

Benchmark Model of a Capacitively Coupled Plasma

The underlying physics of a capacitively coupled plasma is rather complicated, even for rather simple geometric configurations and plasma chemistries. This model benchmarks the Plasma, Time Periodic 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 driftdiffusion equations for the electron density and mean electron energy. For detailed information on electron transport, see Theory for the Drift Diffusion Interface in the Plasma Module User's Guide.

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

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

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:

$$\mathbf{D}_{e} = \mu_{e} T_{e}, \mu_{\varepsilon} = \left(\frac{5}{3}\right) \mu_{e}, \mathbf{D}_{\varepsilon} = \mu_{\varepsilon} T_{e}$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. 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_i is the mole fraction of the target species for reaction j, k_i 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: m²), and f is the electron energy distribution function. In this case, a Maxwellian EEDF is assumed.

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*.

In Ref. 1 the ion diffusivity is defined as:

$$D = 0.10901(a\lambda^3)^{\frac{1}{2}}$$

and the mobility, µ as:

$$\mu E = 0.79788(\alpha\lambda)^{\frac{1}{2}}$$

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 that, go to the **Mobility Specification** and choose the High field ion mobility model with a Cross section σ equal to $3.10^{-19}~\text{m}^2$ 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

$$\mathbf{n} \cdot \Gamma_e = \left(\frac{1-r}{1+r}\right) \left(\frac{1}{2} \mathbf{v}_{e, \, \text{th}} n_e\right) \tag{1}$$

and the electron energy flux

$$\mathbf{n} \cdot \Gamma_{\varepsilon} = \left(\frac{1-r}{1+r}\right) \left(\frac{5}{6} \mathbf{v}_{e, \, \text{th}} n_{\varepsilon}\right) \tag{2}$$

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_n 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 toward the wall:

$$\mathbf{n}\cdot\mathbf{j}_k=M_wc_kZ\mu_k(\mathbf{E}\cdot\mathbf{n})[Z_k\mu_k(\mathbf{E}\cdot\mathbf{n})>0]$$

PLASMA CHEMISTRY

The reference paper suggests a simplistic plasma chemistry for helium consisting of only 3 reactions and 4 species (electron impact cross-sections are obtained from Ref. 2):

TABLE I: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	ТҮРЕ	$\Delta\epsilon(eV)$
I	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 $0.2~\text{A/m}^2$. At lower pressures the ion current density profile is more smooth across the gap. At 300 mtorr 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.

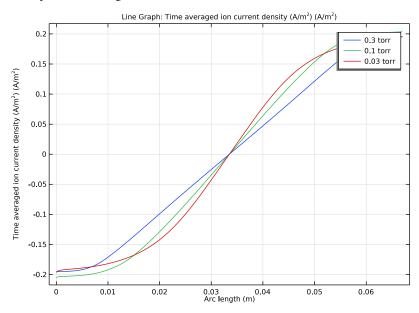


Figure 1: Plot of the period averaged ion current as a function of the distance from the left electrode.

The period averaged excitation and ionization rates are plotted in Figure 2 and Figure 3.

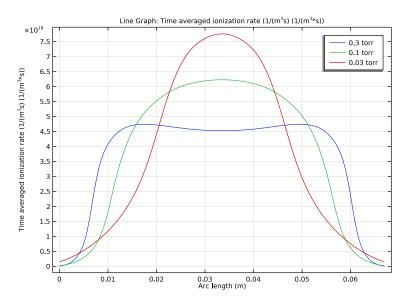


Figure 2: Plot of the period averaged ionization rate as a function of the distance from the left electrode.

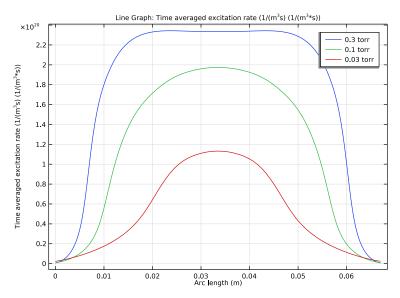


Figure 3: Plot of the period averaged excitation rate as a function of the distance from the left electrode.

The results for the ionization and excitation rates agree well with Ref. 1 in both absolute value and spatial distribution. The period averaged electron power deposition is plotted in Figure 4. The COMSOL results are again, in good agreement with the reference paper.

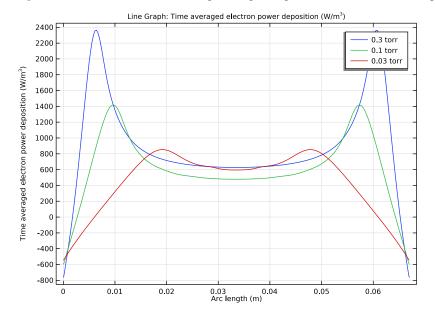


Figure 4: Plot of the period averaged electron power deposition as a function of the distance from the left electrode.

Figure 5 and Figure 6 plot the period 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 toward the wall via the plasma potential.

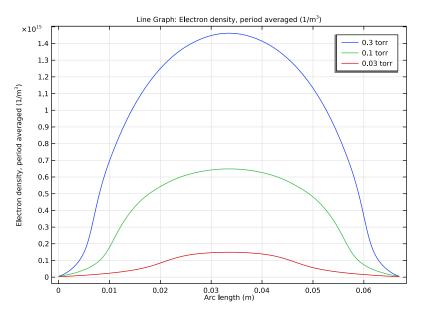


Figure 5: Plot of the period averaged electron density at different operating pressures.

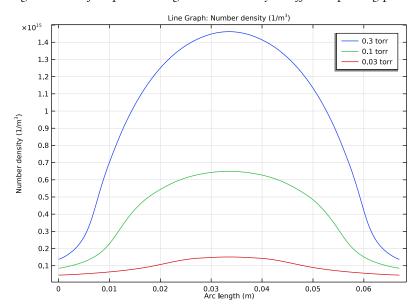


Figure 6: Plot of the period averaged ion density for different operating pressures.

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)	$V_{rf}(V)$	$n_e(\text{cm}^{-3})$	ε(eV)	$P_{\text{tot}}(\text{mWcm}^2)$	$j_{\text{pos}}(\text{mAcm}^{-2})$	$I_{rf}(\text{mAcm}^{-2})$
30	364.8	1.50×10 ⁸	13.5	2.96	0.0196	0.97
100	196.9	6.57×10 ⁸	7.05	4.17	0.0205	0.99
300	128.8	1.47×10 ⁹	5.08	6.02	0.0196	0.99

Reference

- 1. M. Surendra, "Radiofrequency discharge benchmark model comparison," *Plasma Sources Sci. Technol.*, vol. 4, pp 56–73, 1995.
- 2. Phelps database, www.lxcat.net, retrieved 2017.

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

- I In the Model Wizard window, click ID.
- 2 In the Select Physics tree, select Plasma>Plasma, Time Periodic (ptp).
- 3 Click Add.
- 4 Click Study.
- 5 In the Select Study tree, select Preset Studies for Selected Physics Interfaces> Time Periodic.
- 6 Click M Done.

Start by drawing the geometry, which is simply a line of length 0.067m.

GEOMETRY I

Interval I (iI)

- I In the Model Builder window, under Component I (compl) right-click Geometry I 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		
0.067		

Define a parameter for the pressure, which will be used when sweeping over pressure in the study.

4 Click Build All Objects.

GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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]	39.997 Pa	Pressure

Define an expression for the input power. The expression is designed to obtain the same current density of 1 mA/cm² for each value of pressure.

DEFINITIONS (COMPI)

Variables 1

- I In the Model Builder window, under Component I (compl) 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
Pin	if(p0==0.03[torr],11.6,9.4)		Input power

Turn off the source stabilization, since it is not needed in this example. Use the Fick's law diffusion model to be consistent with the reference.

PLASMA, TIME PERIODIC (PTP)

- I In the Model Builder window, under Component I (compl) click Plasma, Time Periodic (ptp).
- 2 In the Settings window for Plasma, Time Periodic, locate the Cross-Section Area section.
- 3 In the A text field, type $0.1[m^2]$.
- 4 Locate the Electron Energy Distribution Function Settings section. From the Electron energy distribution function list, choose Maxwellian.
- 5 Locate the Diffusion Model section. From the Diffusion model list, choose Fick's law.

Cross Section Import 1

- I In the Physics toolbar, click A 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 He xsecs.txt.
- 5 Click | Import.

Species: He

- I In the Model Builder window, 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. From the Preset species data list, choose He.

Species: Hes

- I In the Model Builder window, click Species: Hes.
- 2 In the Settings window for Species, locate the General Parameters section.
- 3 From the Preset species data list, choose He.
- **4** In the D_f text field, type 0.8[m²/s].

Load in a table for the helium reduced ion mobility as a function of the reduced electric field. This table corresponds to the high field limit described in the reference.

Species: He+

I In the Model Builder window, 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 Locate the Mobility and Diffusivity Expressions section. From the Specification list, choose Specify mobility, compute diffusivity.
- 6 From the lon temperature list, choose Use local field approximation.
- 7 Locate the Mobility Specification section. From the Specify using list, choose Lookup table.
- 8 From the Mobility a function of list, choose Reduced electric field.
- **9** Find the **Reduced ion mobility** subsection. Click **Load from File**.
- **10** Browse to the model's Application Libraries folder and double-click the file ccp benchmark He mobility.txt.

Surface Reaction 1

- I 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 He+=>He.
- 4 Locate the Boundary Selection section. From the Selection list, choose All boundaries.
- **5** Locate the **Reaction Parameters** section. In the γ_f text field, type **0**.
- **6** Locate the **Secondary Emission Parameters** section. In the γ_i text field, type 0.
- 7 In the ε_i text field, type 0.
- 2: He+=>He
- I Right-click I: He+=>He and choose **Duplicate**.
- 2 In the Settings window for Surface Reaction, locate the Reaction Formula section.
- 3 In the Formula text field, type Hes=>He.
- **4** Locate the **Reaction Parameters** section. In the γ_f text field, type 1.

Plasma Model I

- I In the Model Builder window, click Plasma Model I.
- 2 In the Settings window for Plasma Model, locate the Model Inputs section.
- **3** In the *T* text field, type 300[K].
- **4** In the p_A text field, type p0.
- 5 Locate the Electron Density and Energy section. From the Electron transport properties list, choose Specify mobility only.

6 In the μ_e text field, type 3.33e24[1/(V*m*s)]/ptp.Nn.

Wall I

- I In the Physics toolbar, click Boundaries and choose Wall.
- 2 In the Settings window for Wall, locate the Boundary Selection section.
- 3 From the Selection list, choose All boundaries.
- **4** Locate the **General Wall Settings** section. In the r_e text field, type 5/11.

Ground I

- I In the Physics toolbar, click Boundaries and choose Ground.
- 2 Select Boundary 1 only.

Metal Contact 1

- I In the Physics toolbar, click Boundaries and choose Metal Contact.
- 2 In the Settings window for Metal Contact, locate the Terminal section.
- 3 From the Source list, choose RF.
- **4** Select Boundary 2 only.
- **5** Locate the **RF Source** section. In the $P_{
 m rf}$ text field, type Pin.

MESH I

Edge 1

In the Mesh toolbar, click A Edge.

Distribution I

- I Right-click **Edge I** 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 150.
- 5 In the Element ratio text field, type 10.
- 6 From the Growth rate list, choose Exponential.
- 7 Select the Symmetric distribution check box.
- 8 Click III Build All.

STUDY I

Step 1: Time Periodic

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

- 2 In the Settings window for Time Periodic, click to expand the Study Extensions section.
- 3 Select the Auxiliary sweep check box.
- 4 Click + Add.
- **5** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
p0 (Pressure)	0.3 0.1 0.03	torr

- 6 In the Model Builder window, click Study 1.
- 7 In the Settings window for Study, locate the Study Settings section.
- **8** Clear the **Generate convergence plots** check box.
- **9** Clear the **Generate default plots** check box.
- 10 In the Home toolbar, click **Compute**.

RESULTS

Create some plots to compare with the reference.

ID Plot Group I

In the Home toolbar, click Add Plot Group and choose ID Plot Group.

We need to use a built in operator to average over the extra dimension. This allows us to plot period averaged quantities for any variable.

Line Graph 1

- I Right-click ID Plot Group I and choose Line Graph.
- 2 In the Settings window for Line Graph, locate the Selection section.
- 3 From the Selection list, choose All domains.
- 4 Locate the y-Axis Data section. In the Expression text field, type ptp.xdintop ptp1(ptp.Jix wHe 1p/ptp.xdim).
- 5 Click to expand the Quality section. From the Resolution list, choose No refinement.
- 6 Locate the y-Axis Data section.
- 7 Select the **Description** check box. In the associated text field, type Time averaged ion current density (A/m²).
- 8 Click to expand the Legends section. Select the Show legends check box.
- 9 In the ID Plot Group I toolbar, click on Plot.

Time Averaged Ion Current Density

- I In the Model Builder window, under Results click ID Plot Group I.
- 2 In the **Settings** window for **ID Plot Group**, type Time Averaged Ion Current Density in the **Label** text field.
- 4 Click the Zoom Extents button in the Graphics toolbar.

Time Averaged Ionization Rate

- I Right-click Time Averaged Ion Current Density and choose Duplicate.
- 2 In the Settings window for ID Plot Group, type Time Averaged Ionization Rate in the Label text field.

Line Graph I

- I In the Model Builder window, expand the 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 ptp.Re av.
- 4 In the **Description** text field, type Time averaged ionization rate (1/(m³s).
- 5 In the Time Averaged Ionization Rate toolbar, click **1** Plot.
- 6 Click the Zoom Extents button in the Graphics toolbar.

Time Averaged Excitation Rate

- I In the Model Builder window, right-click Time Averaged Ionization Rate and choose Duplicate.
- 2 In the Settings window for ID Plot Group, type Time Averaged Excitation Rate in the Label text field.

Line Graph 1

- I In the Model Builder window, expand the 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 ptp.xdintop_ptp1(ptp.R_wHes*N_A_const/ptp.xdim).
- **4** In the **Description** text field, type Time averaged excitation rate (1/(m³s).
- 5 In the Time Averaged Excitation Rate toolbar, click Plot.

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

Time Averaged Electron Power Deposition

- I In the Model Builder window, right-click Time Averaged Excitation Rate and choose Duplicate.
- 2 In the Settings window for ID Plot Group, type Time Averaged Electron Power Deposition in the Label text field.

Line Graph 1

- I In the Model Builder window, expand the Time Averaged Electron 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 ptp.Pcap_ele_ions_av-ptp.Pcap_ions_av.
- 4 In the Description text field, type Time averaged electron power deposition.
- 5 In the Time Averaged Electron Power Deposition toolbar, click **Plot**.
- 6 Click the Zoom Extents button in the Graphics toolbar.
- 7 In the Time Averaged Electron Power Deposition toolbar, click Plot.

Time Averaged Electron Density

- I In the Model Builder window, right-click Time Averaged Electron Power Deposition and choose **Duplicate**.
- 2 In the Settings window for ID Plot Group, type Time Averaged Electron Density in the Label text field.

Line Graph 1

- I In the Model Builder window, expand the Time Averaged Electron 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 I (compl)>Plasma, Time Periodic>Electron density>ptp.neav - Electron density, period averaged - I/m3.
- **3** Locate the **y-Axis Data** section. Clear the **Description** check box.
- 4 In the Time Averaged Electron Density toolbar, click **Plot**.
- 5 Click the Zoom Extents button in the Graphics toolbar.

Time Averaged Ion Density

I In the Model Builder window, right-click Time Averaged Electron Density and choose Duplicate.

2 In the Settings window for ID Plot Group, type Time Averaged Ion Density in the Label text field

Line Graph 1

- I In the Model Builder window, expand the Time Averaged Ion 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 I (comp I)>Plasma, Time Periodic>Number densities>ptp.n_wHe_Ip_av Number density I/m³.
- 3 In the Time Averaged Ion Density toolbar, click Plot.
- **4** Click the **Zoom Extents** button in the **Graphics** toolbar.

Study I/Solution I (2) (soll)

- I In the Model Builder window, expand the Results>Datasets node.
- 2 Right-click Results>Datasets>Study I/Solution I (soll) and choose Duplicate.
- 3 In the Settings window for Solution, locate the Solution section.
- 4 From the Component list, choose Extra Dimension from Plasma, Time Periodic (ptp_xdim).

Electric Potential

- I In the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Dataset list, choose Study I/Solution I (2) (soll).
- 4 In the Label text field, type Electric Potential.

Line Graph 1

- I Right-click Electric Potential and choose Line Graph.
- 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 I (compl)>Plasma, Time Periodic>Metal Contact I> ptp.mctl.V Electric potential V.
- **5** Locate the **Legends** section. Select the **Show legends** check box.
- 6 In the Electric Potential toolbar, click **Plot**.
- **7** Click the **Zoom Extents** button in the **Graphics** toolbar.

Cut Point ID I

I In the Results toolbar, click More Datasets and choose Cut Point ID.

- 2 In the Settings window for Cut Point ID, locate the Point Data section.
- 3 In the X text field, type 0.067/2.

Point Evaluation 1

- I In the Model Builder window, under Results right-click Derived Values and choose Point Evaluation.
- 2 In the Settings window for Point Evaluation, locate the Data section.
- 3 From the Dataset list, choose Cut Point ID 1.
- 4 Click Replace Expression in the upper-right corner of the Expressions section. From the menu, choose Component I (compl)>Plasma, Time Periodic>Electron density>ptp.neav -Electron density, period averaged - I/m3.
- **5** Locate the **Expressions** section. In the table, enter the following settings:

Expression Unit		Description
ptp.neav	1/m^3	Electron density, period averaged
(3/2)*ptp.Teav	V	Mean electron energy, period averaged

6 Click **= Evaluate**.

Line Average 1

- I In the Results toolbar, click \$\frac{8.85}{6.12}\$ More Derived Values and choose Average>Line Average.
- 2 In the Settings window for Line Average, locate the Data section.
- 3 From the Dataset list, choose Study I/Solution I (2) (soll).
- 4 Locate the Selection section. From the Selection list, choose All domains.
- **5** Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
atxd0(0.067,ptp.nJt)	mA/cm^2	Period averaged ion current density

6 Click ▼ next to **= Evaluate**, then choose **Table I - Point Evaluation I**.