below 50 kV/cm (at atmospheric pressure).

Model Definition

The model is one dimensional and describes the transient behavior of an initial electron seed in the presence of a strong electric field using fluid-type equations.

The simulation is design with emphasis in the streamer propagation. The streamer develops from an initial small electron density placed near the cathode. Without pre-ionization only a negative streamer develops towards the anode. The initial number density and exact location of the seed are chosen to form a streamer long before it reaches

the anode. The distance between electrodes is 1.15 mm. The cathode (placed on the left) is grounded and at the anode is given a constant electric field of -100 kV/cm. A constant electric field ahead of the streamer allows for an equilibrium in the electron density growth and a constant propagation velocity.

The model solves the electron and ion continuity and momentum equations, in the drift-diffusion approximation, self-consistently coupled with Poisson's equation. The local field approximation is used, which means that transport and source coefficients are assumed to be well parametrized through the reduced electric field (E/N). In the local field approximation the fluid equation for the mean electron energy is not solved, which reduces significantly the complexity of the numerical problem.

The local field approximation is valid in a situation where the rate of electron energy gain from the electric field is locally balanced by the energy loss rate. When this condition is met the electrons are said to be in local equilibrium with the electric field and the electron mean properties can be expressed as a function the reduced electric field.

DOMAIN EQUATIONS

The electron density is computed by solving the drift-diffusion equation for the electron density.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e \tag{1}$$

Convection of electrons due to fluid motion is neglected. For more detailed information on electron transport see the section Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

When using the local field approximation the electron energy density equation is not solved and the transport and source coefficients are mapped by the reduced electric field. In practice, when using the local field approximation or the local energy approximation, the transport and source coefficients are still given as a function of the mean electron energy. When using the local field approximation however, a function that relates the mean electron energy and the reduced electric field must be provided:

$$\varepsilon = F(E/N)\,. \tag{2}$$

The electron source R_e is defined later. The electron diffusivity and electron mobility are provided as a function of the mean electron energy.

The source coefficients in the above equation is determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay

of electron density and P inelastic electron-neutral collisions. In general $P \gg M$. In the case of rate coefficients, the electron source term is given by

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e \tag{3}$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). For drift-dominated discharges it is better practice to use Townsend coefficients instead of rate coefficients to define reaction rates. Townsend coefficients provide a better description of what happens in the cathode fall region Ref. 2. When Townsend coefficients are used, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j \alpha_j N_n |\Gamma_e| \tag{4}$$

where α_j is the Townsend coefficient for reaction j (m^2) and Γ_e is the electron flux as defined above ($1/(\mathrm{m}^2 \cdot \mathrm{s})$). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with streamers.

For non-electron species, the following equation is solved for the mass fraction of each species:

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k \tag{5}$$

For detailed information on the transport of the non-electron species see the section Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

The electrostatic field is computed using the equation

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho \tag{6}$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right) \tag{7}$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

Boundary Conditions

The present simulation is arranged in a way that the charged particle interaction with the wall is irrelevant to what happen to the streamer propagation. Nevertheless boundary conditions must be given. Electrons are lost to the wall due to random motion within a few mean free paths of the wall resulting in the boundary condition for the electron flux

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1}{2} \nu_{e,\,\mathrm{th}} n_e\right). \tag{8}$$

For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z \mu_k (\mathbf{E} \cdot \mathbf{n})[Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0] \tag{9}$$

The streamer propagates (from left to right) with a constant electric field ahead of -100 kV/cm. The cathode on the left is grounded,

PLASMA CHEMISTRY

The chemistry of a plasma sustained in nitrogen can be very complex and a detailed study of the main excited states could easily have hundreds of reactions. The main goal of this model is to study the charge particle density profiles in the presence of strong electric fields. With that in mind it is used one single ionization reaction as presented in Table 1 that describes correctly the creation of charged species in a background of nitrogen. In this work it is used the Townsend coefficient as a function of the mean electron energy provided in Ref. 1.

TABLE 1: IONIZATION REACTION

Reaction	Formula	Type	$\Delta\varepsilon$ (eV)	k_f (m^3/s)
1	e+N=>2e+N+	Ionization	15.5	-

In addition to the volumetric reactions, the following surface reaction is implemented:

TABLE 2: TABLE OF SURFACE REACTION.

Reaction	Formula	Sticking coefficient
1	N+=>N	1

When an ions reach the wall, they are assumed to change back to neutral atoms.

Results and Discussion

The results in this section are for a streamer propagating in a background gas kept at a constant density as obtained by the ideal gas law at atmospheric pressure and at a temperature of 293.15 K. All transport and source coefficients used in this simulation are form Ref. 1. There, the electron mobility and diffusion coefficients, the Townsend coefficient, and the mean electron energy as a function of the reduced electric field are obtain using particle swarm simulations.

Figure 1 presents the spatial distribution of the electron and ion density for several instants during the streamer simulation. The streamer is initiated by a localized number of electrons near the cathode (left in all figures below). In a first phase there is electron drift and growth in an unperturbed electric field. The first instant in Figure 1 marks the end of this period. A streamer is formed if the amplification of the electron density is enough to generate intense space-charge electric fields and electric shielding before the streamer arrives to the anode. The last three instants of Figure 1correspond to the streamer phase.

In the streamer phase the maximum electron and ion density reach a constant value and propagate at constant velocity (because the electric field ahead of the streamer is kept constant). The streamer morphology is composed of (i) a region of strong charge separation and strong density gradients (the streamer head), and (ii) a quasi-neutral region with flat profiles (the streamer body) that increases its length with the streamer propagation.

Figure 2, Figure 3 and Figure 4 shows the spatial distribution of the electric field, space-charge density and mean electron energy for several instants during the streamer simulation. Note how the quasi-neutral streamer body shields the electric field to very small values causing the electrons to cool down. This makes the electron creation in the body negligible.

On the left there is also a charge separation region. This region is created because the electrons are pulled towards the anode leaving the created ions behind. The ions, being much less mobile than electrons do not have time to drift in this 0.9 ns simulation. Note also that this charge separation region does not move in time, which is achieved by setting low levels of pre-ionization.

The ionization front moves with a velocity larger than the electron drift velocity

$$v_d = \mu_e |\boldsymbol{E}| \,. \tag{10}$$

determined solely by the electric field in the leading edge of the streamer. The ionization front velocity has also contributions from electron diffusion and creation of new electrons

and can be given by the expression Ref. 1

$$v_f = \mu_e |E| + 2\sqrt{D_e \mu_e |E| a}\,. \tag{11}$$

The values of the electron drift velocity and the ionization front propagation are plotted in Ref. 5. Equation 11 is an analytic solution obtained for planar fronts.

There is a general excellent agreement with the results from the model here presented and the ones from the fluid model presented in Ref. 1 when comparing values of peak electron density, ionization level in the body, electron mean energy, streamer propagation velocity, and spatial profiles of different quantities.

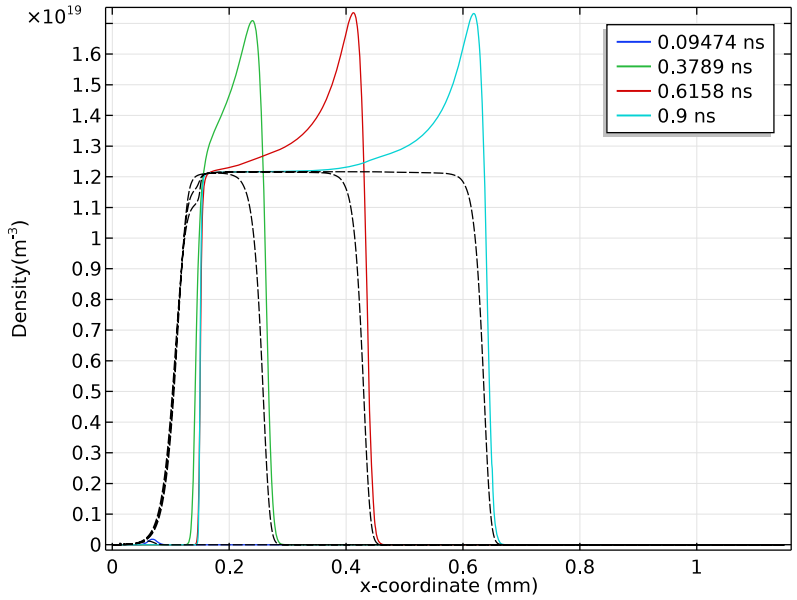

Figure 1: Spatial distribution of the electron (colored solid lines) and ion number density (black dashed lines) for four time instants during the streamer propagation.

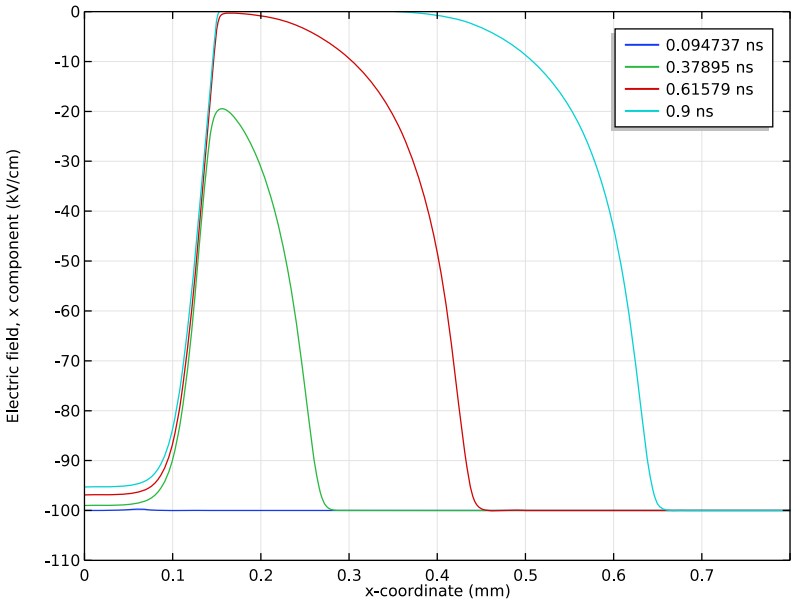

Figure 2: Electric field spatial distribution for four time instants during the streamer propagation.

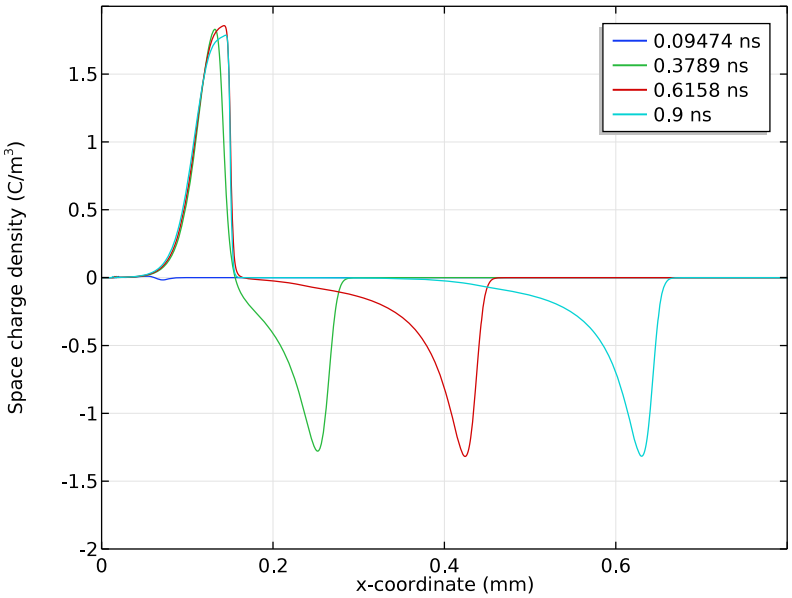

Figure 3: Space charge density for four time instants during the streamer propagation.

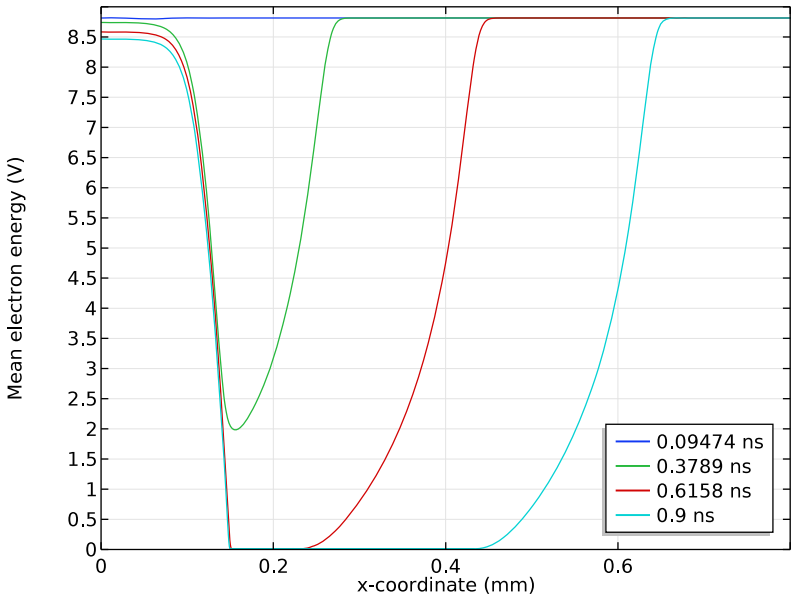

Figure 4: Mean electron energy for four time instants during the streamer propagation.

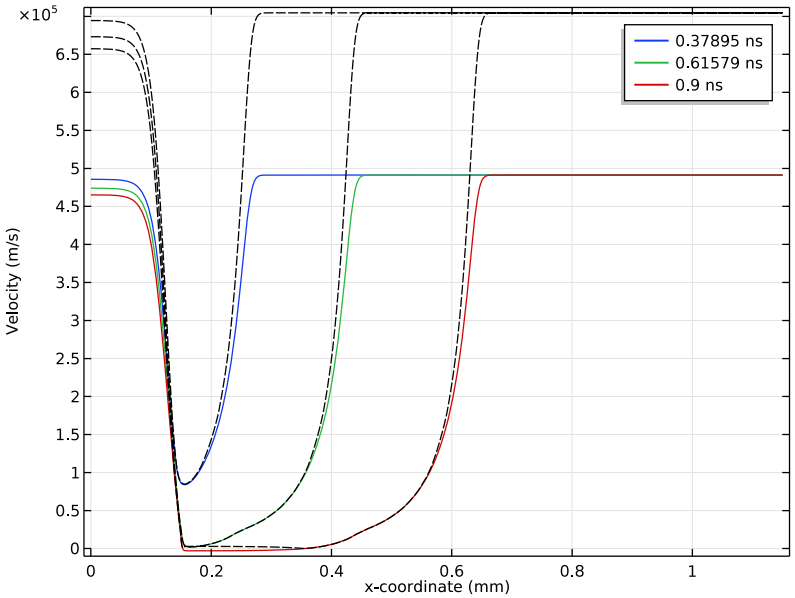

Figure 5: Electron drift velocity (colored solid lines) and velocity computed using Equation 11 *(black dashed lines) for three time instants during the streamer propagation.*

Reference

1. C. Li, W. J. M. Brok, U. Ebert, J. J. A. M. van der Mullen, "Deviations from the local field approximation in negative streamer heads", *J. Appl. Phys.*, vol. 101, pp. 123305–1–11, 2007.

2. M.A. Lieberman and A.J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, John Wiley & Sons, 2005.

Application Library path: `Plasma_Module/Direct_Current_Discharges/streamer_1d`

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 **1D**.
2. In the **Select Physics** tree, select **Plasma>Plasma (plas)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies>Time Dependent**.
6. Click **Done**.

GEOMETRY 1

Follow the steps below to create the model geometry: a simple 1D geometry consisting of a grounded electrode on the left (cathode) and a boundary condition to fix a constant electric field on the rigth (anode).

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**.

Interval 1 (i1)

1. On the **Geometry** toolbar, click **Interval**.
2. In the **Settings** window for **Interval**, locate the **Interval** section.
3. In the **Right endpoint** text field, type `1.15`.

Interval 2 (i2)

1. On the **Geometry** toolbar, click **Interval**.
2. In the **Settings** window for **Interval**, locate the **Interval** section.
3. In the **Left endpoint** text field, type `1.15`.
4. In the **Right endpoint** text field, type `1.151`.
5. Click **Build All Objects**.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
ne0	ne0max*exp(-((x-x0)/sigma)^2)+ ne0min	1/m³	
ne0min	1e-15[m^-3]	1/m³	
ne0max	5e16[m^-3]	1/m³	
x0	0.02e-3[m]	m	
sigma	0.01e-4[m]	m	

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
Efield	-100[kV/cm]	-1E7 V/m	

4 In the **Model Builder** window's toolbar, click the **Show** button and select **Stabilization** in the menu.

PLASMA (PLAS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Plasma (plas)**.

2 In the **Settings** window for **Plasma**, click to expand the **Stabilization** section.

3 Clear the **Source stabilization** check box.

4 Clear the **Reaction source stabilization** check box.

5 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** check box.

This model uses the local field approximation to parametrize in space source and trasnport coefficients

6 From the **Mean electron energy** list, choose **Local field approximation**.

Electron Impact Reaction 1

1 On the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

Add an ionization reaction.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+N=>2e+N+`.

4 Locate the **Collision Type** section. From the list, choose **Ionization**.

5 In the Δε text field, type `15.6`.

Import the ionization Townsend coefficient

6 Locate the **Collision** section. From the **Specify reaction using** list, choose **Use lookup table**.

7 Locate the **Reaction Parameters** section. From the **Rate constant form** list, choose **Townsend coefficient**.

8 Click **Load from File**.

9 Browse to the model's Application Libraries folder and double-click the file `alphaN2.txt`.

Species: N

When solving any type of reacting flow problem one species must always be chosen to fulfill the mass constraint. This should be taken as the species with the largest mass fraction.

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: N**.

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 **N2**.

Species: N+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Species: N+**.

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 **N2**.

Surface Reaction 1

1 On 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 `N+=>N`.

4 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

5 In the list, select **3**.

6 Click **Remove from Selection**.

7 Select Boundaries 1 and 2 only.

Plasma Model 1

Import the tables of the electron mobility and diffusivity, and the mean electron energy as a function of the reduced electric field.

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Plasma Model 1**.

2 In the **Settings** window for **Plasma Model**, locate the **Electron Density and Energy** section.

3 From the **Electron transport properties** list, choose **Use lookup tables**.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `muN2.txt`.

6 Click **Load from File**.

7 Browse to the model's Application Libraries folder and double-click the file `DN2.txt`.

8 Click to expand the **Mean electron energy specification** section. Locate the **Mean Electron Energy Specification** section. From the **Specify using** list, choose **Use lookup table**.

9 Click **Load from File**.

10 Browse to the model's Application Libraries folder and double-click the file `EN_to_NrgN2.txt`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `ne0`.

Wall 1

1 On 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**.

Ground 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Ground**.

2 Select Boundary 1 only.

Electric Displacement Field 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Electric Displacement Field**.

2 In the **Settings** window for **Electric Displacement Field**, locate the **Electric Displacement Field** section.

3 Specify the $\mathbf{D}_0$ vector as

Efield*epsilon0_const	x

4 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

Charge Conservation 1

1 On the **Physics** toolbar, click **Domains** and choose **Charge Conservation**.

2 In the **Settings** window for **Charge Conservation**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 In the list, select **1**.

5 Click **Remove from Selection**.

6 Select Domain 2 only.

7 Locate the **Electric Field** section. From the ε_r list, choose **User defined**. In the associated text field, type 10.

MESH 1

Distribution 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edge**.

2 Right-click **Edge 1** and choose **Distribution**.

3 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

4 In the list, select **2**.

5 Click **Remove from Selection**.

6 Select Domain 1 only.

7 Locate the **Distribution** section. In the **Number of elements** text field, type 2000.

Distribution 1

1 Right-click **Edge 1** and choose **Duplicate**.

2 In the **Model Builder** window, expand the **Edge 2** node, then click **Distribution 1**.

3 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

4 From the **Selection** list, choose **All domains**.

5 In the list, select **1**.

6 Click **Remove from Selection**.

7 Select Domain 2 only.

8 Locate the **Distribution** section. In the **Number of elements** text field, type `10`.

9 Click **Build All**.

STUDY 1

1 In the **Settings** window for **Study**, locate the **Study Settings** section.

2 Clear the **Generate default plots** check box.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 From the **Time unit** list, choose **ns**.

4 In the **Times** text field, type `range(0,0.9/19,0.9)`.

5 Click to expand the **Results while solving** section. Locate the **Results While Solving** section. Select the **Plot** check box.

6 From the **Update at** list, choose **Time steps taken by solver**.

Get the initial values to prepare a plot to show the electron and ion densities while the solver runs.

Study 1

On the **Study** toolbar, click **Get Initial Value**.

RESULTS

1D Plot Group 1

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Charged Species` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Plot Settings** section. Select the **y-axis label** check box.

6 In the associated text field, type `Density (m<sup>-3</sup>)`.

7 Locate the **Axis** section. Select the **Manual axis limits** check box.

8 In the **x minimum** text field, type `0`.

9 In the **x maximum** text field, type `0.8`.

10 In the **y minimum** text field, type `0`.

11 In the **y maximum** text field, type `2.15e19`.

Line Graph 1

1 Right-click **Charged Species** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Electrons` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `x`.

6 Click to expand the **Legends** section. Select the **Show legends** check box.

Electrons 1

1 Right-click **Results>Charged Species>Electrons** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, type `Ions` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.n_wN_1p`.

4 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Black**.

6 Click to expand the **Legends** section. Clear the **Show legends** check box.

7 On the **Home** toolbar, click **Compute**.

Charged Species

1 In the **Model Builder** window, under **Results** click **Charged Species**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Time selection** list, choose **From list**.

4 In the **Times (ns)** list, choose **0.094737**, **0.37895**, **0.61579**, and **0.9**.

5 On the **Charged Species** toolbar, click **Plot**.

Electrons

1 In the **Model Builder** window, under **Results>Charged Species** click **Electrons**.

2 In the **Settings** window for **Line Graph**, click to expand the **Legends** section.

3 Select the **Show legends** check box.

1D Plot Group 2

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Mean electron energy` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **From list**.

4 In the **Times (ns)** list, choose **0.094737**, **0.37895**, **0.61579**, and **0.9**.

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Axis** section. Select the **Manual axis limits** check box.

7 In the **x minimum** text field, type `0`.

8 In the **x maximum** text field, type `0.8`.

9 In the **y minimum** text field, type `0`.

10 In the **y maximum** text field, type `9`.

11 Locate the **Title** section. From the **Title type** list, choose **None**.

12 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Line Graph 1

1 Right-click **Mean electron energy** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `plas.ebar`.

4 Select Domain 1 only.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Locate the **Legends** section. Select the **Show legends** check box.

8 On the **Mean electron energy** toolbar, click **Plot**.

Mean electron energy 1

1 In the **Model Builder** window, under **Results** right-click **Mean electron energy** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Space charge` in the **Label** text field.

3 Locate the **Axis** section. In the **y minimum** text field, type `-2`.

4 In the **y maximum** text field, type `2`.

5 Locate the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Legend** section. From the **Position** list, choose **Upper right**.

Line Graph 1

1 In the **Model Builder** window, expand the **Results>Space charge** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `plas.scharge`.

4 On the **Space charge** toolbar, click **Plot**.

1D Plot Group 4

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Velocity` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **From list**.

4 In the **Times (ns)** list, choose **0.37895**, **0.61579**, and **0.9**.

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Plot Settings** section. Select the **y-axis label** check box.

7 In the associated text field, type `Velocity (m/s)`.

Line Graph 1

1 Right-click **Velocity** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Drift velocity` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.mflux_nex/plas.ne`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Click to expand the **Legends** section. Select the **Show legends** check box.

Line Graph 2

1 In the **Model Builder** window, under **Results** right-click **Velocity** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Analytic` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.muexx*abs(plas.Ex)+2*sqrt(plas.Dexx*plas.muexx*abs(plas.Ex)*plas.alpha_1*plas.Nn)`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

8 From the **Color** list, choose **Black**.

Velocity

1 In the **Model Builder** window, under **Results** click **Velocity**.

2 On the **Velocity** toolbar, click **Plot**.

Mean electron energy 1

1 In the **Model Builder** window, under **Results** right-click **Mean electron energy** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Electric field` in the **Label** text field.

3 Locate the **Axis** section. In the **y maximum** text field, type `-110`.

4 Locate the **Legend** section. From the **Position** list, choose **Upper right**.

Line Graph 1

1 In the **Model Builder** window, expand the **Results>Electric field** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `plas.Ex`.

4 In the **Unit** field, type `kV/cm`.

5 On the **Electric field** toolbar, click **Plot**.

Surface Chemistry Tutorial

Introduction

Surface chemistry is often the most important and most overlooked aspect of reacting flow modeling. Surface rate expressions can be hard to find or not even exist at all. Often it is preferable to use sticking coefficients to describe surface reactions because they can be estimated intuitively.

Model Definition

The tutorial model simulates outgassing from a wafer during a chemical vapor deposition (CVD) process. Careful attention is paid to the overall mass balance in the system and the difference between the mass averaged velocity and diffusion velocity is explored.

The same physical problem is investigated first with a global (volume-averaged) model and after with a space dependent model. Starting to study a problem with a global model is a good approach when the knowledge about the system is still limited. One reason being that the global model has reduced computational times allowing for fast iterations in an initial trial and error tuning of the model. The fast computational time of global models is also a great advantage to investigate a broad region of parameters with a complex chemistry.

In some cases a volume-average model might produce enough knowledge and be accurate enough for one needs. If, however, space dependent information is necessary a space dependent model can be implemented in a posterior study.

The geometry and operating principle for the model is shown in Figure 1. Initially the closed container is full of 99.9% silicon hydride and 0.1% hydrogen (measured by molar content).

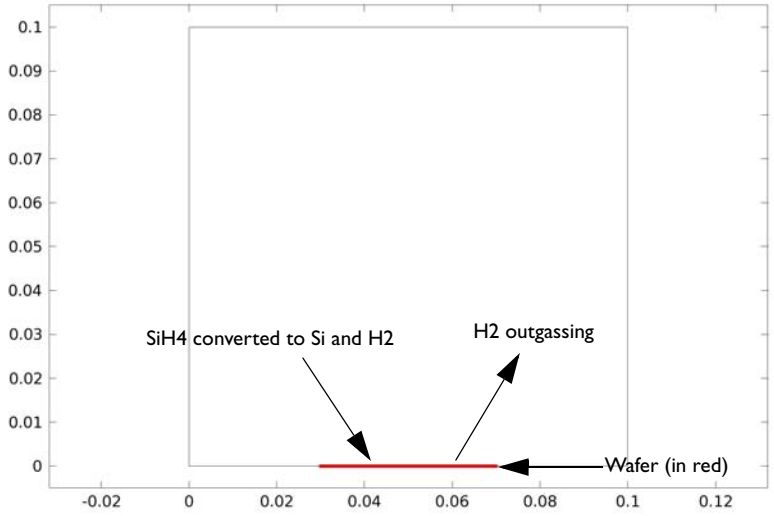

Figure 1: Geometry and basic operating principle for the surface chemistry tutorial model.

A surface reaction begins to occur on the wafer which consumes the silicon hydride, releases hydrogen into the domain, alters the composition of the absorbed species on the wafer surface and deposits bulk silicon. The following reactions are considered on the surface of the wafer:

TABLE 0-1: SURFACE REACTIONS CONSIDERED

REACTION	STICKING COEFFICIENT
SiH4+2Si(s)=>Si(b)+2SiH(s)+H2	1E-4
SiH(s)=>Si(s)+0.5H2	1E-4

The (s) here denotes "surface species" which means that the species only exists on the surfaces where the reaction is occurring. To indicate that a species is bulk, append (b) to the end of the species. Since bulk species cannot participate in surface reactions, they must only be products and not reactants in a surface reaction. The net result of these two competing reactions is `SiH4=>Si(b)+2H2`, which means it is expected that the silane is replaced by hydrogen inside the reactor, and layers of silicon deposited on the wafer surface.

MODEL EQUATIONS - SURFACE REACTIONS AND SURFACE SPECIES

The surface reaction rate for reaction i is given by:

$$q_i = k_{f,i} \prod_{k=1}^{K} c_k^{\nu_{ki}^f}$$

where the rate constant, k_f is given by:

$$k_{\mathrm{f},i} = \left(\frac{\gamma_i}{1-\gamma_i/2}\right) \frac{1}{(\Gamma_{\mathrm{tot}})^m} \left(\frac{1}{4}\right) \sqrt{\frac{8RT}{\pi M_n}}$$

and c_k is the concentration of species k which may be a volumetric or surface species, m is the reaction order minus 1, T is the surface temperature, R is the gas constant and M_n is the mean molecular weight of the gas mixture. γ_i is the dimensionless sticking coefficient. For the surface species the following equations are solved:

$$\frac{d\Gamma}{dt} = \sum_{i=1}^{N} q_i \Delta\sigma_i$$

where Γ is the surface site concentration (mol/m^2), q_i is the reaction rate for reaction i (mol/m^2), $\Delta\sigma_i$ is the change in site occupancy number for reaction i (dimensionless).

$$\frac{dZ_k}{dt} = \frac{R}{\Gamma_{tot}}$$

where Γ_{tot} is the total surface site concentration (mol/m^2), Z_k is the site fraction (dimensionless) and R is the surface rate expression (mol/m^2).

For the bulk surface species, the following equation is solved for the deposition height:

$$\frac{dh}{dt} = -\frac{RM_w}{\rho}$$

where h is the total growth height (m), M is the molecular weight (kg/mol) and ρ is the density of the bulk species (kg/m^3).

DOMAIN EQUATIONS

Inside the domain, the Navier-Stokes equations are solved for the fluid velocity. The mass fraction of hydrogen is computed by solving:

$$\rho\frac{\partial}{\partial t}(w) + \rho(\mathbf{u}\cdot\nabla)w = \nabla\cdot\mathbf{j}$$

where w is the mass fraction of hydrogen. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*. The mass fraction of silane is not directly computed. It's value comes from the fact that the sum of the mass fractions must equal one. The gas temperature is computed by solving the energy equation.

BOUNDARY CONDITIONS

Fluid Flow

The following boundary conditions are used. The mass averaged velocity is constrained using:

$$\mathbf{u} = -\frac{M_f}{\rho}\mathbf{n}$$

where M_f is the inward (or outward in this example) mass flux which is defined, from the surface chemistry as:

$$M_f = \sum_{k=1}^{K_g} M_k \dot{s}_k$$

where s_k is the surface rate expression for each species which comes from summing the surface reaction rates multiplied by their stoichiometric coefficients over all surface reactions:

$$\dot{s}_k = \sum_{i=1}^{I} \nu_{ki} q_i$$

Hydrogen Mass Fraction

The flux of hydrogen at the surface of the wafer comes from the surface reactions:

$$\mathbf{n}\cdot\mathbf{j} = M_k s_k$$

Energy Equation

For the energy equation, the following boundary condition is used:

$$\mathbf{n} \cdot \kappa \nabla T = \sum_{i=1}^{I} q_i h_i$$

where hi is the molar enthalpy change due to reaction i.

GLOBAL MODEL EQUATIONS

The global model used in this work considers that the spatial information of the different quantities in the plasma reactor can be treated as uniform. Without the spatial derivatives the numerical solution of the equation set becomes considerably simpler and the computational time is reduced. For detailed information on the global model see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*. For heavy species the following equation is solved for the mass fraction

$$V\rho\frac{d}{dt}(w_k) = VR_k + \sum_l h_l A_l R_{surf,k,l} M_k - w_k \sum_l h_l A_l M_{f,l}$$

where ρ is the mass density (SI unit: kg/m^3), w_k is the mass fraction, and R_k is the rate expression (SI unit: kg/(m^3.s)). The fourth term on the right hand side accounts for surface losses and creation, where A_l is the surface area, h_l is a dimensionless correction, V is the reactor volume, M_k is the species molar mass (SI unit: kg/mol) and $R_{surf,k,l}$ is the surface rate expression (SI unit: mol/(m^2.s)) at a surface l. The last term on the right hand side is introduce because the species mass balance equations are written in the non-conservative form and it was used the mass-continuity equation to replace for the mass density time derivative. In the last term $M_{f,l}$ is the inward mass flux of surface l (SI unit: kg/(m^2·s)). The sum in the last two terms is over all surfaces where there are surface reactions.

To take into account possible variations of the system total mass or pressure the mass-continuity equation is also solved

$$V\frac{d\rho}{dt} = \sum_l h_l A_l M_{f,l}\,.$$

The gas temperature is set to a constant value. The model for the surface chemistry is exactly the same.

Results and Discussion

In this section both space dependent and global model results are presented and discussed. For this particular physical system the results from the global model and the space dependent model are in a very good agreement. Therefore, no special discussion is made between the results of the two models.

The y-component of the mass averaged velocity is plotted in Figure 2. The mass averaged velocity is negative at the surface of the wafer. This means that overall, mass is leaving the system. This is to be expected since silane is being consumed, which has a molecular weight of 0.032 kg/mol and replacing it with hydrogen, which has a lower molecular weight of 0.002 kg/mol.

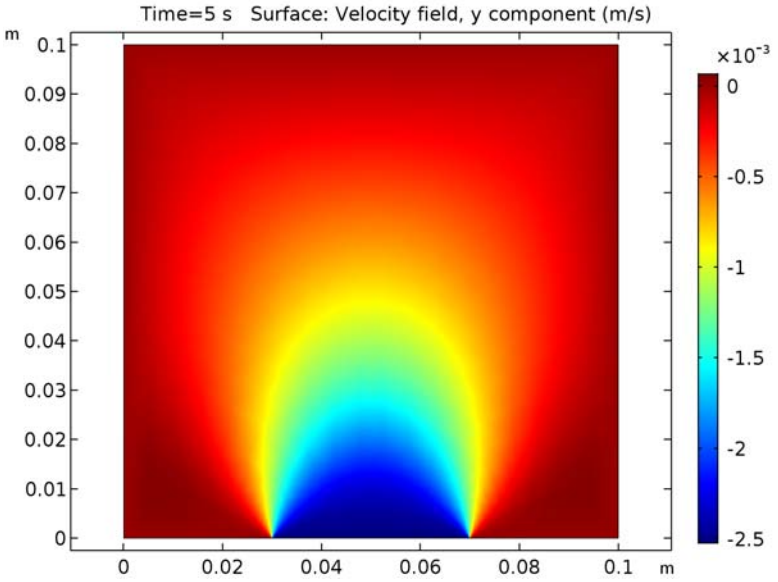

Figure 2: Plot of the mass averaged velocity field after 5 seconds.

The surface reactions begin to consume the silane which results in concentration gradients within the reactor. The outward mass flux at the wafer surface leads to a mass averaged velocity everywhere inside the reactor. The combination of concentration gradients and convection due to the mass averaged velocity tends to draw silane to wards the wafer. The first surface reaction is exothermic while the second surface reaction is endothermic. The amount of heat released by the exothermic reaction dominates, so the temperature begins to increase. The temperature is plotted in Figure 3 and is highest on the wafer surface.

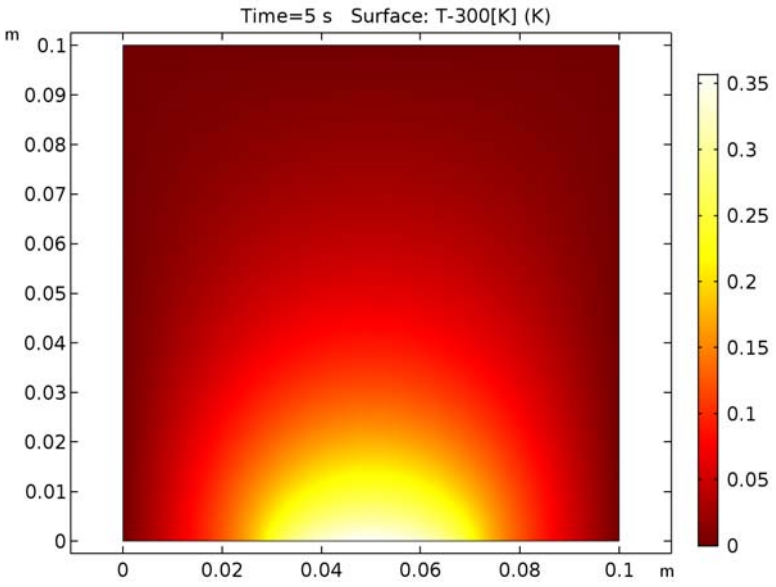

Figure 3: Plot of the change in gas temperature after 5 seconds. The higher temperature is observed at the wafer surface due to the heat released in the surface reactions.

From the net reaction `SiH4=>Si(b)+2H2` there should be a molar inflow of hydrogen at twice the rate that silane is leaving. Although this condition is not applied explicitly, it is implicit from the equations solved in the Heavy Species transport interface. Despite the fact that there is a negative mass averaged velocity, there is a positive diffusion velocity for the hydrogen at the wafer surface. The y-component of the diffusion velocity for hydrogen is plotted in Figure 4.

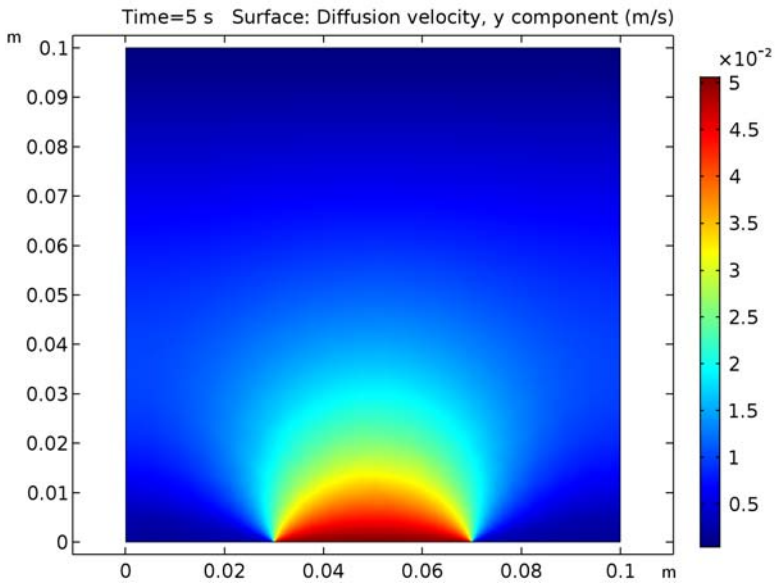

Figure 4: Plot of the y-component of the diffusion velocity for hydrogen after 5 seconds. Even though the mass averaged velocity is negative, the diffusion velocity is positive indicating an inflow of hydrogen and a net outflow of total mass.

Figure 5 plots the integrated pressure in the reactor divided by the initial average pressure in the reactor. Once the problem reaches steady state the average pressure in the reactor has increased by a factor of 2. This is expected since every mole of silane is being replaced by two moles of hydrogen. The silane in the reactor is completely consumed after around 200 seconds.

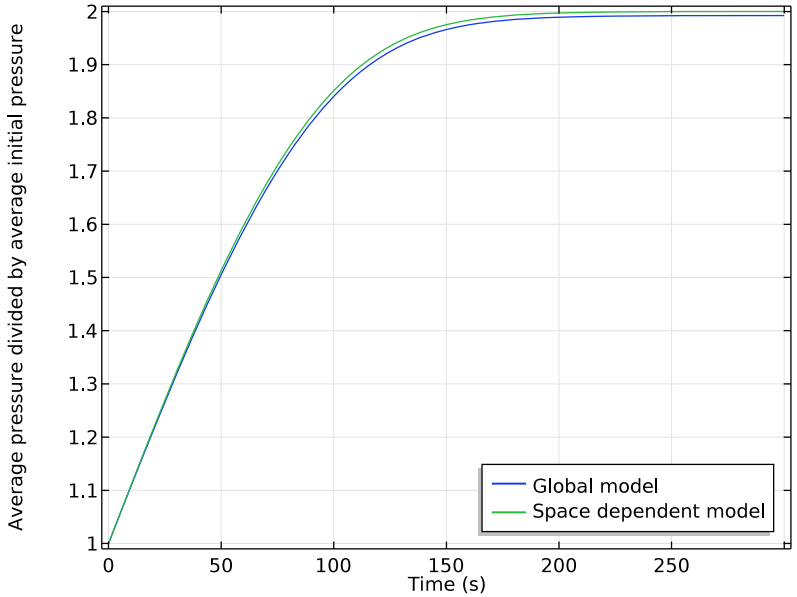

Figure 5: Plot of the ratio of the average pressure by the average initial pressure computed with the global model (blue) and the space dependent model (green).

In Figure 6 the total mass initially present in the reactor divided by the total mass in the reactor is plotted. The total mass in the reactor drops by a factor of 8, which is expected since the silane with molecular mass 0.032 kg/mol is replaced with two moles of hydrogen which has a molecular weight of 2·0.002=0.004 kg/mol.

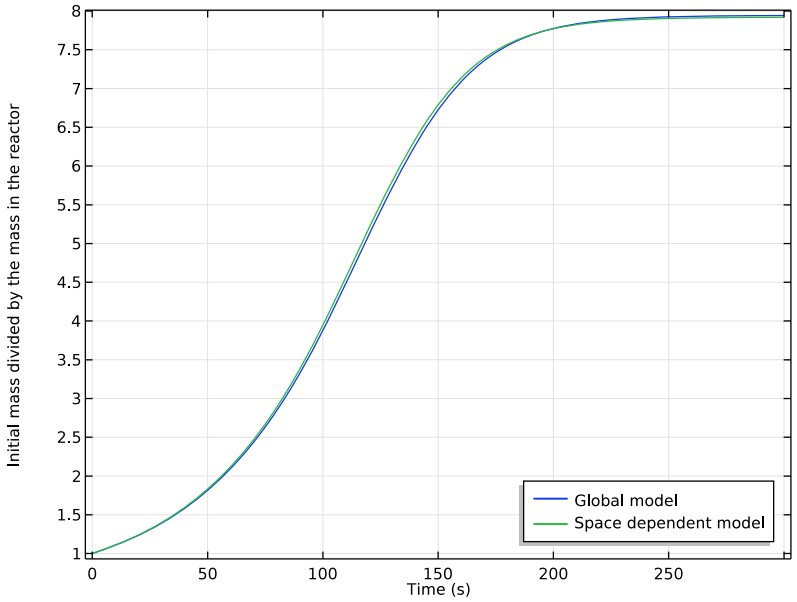

Figure 6: Plot of the ratio of the total mass by the total mass computed with the global model (blue) and the space dependent model (green).

Another way of verifying the correctness of the model is to compare the mass lost inside the reactor to the mass accumulated on the wafer surface. The two quantities should be equal. The total gain in mass from surface and bulk species is compared to the total loss in mass from the reactor in Figure 7. The two curves agree very well indicating that the total mass in the entire system is conserved.

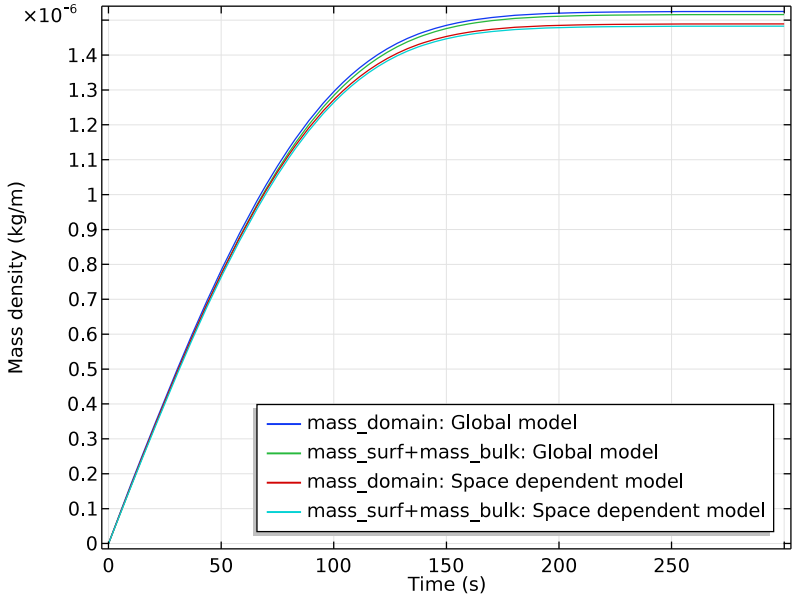

Figure 7: Plot of the total mass lost in the domain (blue: global model, and red: space dependent model) and the total mass gained due to Silicon deposition on the wafer surface (green: global model and cyan: space dependent model).

The ultimate goal of most CVD models is to determine the total growth height and growth rate on the surface of the wafer. The total growth height is plotted in Figure 8 and saturates at about 159 Angstroms. The total growth rate saturates because all the silane in the reactor is consumed after around 200 seconds. The accumulated growth height is also very uniform across the surface of the wafer. The global model and space dependent model results for the total growth height agrees very well (not shown).

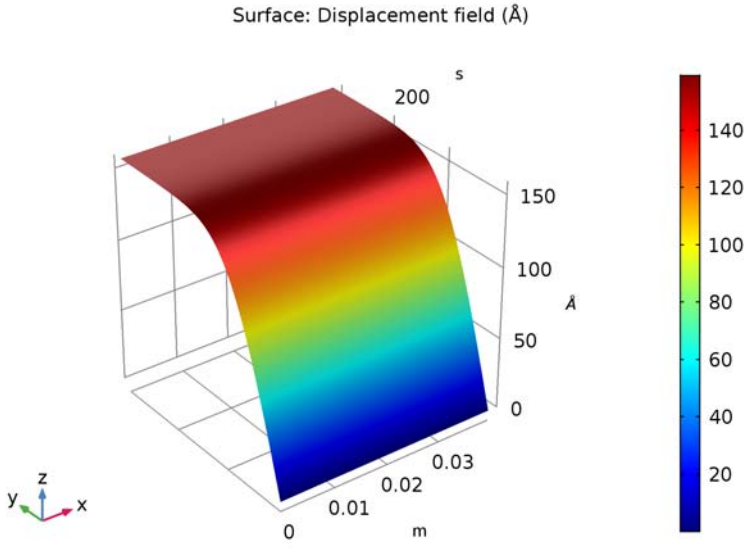

Figure 8: Plot of the growth height (surface and z-axis) vs. the wafer arc length (x-axis) and time (y-axis). The final height of deposited silicon is 158 Å.

Reference

1. R.J. Kee, M.E. Coltrin, and P. Glarborg, *Chemically Reacting Flow Theory and Practice*, John Wiley & Sons, 2003.

Application Library path: `Plasma_Module/Chemical_Vapor_Deposition/surface_chemistry_tutorial`

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 **2D**.

2 In the **Select Physics** tree, select **Plasma>Heavy Species Transport (hs)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

6 Click **Done**.

GEOMETRY 1

Square 1 (sq1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Square**.

2 In the **Settings** window for **Square**, locate the **Size** section.

3 In the **Side length** text field, type `0.1`.

Polygon 1 (pol1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Polygon**.

2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

3 In the **x** text field, type `0.03 0.07`.

4 In the **y** text field, type `0 0`.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `surface_chemistry_tutorial_variables.txt`.

Integration 1 (intop1)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

Integration 2 (intop2)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

HEAVY SPECIES TRANSPORT (HS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heavy Species Transport (hs)**.

2 In the **Settings** window for **Heavy Species Transport**, locate the **Transport Settings** section.

3 From the **Diffusion model** list, choose **Global**.

Surface Reaction 1

1 On 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 `SiH4+2Si(s)=>Si(b)+2SiH(s)+H2`.

4 Select Boundary 4 only.

5 Locate the **Reaction Parameters** section. In the γ_f text field, type `1e-4`.

Surface Reaction 2

1 On 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 `SiH(s)=>Si(s)+0.5H2`.

4 Select Boundary 4 only.

5 Locate the **Reaction Parameters** section. In the γ_f text field, type `1e-4`.

Species: SiH4

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **Species: SiH4**.

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 **SiH4**.

Species: H2

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **Species: H2**.

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **H2**.

4 In the x_0 text field, type `1E-3`.

Species: Si(s)

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **Species: Si(s)**.

2 In the **Settings** window for **Surface Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **Si**.

4 Locate the **Surface Species Parameters** section. In the $Z_{k,\,0}$ text field, type `0.995`.

Species: Si(b)

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **Species: Si(b)**.

2 In the **Settings** window for **Surface Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **Si**.

Species: SiH(s)

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **Species: SiH(s)**.

2 In the **Settings** window for **Surface Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **SiH**.

4 Locate the **Surface Species Parameters** section. In the $Z_{k,\,0}$ text field, type `0.005`.

Global Model

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **Global Model**.

2 In the **Settings** window for **Global Model**, locate the **Model Inputs** section.

3 In the p_0 text field, type `13.3`.

STUDY 1

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Global model` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

4 Clear the **Generate convergence plots** check box.

GLOBAL MODEL

Step 1: Time Dependent

1 In the **Model Builder** window, under **Global model** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,5,300)`.

4 On the **Home** toolbar, click **Compute**.

RESULTS

1D Plot Group 1

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Average Pressure Divided by Average Initial Pressure` in the **Label** text field.

3 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Average Pressure Divided by Average Initial Pressure** and choose **Global**.

2 In the **Settings** window for **Global**, type `Global model` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Global model/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`hs.pA/at(0,hs.pA)`	1	

5 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Global model`

7 On the **Average Pressure Divided by Average Initial Pressure** toolbar, click **Plot**.

1D Plot Group 2

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Density ratio` in the **Label** text field.

3 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Density ratio** and choose **Global**.

2 In the **Settings** window for **Global**, type `Global model` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Global model/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
at(0,hs.rho)/hs.rho	1	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
Global model

7 On the **Density ratio** toolbar, click **Plot**.

1D Plot Group 3

1 On the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Total Reactor Mass` in the **Label** text field.

3 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Total Reactor Mass** and choose **Global**.

2 In the **Settings** window for **Global**, type `Global model` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Global model/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
mass_domain	kg/m	Mass change in the domain
mass_surf+mass_bulk	kg/m	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
mass_domain: Global model
mass_surf+mass_bulk: Global model

7 On the **Total Reactor Mass** toolbar, click **Plot**.

Edge 2D 1

1 On the **Results** toolbar, click **More Data Sets** and choose **Edge 2D**.

2 Select Boundary 4 only.

2D Plot Group 4

1 On the **Results** toolbar, click **More Data Sets** and choose **Parametric Extrusion 1D**.

2 On the **Results** toolbar, click **2D Plot Group**.

3 In the **Settings** window for **2D Plot Group**, type `Parametric Extrusion 1D 1 - Global model` in the **Label** text field.

4 Locate the **Data** section. From the **Data set** list, choose **Parametric Extrusion 1D 1**.

Surface 1

1 Right-click **Parametric Extrusion 1D 1 - Global model** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `h_Si_bulk`.

4 From the **Unit** list, choose **Å**.

Height Expression 1

1 Right-click **Results>Parametric Extrusion 1D 1 - Global model>Surface 1** and choose **Height Expression**.

Add the physic interfaces necessary for the space dependent simulations.

ADD PHYSICS

1 On the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

4 Click **Add to Component** in the window toolbar.

ADD PHYSICS

1 Go to the **Add Physics** window.

2 In the tree, select **Heat Transfer>Heat Transfer in Fluids (ht)**.

3 Click **Add to Component** in the window toolbar.

HEAT TRANSFER IN FLUIDS (HT)

On the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

HEAVY SPECIES TRANSPORT (HS)

On the **Physics** toolbar, click **Heat Transfer in Fluids (ht)** and choose **Heavy Species Transport (hs)**.

Change the Diffusion Model to Mixture-averaged for the space dependent simulations.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heavy Species Transport (hs)**.
2 In the **Settings** window for **Heavy Species Transport**, locate the **Transport Settings** section.
3 From the **Diffusion model** list, choose **Mixture-averaged**.
4 Select the **Calculate thermodynamic properties** check box.
5 Clear the **Migration in electric field** check box.
6 Select the **Convection** check box.

Convection and Diffusion

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **Convection and Diffusion**.
2 In the **Settings** window for **Convection and Diffusion**, locate the **Model Inputs** section.
3 From the $\mathbf{u}$ list, choose **Velocity field (spf)**.
4 From the T list, choose **Temperature (ht)**.
5 From the p_A list, choose **Absolute pressure (spf)**.

LAMINAR FLOW (SPF)

On the **Physics** toolbar, click **Heavy Species Transport (hs)** and choose **Laminar Flow (spf)**.

Since the density variation is not small, the flow cannot be regarded as incompressible. Therefore set the flow to be compressible.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.
2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.
3 From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Define the pressure reference level in the interface properties.

4 Find the **Reference values** subsection. In the p_{ref} text field, type `13.3`.
5 In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.
6 In the **Model Builder** window's toolbar, click the **Show** button and select **Stabilization** in the menu.
7 In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.

8 Click to expand the **Consistent stabilization** section. Locate the **Consistent Stabilization** section. Find the **Navier-Stokes equations** subsection. Clear the **Crosswind diffusion** check box.

9 Click to expand the **Discretization** section. From the **Discretization of fluids** list, choose **P2+P1**.

Fluid Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Laminar Flow (spf)** click **Fluid Properties 1**.

2 In the **Settings** window for **Fluid Properties**, locate the **Fluid Properties** section.

3 From the ρ list, choose **Density (hs/cdm1)**.

4 From the μ list, choose **Dynamic viscosity (hs/cdm1)**.

5 In the **Model Builder** window, click **Laminar Flow (spf)**.

Inlet 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

4 From the list, choose **Mass flow**.

5 Locate the **Mass Flow** section. From the **Mass flow type** list, choose **Pointwise mass flux**.

6 From the M_f list, choose **Inward mass flux (hs)**.

Reaction forces must apply to the velocities only in order to avoid undesired couplings to the surface reactions, so use a unidirectional constraint.

7 Click to expand the **Constraint settings** section. Locate the **Constraint Settings** section. From the **Apply reaction terms on** list, choose **Individual dependent variables**.

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (ht)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Model Input** section.

3 From the p_A list, choose **Absolute pressure (spf)**.

4 From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

5 Locate the **Heat Conduction, Fluid** section. From the k list, choose **Thermal conductivity (hs/cdm1)**.

6 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Ideal gas**.

7 From the **Gas constant type** list, choose **Mean molar mass**.

8 From the M_n list, choose **Mean molar mass (hs/cdm1)**.

9 From the C_p list, choose **Mass-averaged mixture specific heat (hs/cdm1)**.

10 In the **Model Builder** window, click **Heat Transfer in Fluids (ht)**.

Temperature 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 In the **Settings** window for **Temperature**, locate the **Temperature** section.

3 In the T_0 text field, type `300`.

4 Select Boundaries 1, 3, and 6 only.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (ht)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, type `300` in the T text field.

Boundary Heat Source 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Boundary Heat Source**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Boundary Heat Source**, locate the **Boundary Heat Source** section.

4 From the Q_b list, choose **Total surface heat source of reaction (hs)**.

MESH 1

Size 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Points 3 and 4 only.

5 Locate the **Element Size** section. From the **Predefined** list, choose **Extremely fine**.

6 Click the **Custom** button.

7 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

8 In the associated text field, type `0.0002`.

Edge 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **More Operations>Edge**.

2 Select Boundary 4 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely fine**.

Free Triangular 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

Add a new study to perform the space dependent simulations.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies**.

4 In the **Select Study** tree, select **Preset Studies>Time Dependent**.

5 Click **Add Study** in the window toolbar.

STUDY 2

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 In the **Times** text field, type `range(0,5,300)`.

3 In the **Model Builder** window, click **Study 2**.

4 In the **Settings** window for **Study**, type `Space dependent model` in the **Label** text field.

Solution 2 (sol2)

On the **Study** toolbar, click **Show Default Solver**.

SPACE DEPENDENT MODEL

Solution 2 (sol2)

1 In the **Model Builder** window, expand the **Solution 2 (sol2)** node.

2 In the **Model Builder** window, under **Space dependent model>Solver Configurations> Solution 2 (sol2)** click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Absolute tolerance** section.

4 Locate the **Absolute Tolerance** section. From the **Global method** list, choose **Unscaled**.

5 Click to expand the **Time stepping** section. Locate the **Time Stepping** section. In the **Initial step** text field, type `0.001`.

6 Click **Compute**.

RESULTS

Velocity (spf)

1 In the **Model Builder** window, under **Results** click **Velocity (spf)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **5**.

Surface

1 In the **Model Builder** window, expand the **Velocity (spf)** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `v`.

4 On the **Velocity (spf)** toolbar, click **Plot**.

Temperature (ht)

1 In the **Model Builder** window, under **Results** click **Temperature (ht)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **5**.

Surface

1 In the **Model Builder** window, expand the **Temperature (ht)** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `T-300[K]`.

4 On the **Temperature (ht)** toolbar, click **Plot**.

2D Plot Group 10

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Diffusion Velocity, Hydrogen` in the **Label** text field.

3 Locate the **Data** section. From the **Time (s)** list, choose **5**.

4 From the **Data set** list, choose **Space dependent model/Solution 2 (sol2)**.

Surface 1

1 Right-click **Diffusion Velocity, Hydrogen** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `hs.Vdy_wH2`.

4 On the **Diffusion Velocity, Hydrogen** toolbar, click **Plot**.

Plot the global model and space dependent simulation together.

Average Pressure Divided by Average Initial Pressure

1 In the **Model Builder** window, under **Results** click **Average Pressure Divided by Average Initial Pressure**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section. Select the **y-axis label** check box.

5 In the associated text field, type `Average pressure divided by average initial pressure`.

Global 2

1 Right-click **Results>Average Pressure Divided by Average Initial Pressure** and choose **Global**.

2 In the **Settings** window for **Global**, type `Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Space dependent model/ Solution 2 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`intop1(spf.pA)/at(0,intop1(spf.pA))`	1	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Space dependent model`

7 On the **Average Pressure Divided by Average Initial Pressure** toolbar, click **Plot**.

Density ratio

1 In the **Model Builder** window, under **Results** click **Density ratio**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section. Select the **y-axis label** check box.

5 In the associated text field, type `Initial mass divided by the mass in the reactor`.

Global 2

1 Right-click **Results>Density ratio** and choose **Global**.

2 In the **Settings** window for **Global**, type `Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Space dependent model/ Solution 2 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`at(0,intop1(hs.rho))/intop1(hs.rho)`	1	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Space dependent model`

7 On the **Density ratio** toolbar, click **Plot**.

Total Reactor Mass

1 In the **Model Builder** window, under **Results** click **Total Reactor Mass**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section. Select the **y-axis label** check box.

5 In the associated text field, type `Mass density (kg/m)`.

Global 2

1 Right-click **Results>Total Reactor Mass** and choose **Global**.

2 In the **Settings** window for **Global**, type `Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Space dependent model/ Solution 2 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
mass_domain	kg/m	Mass change in the domain
mass_surf+mass_bulk	kg/m	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
mass_domain: Space dependent model
mass_surf+mass_bulk: Space dependent model

7 On the **Total Reactor Mass** toolbar, click **Plot**.

Data Sets

Plot the Si growth height computed with the space dependent model.

Edge 2D 2

1 On the **Results** toolbar, click **More Data Sets** and choose **Edge 2D**.

2 In the **Settings** window for **Edge 2D**, locate the **Data** section.

3 From the **Data set** list, choose **Space dependent model/Solution 2 (sol2)**.

4 Select Boundary 4 only.

Parametric Extrusion 1D 2

1 On the **Results** toolbar, click **More Data Sets** and choose **Parametric Extrusion 1D**.

2 In the **Settings** window for **Parametric Extrusion 1D**, locate the **Data** section.

3 From the **Data set** list, choose **Edge 2D 2**.

Parametric Extrusion 1D 1 - Global model 1

1 In the **Model Builder** window, under **Results** right-click **Parametric Extrusion 1D 1 - Global model** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Parametric Extrusion 1D 1 - Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Parametric Extrusion 1D 2**.

4 On the **Parametric Extrusion 1D 1 - Space dependent model** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

Thermal Plasma

Introduction

Low pressure discharges are characterized by the fact that the electron temperature is much higher than the neutral gas temperature. As the gas pressure increases, the number of collisions between the electrons and neutrals increases. At high enough pressures the electron temperature becomes equal to the gas temperature. At this point the plasma is in local thermodynamic equilibrium and a much simpler MHD model can be used to model the plasma.

This model simulates a plasma at medium pressure (2 torr) where the gas temperature cannot be assumed to be constant but the plasma is still not in local thermodynamic equilibrium. In Figure 1 the electron (blue) and gas (black) temperatures are plotted as a function of pressure. At low pressures the two temperatures are decoupled but as the pressure increases the temperatures tend towards the same limit. There are no axes on the plot since the exact temperature and pressure depends strongly on the gas in question.

Molecular gases tend to heat more easily than atomic gases for to the following reasons:

- Continual dissociation and recombination of the molecule. An electron impact reaction may dissociate a molecule into its atomic components. The energy lost by the electron when this reaction occurs is given back to the gas in the form of thermal energy during recombination.
- Vibrational excitation and relaxation. The threshold energy for vibrational excitation is much smaller than the threshold energy for dissociation. The continuous vibrational excitation and relaxation of the molecules can cause the gas temperature to increase.

Note: This application requires the Plasma Module and AC/DC Module.

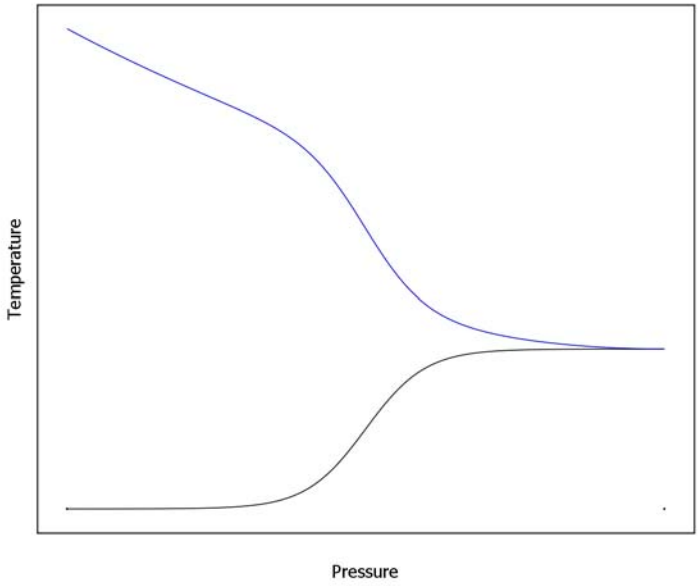

Figure 1: Plot of electron (blue) and gas (black) temperature v.s. pressure. At higher pressures the two temperatures become equal.

Model Definition

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the *Plasma Module User's Guide*.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\boldsymbol{\mu}_e \bullet \mathbf{E}) - \mathbf{D}_e \bullet \nabla n_e] = R_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot [-n_\varepsilon(\boldsymbol{\mu}_\varepsilon \bullet \mathbf{E}) - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon] + \mathbf{E} \cdot \boldsymbol{\Gamma}_e = R_\varepsilon$$

The electron source R_e and the energy loss due to inelastic collisions R_ε are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are M reactions that contribute to the growth or decay of electron density and P inelastic electron-neutral collisions. In general, $P >> M$. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (SI unit: m^3/s), and N_n is the total neutral number density (SI unit: $1/\mathrm{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon$$

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\mathrm{C}^{1/2}/\mathrm{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see Theory for the Heavy Species Transport Interface in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

For detailed information about electrostatics see Theory for the Electrostatics Interface in the *Plasma Module User's Guide*.

PLASMA CHEMISTRY

Argon is one of the simplest mechanisms to implement at low pressures. The electronically excited states can be lumped into a single species which results in a chemical mechanism consisting of only 3 species and 7 reactions:

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	-

Stepwise ionization (reaction 5) can play an important role in sustaining low pressure argon discharges. Excited argon atoms are consumed via superelastic collisions with electrons, quenching with neutral argon atoms, ionization or Penning ionization where two metastable argon atoms react to form a neutral argon atom, an argon ion and an electron. Reaction number 1, elastic collisions with electrons is primarily responsible for heating of the gas. In addition to volumetric reactions, the following surface reactions are implemented:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When a metastable argon atom makes contact with the wall, it reverts to the ground state argon atom with some probability (the sticking coefficient).

ELECTRICAL EXCITATION

The reactor geometry is simply a cylindrical glass tube with a 4 turn coil wrapped around it. Gas flows in from the bottom and exits out of the top. The gas is heated through elastic and inelastic collisions. The inelastic collisions are responsible for the bulk of the gas heating. A fixed power of 700 W is applied to the coil.

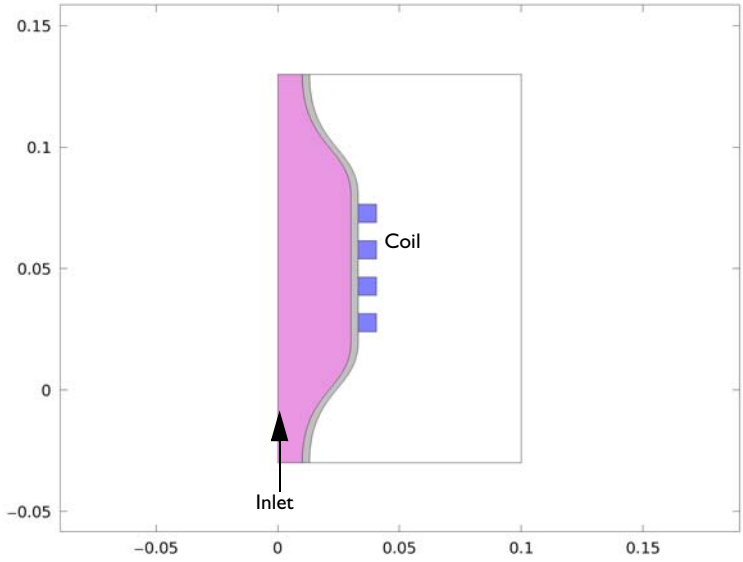

Figure 2: Schematic of the ICP reactor. Flow enters from the base and leaves out the top.

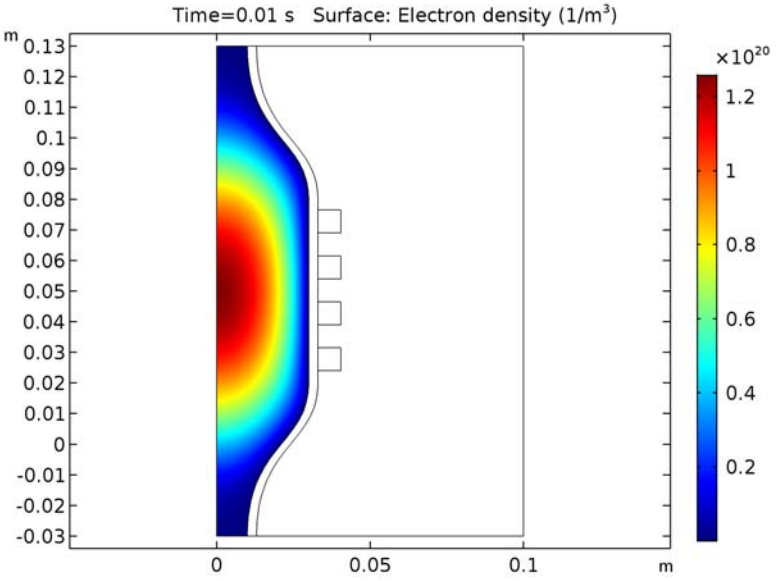

Figure 3: Surface plot of electron density inside the column.

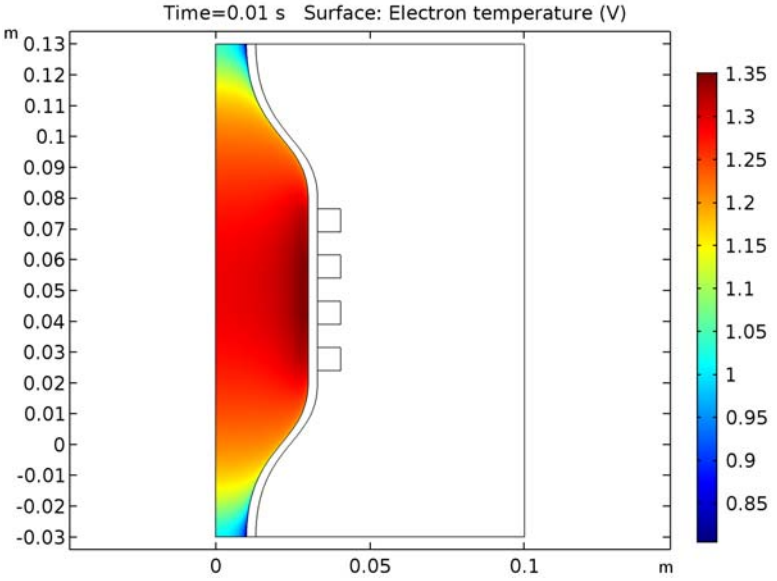

Figure 4: Plot of the electron temperature inside the plasma source.

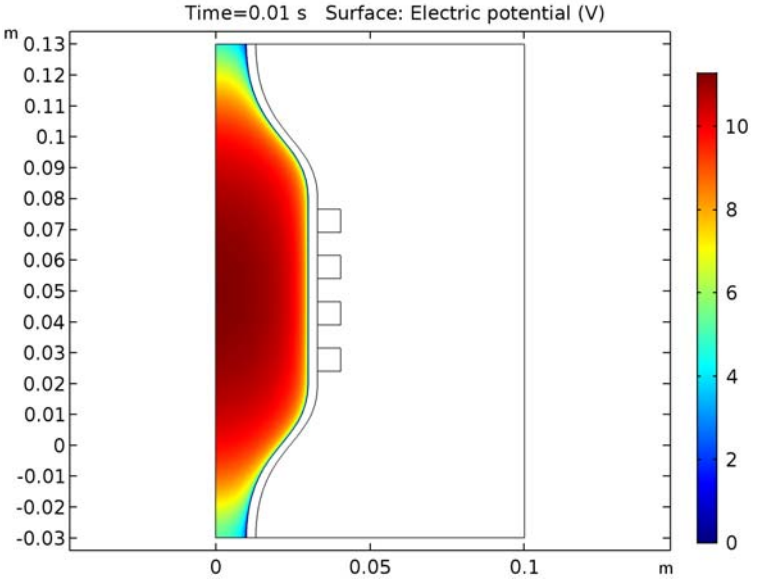

Figure 5: Plot of the plasma potential inside the plasma source.

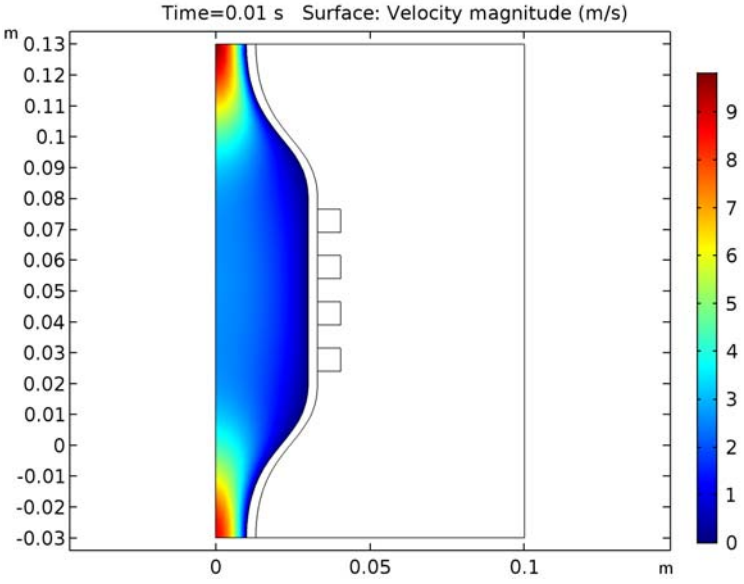

Figure 6: Plot of the velocity field.

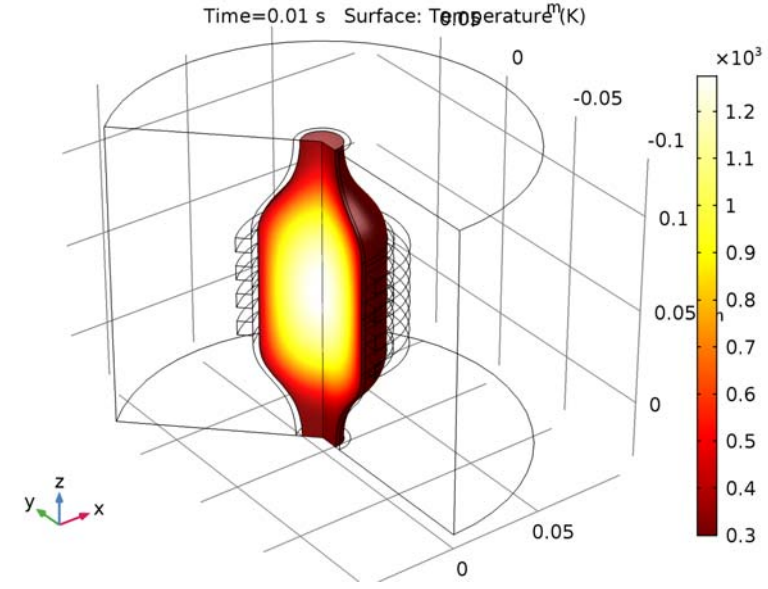

Figure 7: Revolved plot of the temperature inside the plasma source.

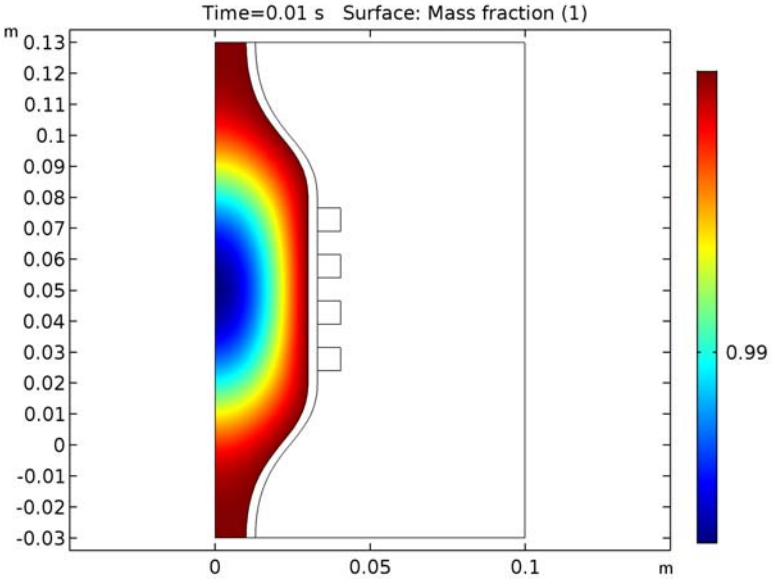

Figure 8: Plot of the mass fraction of ground state argon.

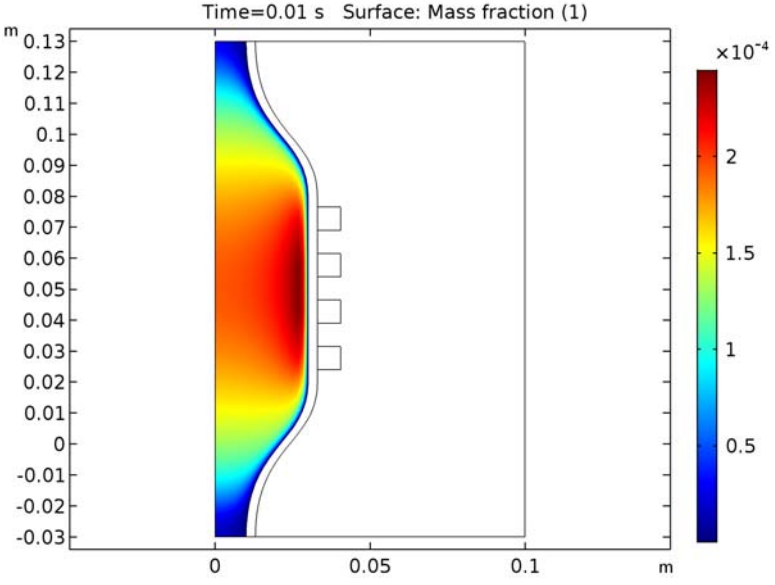

Figure 9: Plot of the mass fraction of electronically excited argon atoms.

Reference

1. M.A. Lieberman and A.J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, John Wiley & Sons, 2005.

Application Library path: `Plasma_Module/Inductively_Coupled_Plasmas/thermal_plasma`

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 **2D Axisymmetric**.
2. In the **Select Physics** tree, select **Plasma>Inductively Coupled Plasma**.
3. Click **Add**.
4. In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.
5. Click **Add**.
6. In the **Select Physics** tree, select **Heat Transfer>Heat Transfer in Fluids (ht)**.
7. Click **Add**.
8. Click **Study**.
9. In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Frequency-Transient**.
10. Click **Done**.
11. In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.
12. In the **Model Builder** window's toolbar, click the **Show** button and select **Stabilization** in the menu.

GEOMETRY 1

Import 1 (imp1)

1 On the **Home** toolbar, click **Import**.

2 In the **Settings** window for **Import**, locate the **Import** section.

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `thermal_plasma.mphbin`.

5 Click **Import**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
p0	1[torr]	133.3 Pa	Initial and outlet pressure

DEFINITIONS

Explicit 1

1 On the **Definitions** toolbar, click **Explicit**.

2 Select Domain 1 only.

3 Right-click **Explicit 1** and choose **Rename**.

4 In the **Rename Explicit** dialog box, type `Plasma` in the **New label** text field.

5 Click **OK**.

Explicit 2

1 On the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 9, 10, 34, and 35 only.

5 Right-click **Explicit 2** and choose **Rename**.

6 In the **Rename Explicit** dialog box, type `Walls` in the **New label** text field.

7 Click **OK**.

Explicit 3

1 On the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

5 Right-click **Explicit 3** and choose **Rename**.

6 In the **Rename Explicit** dialog box, type `Outlet` in the **New label** text field.

7 Click **OK**.

Explicit 4

1 On the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 12, 13, 15–17, 19, 21, 22, 24–26, and 28–32 only.

5 Right-click **Explicit 4** and choose **Rename**.

6 In the **Rename Explicit** dialog box, type `Coil Walls` in the **New label** text field.

7 Click **OK**.

Start by importing the cross sections for argon and by activating the convection and thermodynamic property evaluation.

PLASMA (PLAS)

1 In the **Settings** window for **Plasma**, locate the **Domain Selection** section.

2 From the **Selection** list, choose **Plasma**.

3 In the **Model Builder** window, expand the **Plasma (plas)** node.

Cross Section Import 1

1 Right-click **Component 1 (comp1)>Plasma (plas)** 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`.

5 In the **Model Builder** window, click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Transport Settings** section.

7 Select the **Convection** check box.

8 Select the **Calculate thermodynamic properties** check box.

9 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** check box.

Reaction 1

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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 `3.734E8`.

Reaction 2

1 Right-click **Plasma (plas)** and choose the domain setting **Heavy Species Transport> 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`.

Ground 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Electrostatics>Ground**.

2 In the **Settings** window for **Ground**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Walls**.

Surface Reaction 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Walls**.

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ar+=>Ar`.

Surface Reaction 2

1 Right-click **Plasma (plas)** and choose the boundary condition **Heavy Species Transport> Surface Reaction**.

2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Walls**.

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ars=>Ar`.

Wall 1

1 Right-click **Plasma (plas)** and choose the boundary condition **Drift Diffusion>Wall**.

2 In the **Settings** window for **Wall**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Walls**.

Outflow 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** right-click **Species: Ars** and choose **Outflow**.

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

Outflow 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** right-click **Species: Ar+** and choose **Outflow**.

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

Species: Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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, under **Component 1 (comp1)>Plasma (plas)** click **Species: Ars**.

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the x_0 text field, type `1E-4`.

4 From the **Preset species data** list, choose **Ar**.

5 Click to expand the **Species thermodynamic parameters** section. Locate the **Species Thermodynamic Parameters** section. In the Δh text field, type `11.5`.

The thermodynamic properties for the electronically excited Argon atoms can be the same as for the ground state species plus the threshold energy for the electron impact reaction. In this case this corresponds to an energy of 11.5eV. This is added in the text field **Additional enthalpy contribution**.

Species: Ar+

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** 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 **Species thermodynamic parameters** section. Locate the **Species Thermodynamic Parameters** section. In the Δh text field, type `15.8`.

The thermodynamic properties for the Argon ions can be the same as for the ground state species plus the threshold energy for ionization. In this case this corresponds to an energy of 15.8eV. This is added in the text field **Additional enthalpy contribution**.

You can set the gas temperature and pressure in the plasma model to the computed gas pressure and temperature from other physics interfaces. The velocity field is also set to the velocity field computed from the **Laminar Flow** interface.

Plasma Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Plasma Model 1**.

2 In the **Settings** window for **Plasma Model**, locate the **Model Inputs** section.

3 From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

4 From the T list, choose **Temperature (ht)**.

5 From the p_A list, choose **Absolute pressure (spf)**.

6 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `4E24`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,\,0}$ text field, type `1E15`.

4 In the ε_0 text field, type `3`.

MAGNETIC FIELDS (MF)

On the **Physics** toolbar, click **Plasma (plas)** and choose **Magnetic Fields (mf)**.

Coil 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Magnetic Fields (mf)** and choose the domain setting **Coil**.

2 Select Domains 4–7 only.

3 In the **Settings** window for **Coil**, locate the **Coil** section.

4 From the **Coil excitation** list, choose **Power**.

5 Select the **Coil group** check box.

6 In the P_{coil} text field, type `700[W]`.

LAMINAR FLOW (SPF)

Since the density variation is not small, the flow cannot be regarded as incompressible. Therefore set the flow to be weakly compressible.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.

3 From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

4 Click to expand the **Consistent stabilization** section. Locate the **Consistent Stabilization** section. Find the **Navier-Stokes equations** subsection. Clear the **Crosswind diffusion** check box.

Define the pressure reference level to be zero. This means that absolute pressure values are used throughout the model.

5 Locate the **Physical Model** section. Find the **Reference values** subsection. In the p_{ref} text field, type `0`.

6 In the **Model Builder** window, click **Laminar Flow (spf)**.

7 In the **Settings** window for **Laminar Flow**, click to expand the **Consistent stabilization** section.

8 Locate the **Consistent Stabilization** section. Find the **Navier-Stokes equations** subsection. Clear the **Crosswind diffusion** check box.

9 Locate the **Domain Selection** section. Click **Clear Selection**.

10 Select Domain 1 only.

11 Click to expand the **Equation** section. From the **Equation form** list, choose **Stationary**.

Fluid Properties 1

1 In the **Model Builder** window, expand the **Laminar Flow (spf)** node, then click **Fluid Properties 1**.

2 In the **Settings** window for **Fluid Properties**, locate the **Fluid Properties** section.

3 From the ρ list, choose **Density (plas/pes1)**.

4 From the μ list, choose **Dynamic viscosity (plas/pes1)**.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Laminar Flow (spf)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the p text field, type `p0`.

Inlet 1

1 In the **Model Builder** window, right-click **Laminar Flow (spf)** and choose **Inlet**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

4 From the list, choose **Mass flow**.

5 Locate the **Mass Flow** section. From the **Mass flow type** list, choose **Standard flow rate (SCCM)**.

6 From the M_n list, choose **Mean molar mass (plas/pes1)**.

7 In the Q_{sccm} text field, type `100*tanh(1E5*t[1/s])`.

Outlet 1

1 Right-click **Laminar Flow (spf)** and choose **Outlet**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.

4 In the p_0 text field, type `p0`.

HEAT TRANSFER IN FLUIDS (HT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heat Transfer in Fluids (ht)**.

2 In the **Settings** window for **Heat Transfer in Fluids**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domain 1 only.

5 Click to expand the **Equation** section. From the **Equation form** list, choose **Time dependent**.

Fluid 1

1 In the **Model Builder** window, expand the **Heat Transfer in Fluids (ht)** node, then click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Model Input** section.

3 From the p_A list, choose **Absolute pressure (spf)**.

4 From the **u** list, choose **Velocity field (spf)**.

5 Locate the **Heat Conduction, Fluid** section. From the k list, choose **Thermal conductivity (plas/pes1)**.

6 Locate the **Thermodynamics, Fluid** section. From the ρ list, choose **Density (plas/pes1)**.

7 From the C_p list, choose **Mass-averaged mixture specific heat (plas/pes1)**.

8 From the γ list, choose **User defined**.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (ht)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, type 300 in the T text field.

Heat Source 1

1 In the **Model Builder** window, right-click **Heat Transfer in Fluids (ht)** and choose **Heat Source**.

2 Select Domain 1 only.

3 In the **Settings** window for **Heat Source**, locate the **Heat Source** section.

4 From the Q_0 list, choose **Heat source for gas (plas/pes1)**.

Temperature 1

1 Right-click **Heat Transfer in Fluids (ht)** and choose **Temperature**.

2 Select Boundaries 2, 9, 10, 34, and 35 only.

3 In the **Settings** window for **Temperature**, locate the **Temperature** section.

4 In the T_0 text field, type 300.

Outflow 1

1 Right-click **Heat Transfer in Fluids (ht)** and choose **Outflow**.

2 Select Boundary 4 only.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 Select Domain 2 only.

3 In the **Settings** window for **Material**, locate the **Material Contents** section.

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	1	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	4.5	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 1 (mat1)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Dielectric` in the **New label** text field.

7 Click **OK**.

Material 2 (mat2)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 Select Domain 3 only.

3 In the **Settings** window for **Material**, locate the **Material Contents** section.

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Relative permeability	mur	1	1	Basic
Electrical conductivity	sigma	0	S/m	Basic
Relative permittivity	epsilonr	1	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 2 (mat2)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Air` in the **New label** text field.

7 Click **OK**.

Material 3 (mat3)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 Select Domains 4–7 only.

3 In the **Settings** window for **Material**, locate the **Material Contents** section.

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Electrical conductivity	sigma	6E7	S/m	Basic
Relative permeability	mur	1	1	Basic
Relative permittivity	epsilonr	1	1	Basic

5 Right-click **Component 1 (comp1)>Materials>Material 3 (mat3)** and choose **Rename**.

6 In the **Rename Material** dialog box, type `Copper coil` in the **New label** text field.

7 Click **OK**.

A boundary layer mesh is used on the reactor walls so that the region of space charge separation between the ions and electrons can be resolved.

MESH 1

1 In the **Settings** window for **Mesh**, locate the **Mesh Settings** section.

2 From the **Element size** list, choose **Extra fine**.

Edge 1

1 Right-click **Component 1 (comp1)>Mesh 1** and choose **More Operations>Edge**.

2 Select Boundary 2 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>Edge 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely 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 In the associated text field, type `0.001`.

Free Triangular 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 1 only.

Size 1

1 Right-click **Component 1 (comp1)>Mesh 1>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 **Model Builder** window, right-click **Mesh 1** and choose **Boundary Layers**.

2 In the **Settings** window for **Boundary Layers**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 1 only.

Boundary Layer Properties

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1>Boundary Layers 1** click **Boundary Layer Properties**.

2 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Walls**.

4 Locate the **Boundary Layer Properties** section. In the **Number of boundary layers** text field, type `5`.

5 In the **Boundary layer stretching factor** text field, type `1.5`.

Mapped 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Mapped**.

2 In the **Settings** window for **Mapped**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domains 4–7 only.

Distribution 1

1 Right-click **Component 1 (comp1)>Mesh 1>Mapped 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Coil Walls**.

4 Locate the **Distribution** section. From the **Distribution properties** list, choose **Predefined distribution type**.

5 In the **Number of elements** text field, type `35`.

6 In the **Element ratio** text field, type `8`.

7 From the **Distribution method** list, choose **Geometric sequence**.

8 Select the **Symmetric distribution** check box.

Free Triangular 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

STUDY 1

Step 1: Frequency-Transient

1 In the **Settings** window for **Frequency-Transient**, locate the **Study Settings** section.

2 In the **Times** text field, type `0`.

3 Click **Range**.

4 In the **Range** dialog box, choose **Number of values** from the **Entry method** list.

5 In the **Start** text field, type `-8`.

6 In the **Stop** text field, type `-2`.

7 In the **Number of values** text field, type `21`.

8 From the **Function to apply to all values** list, choose **exp10**.

9 Click **Add**.

10 In the **Settings** window for **Frequency-Transient**, locate the **Study Settings** section.

11 In the **Frequency** text field, type `13.56E6`.

12 On the **Home** toolbar, click **Compute**.

RESULTS

Electron Density (plas)

Click the **Zoom Extents** button on the **Graphics** toolbar.

2D Plot Group 11

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Argon Mass Fraction` in the **Label** text field.

Surface 1

1 Right-click **Argon Mass Fraction** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Mass fractions>plas.wAr - Mass fraction**.

3 On the **Argon Mass Fraction** toolbar, click **Plot**.

2D Plot Group 12

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Excited Argon Mass Fraction` in the **Label** text field.

Surface 1

1 Right-click **Excited Argon Mass Fraction** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1> Plasma (Heavy Species Transport)>Mass fractions>plas.wArs - Mass fraction**.

3 On the **Excited Argon Mass Fraction** toolbar, click **Plot**.