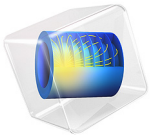

DC Glow Discharge, 1D

Introduction

DC glow discharges in the low pressure regime have long been used for gas lasers and fluorescent lamps. DC discharges are good 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):

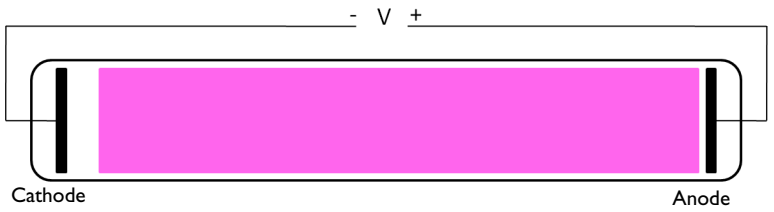

Figure 1: Schematic of the DC discharge. The voltage applied across the electrodes leads to formation of a plasma.

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*.

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

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

where:

$$\Gamma_e = -(\mu_e \bullet \mathbf{E})n_e - \mathbf{D}_e \bullet \nabla n_e$$

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:

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

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 nonelectron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the nonelectron 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 toward the wall:

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

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 (electrons impact cross sections are obtained from Ref. 2):

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 the density of the excited species are 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 because the diffusive loss of electrons to the outer walls and the accumulation of surface charge on the walls are not modeled.

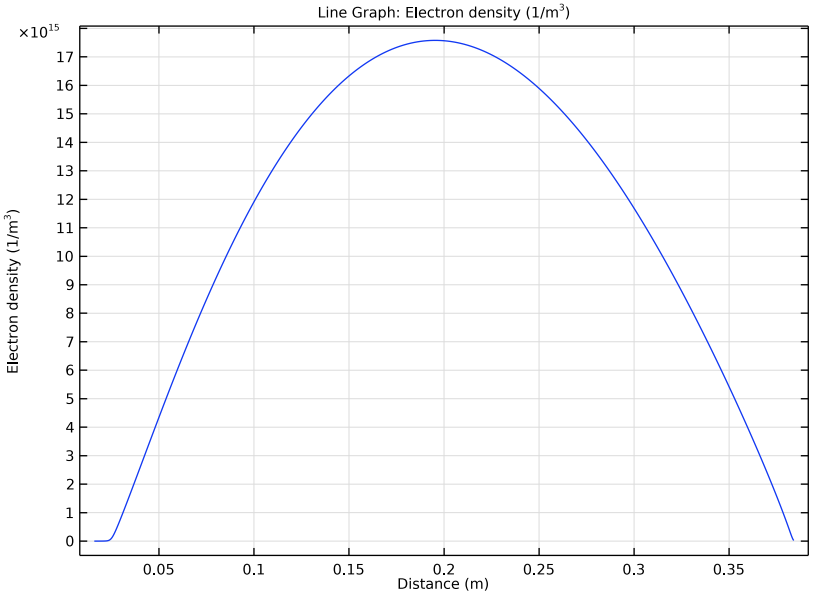

Figure 2: Electron density along the axial length of the positive column.

In Figure 3 the electric potential is plotted along the axial length of the column. Notice that the potential profile is significantly 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.

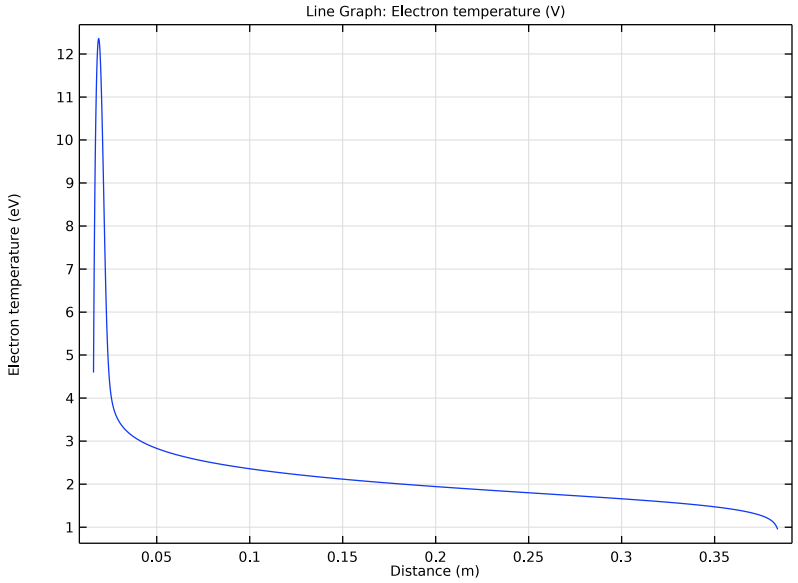

Figure 3: Electron temperature along the axial length of the positive column.

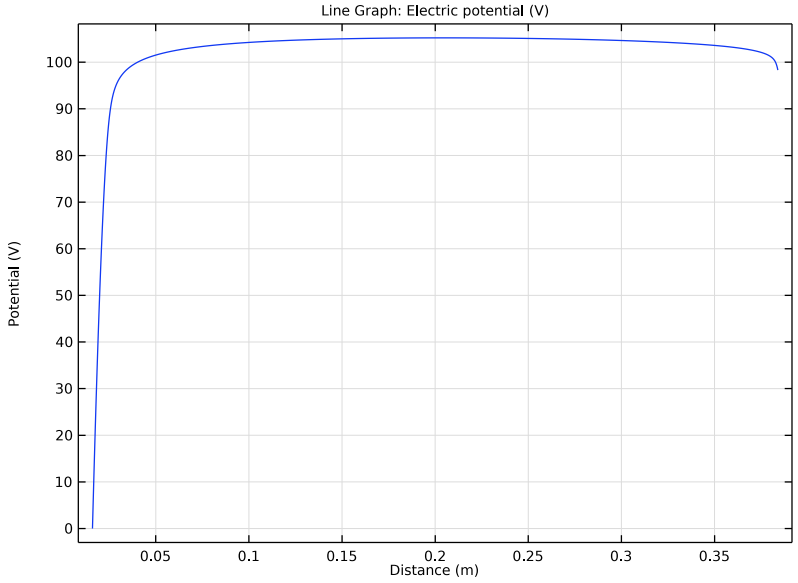

Figure 4: Potential along the axial length of the positive column.

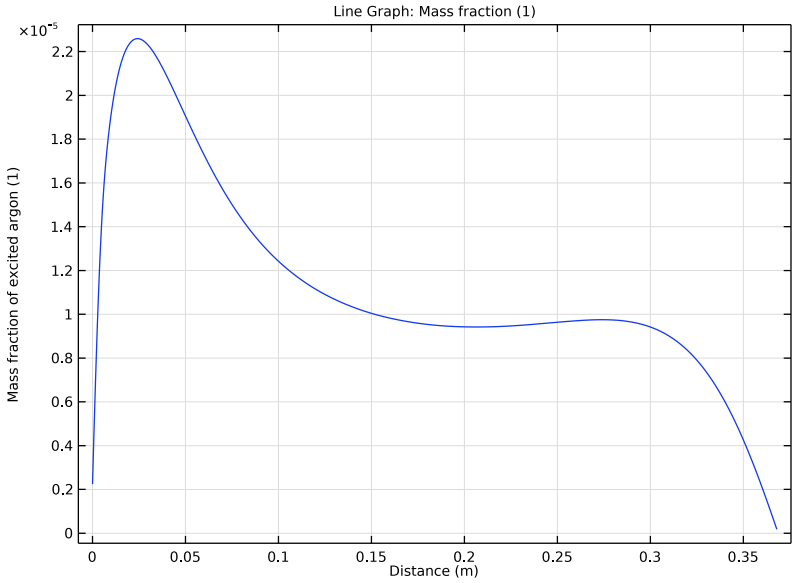

Figure 5: Mass fraction of excited argon atoms along the axial length of the positive column.

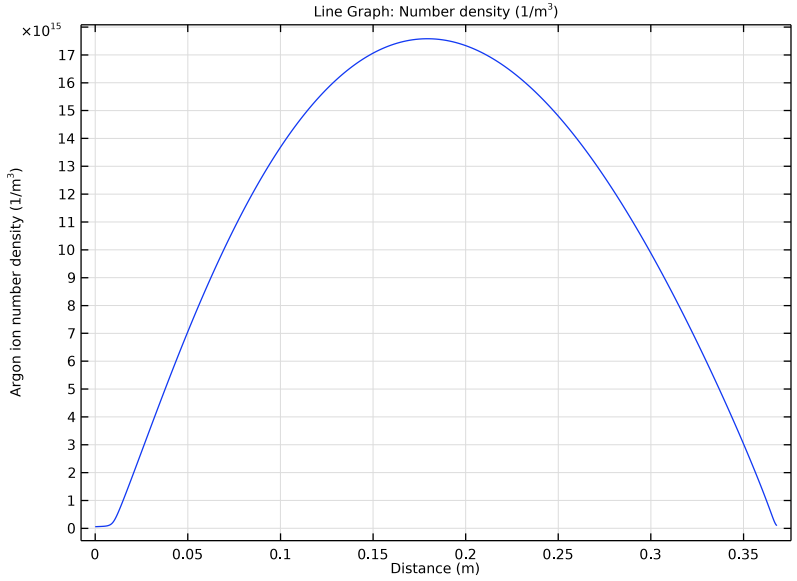

Figure 6: Number density of argon ions along the axial length of the positive column.

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 production of new electrons through electron impact ionization with the background gas.

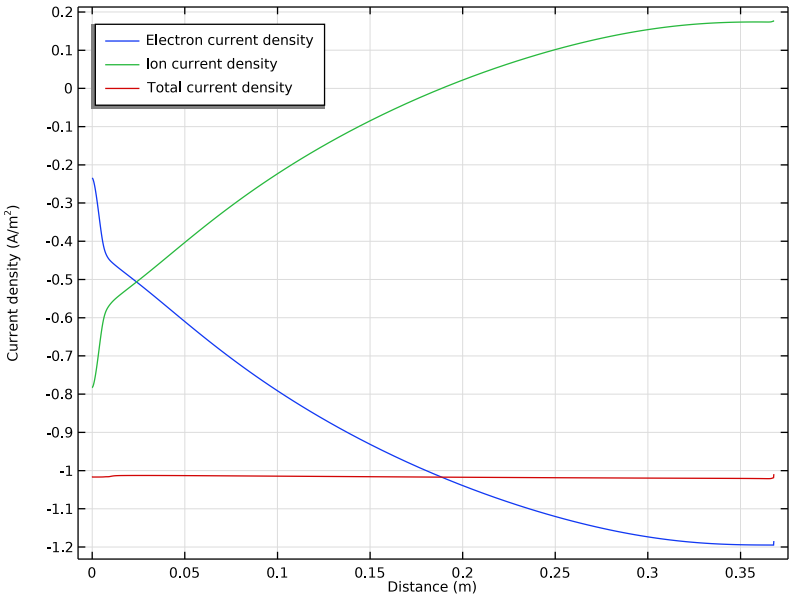

Figure 7: Electron current density (blue), ion current density (green), and total current density (red) along the axial length of the positive column.

References

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

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

Application Library path: `Plasma_Module/Direct_Current_Discharges/positive_column_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 **General Studies>Time Dependent**.

6 Click **Done**.

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

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

3 In the table, enter the following settings:

Coordinates (m)
0.016
0.384

DEFINITIONS

Variables 1

1 In 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	1E24[1/(m*V*s)]	1/(V·m·s)	Electron mobility
V0	200[V]	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 **Global>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 Click **Import**.

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

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

8 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.

9 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, 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, 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 Find the **Townsend coefficient data** subsection. 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, 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 Find the **Townsend coefficient data** subsection. 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 **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 In the **Physics** toolbar, click **Domains** and choose **Reaction**.

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

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

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

Species: Ar

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

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

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

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

When solving a 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: Ars

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

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

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

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, 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 **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.

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

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

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

4 Select Boundary 2 only.

Surface Reaction 3

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

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

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

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

Wall 1

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

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

Ground 1

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

2 Select Boundary 1 only.

Metal Contact 1

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

5 Locate the **Circuit Settings** section. From the **Circuit type** list, choose **Ballast resistor**.

6 In the R_b text field, type `10000[ohm]`.

MESH 1

Edge 1

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

Distribution 1

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

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

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

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

5 In the **Element ratio** text field, type 50.

6 From the **Growth rate** list, choose **Exponential**.

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

8 Click **Build All**.

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 **Output 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 101.

9 From the **Function to apply to all values** list, choose **exp10(x)** – **Exponential function (base 10)**.

10 Click **Add**.

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

RESULTS

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 Locate the **Plot Settings** section.

4 Select the **x-axis label** check box. In the associated text field, type Distance (m).

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

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

Electron Temperature (plas)

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

5 Select the **x-axis label** check box. In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box. In the associated text field, type `Electron temperature (eV)`.

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

Electric Potential (plas)

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

5 Select the **x-axis label** check box. In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box. In the associated text field, type `Potential (V)`.

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

Excited Argon Mass Fraction

1 In 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.

5 Select the **x-axis label** check box. In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box. 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 Select Domain 1 only.

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 (comp1)>Plasma> Mass fractions>plas.wArs - Mass fraction - 1**.

4 In the **Excited Argon Mass Fraction** toolbar, click **Plot**.

Argon Ion Number Density

1 In 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.

5 Select the **x-axis label** check box. In the associated text field, type `Distance (m)`.

6 Select the **y-axis label** check box. 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 Select Domain 1 only.

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 (comp1)>Plasma> Number densities>plas.n_wAr_1p - Number density - 1/m³**.

4 In the **Argon Ion Number Density** toolbar, click **Plot**.

Current Density

1 In the **Model Builder** window, 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 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Line Graph 1

1 In the **Model Builder** window, expand the **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 (comp1)>Plasma> Current>Electron current density - A/m²>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 In 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 (comp1)>Plasma> Species>Species wAr_1p>Ion current density - A/m²>plas.Jix_wAr_1p - Ion current density, x-component**.

3 In 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 In the **Current Density** toolbar, click **Plot**.