

3D ICP Reactor, Argon Chemistry

Although not recommended, 3-dimensional plasma modeling is possible to do in COMSOL. A square coil is placed on top of a dielectric window and it electrically excited at 13.56 MHz. A plasma is formed in the chamber beneath the dielectric window, which contains argon gas at low pressure (20 mtorr). The gas flows into the process chamber from two 2 inch ports and the gas is extracted through a single 4 inch port. The plasma is sustained via electromagnetic induction where power is transferred from the electromagnetic fields to the electrons.

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 (>10¹⁷ 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.

DOMAIN EQUATIONS

The Inductively Coupled Plasma (ICP) reactor interface solves a system of coupled partial differential equations for:

- The electron density.
- The mean electron energy.
- The mass fraction of each of the nonelectron species.
- The electrostatic potential.
- The electric field due to induction currents.

The electron density and mean electron energy are computed by solving a pair of driftdiffusion 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 the Plasma Module User's Guide.

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

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

The electron source R_e and the energy loss due to inelastic collisions R_{ε} are defined later. In this model, the electron diffusivity, energy mobility and energy diffusivity are calculated from the electron mobility, μ_e 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 and are written using either rate coefficients. Suppose that there are M reactions which contribute to the growth or decay of electron density and P electron-neutral collisions. In general P >> M. 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 (m³/s), and N_n is the total neutral number density (1/m³). 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 **Inductively Coupled Plasma** 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 (m²) and f is the electron energy distribution function (EEDF). In this model 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.

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 is automatically defined using the cold plasma approximation:

$$\sigma = \frac{n_e q^2}{m_\rho (v_\rho + j\omega)}$$

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

PLASMA CHEMISTRY

Since 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 (electron impact cross section are obtained from Ref. 3):

TABLE I: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\epsilon(eV)$
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

TABLE I: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	ТҮРЕ	Δε(eV)
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	I
2	Ar+=>Ar	I

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 impedance. The current flowing in the plasma depends on the current applied to the coil and the reaction kinetics. The total plasma current may 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. Since this is a 3D model it is not practical to resolve the skin depth in the driving coil. Instead an impedance boundary condition is used which only computes the coil current density in the tangential direction of the coil surface. This means the mesh does not have to resolve the skin depth in the coil, which at 13.56MHz for copper is only 17 microns.

Results and Discussion

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.

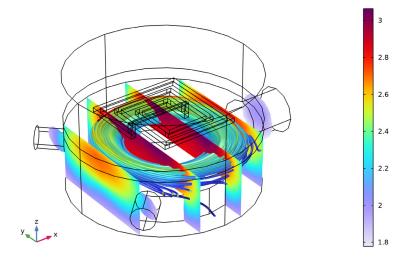


Figure 1: Plot of electron temperature (slice), magnetic vector potential (streamlines) and electric field norm (streamline color).

The electron "temperature" is highest directly underneath the coil, which is where the bulk of the power deposition occurs. The streamlines in Figure 1 show the norm of the electric field. The streamlines are not perfectly circular since the coil is asymmetric.

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. Lymberopoulos 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, pp. 473-494, 1995.
- 3. Phelps database, www.lxcat.net, retrieved 2017.

Application Library path: Plasma Module/Inductively Coupled Plasmas/ argon_3d_icp

Modeling Instructions

From the File menu, choose New.

In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click **3D**.
- 2 In the Select Physics tree, select Fluid Flow>Single-Phase Flow>Laminar Flow (spf).
- 3 Click Add.
- 4 In the Select Physics tree, select Plasma>Inductively Coupled Plasma.
- 5 Click Add.
- 6 Click M Done.

GEOMETRY I

- I Click the Show More Options button in the Model Builder toolbar.
- 2 In the Show More Options dialog box, in the tree, select the check box for the node Physics>Advanced Physics Options.
- 3 Click OK.

Import I (impl)

- I In 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_3d_icp.mphbin.
- 5 Click Import.

DEFINITIONS

Coil boundaries

- I In the **Definitions** toolbar, click **\(\frac{1}{2} \) Explicit**.
- 2 Click the Wireframe Rendering button in the Graphics toolbar.
- **3** Select Domains 4–6, 8, and 9 only.
- 4 In the Settings window for Explicit, type Coil boundaries in the Label text field.
- 5 Locate the Output Entities section. From the Output entities list, choose Adjacent boundaries.

Current density

- I In the **Definitions** toolbar, click **\(\bigcap_{\text{a}} \) Explicit**.
- **2** Select Domain 7 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 Current density.

Plasma

- I In the **Definitions** toolbar, click **\(\bigcap_{\bigcap} \) Explicit**.
- **2** Select Domain 1 only.
- 3 In the Settings window for Explicit, type Plasma in the Label text field.

Inlets

- I In the **Definitions** toolbar, click 堶 **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 and 4 only.
- 5 In the Label text field, type Inlets.

Outlet

- I In the **Definitions** toolbar, click **\(\frac{1}{2} \) Explicit**.
- 2 Select Domain 1 only.
- 3 In the Settings window for Explicit, locate the Input Entities section.
- 4 From the Geometric entity level list, choose Boundary.
- **5** Select Boundary 100 only.
- 6 In the Label text field, type Outlet.

7 Click the Go to Default View button in the Graphics toolbar.

ICP domains

- I In the **Definitions** toolbar, click **\(\frac{1}{2} \) Explicit**.
- 2 Select Domains 1–3 only.
- 3 In the Settings window for Explicit, type ICP domains in the Label text field.

Plasma walls

- I In the **Definitions** toolbar, click **\(\bigcap_{\text{a}} \) 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 2, 3, 5–9, 12, 17–23, 70, 73–75, and 96–99 only.
- 5 In the Label text field, type Plasma walls.

View I

- I In the Model Builder window, under Component I (compl)>Definitions click View I.
- 2 In the Settings window for View, locate the View section.
- 3 Clear the Show grid check box.
- 4 Click the Go to Default View button in the Graphics toolbar.

Variables I

- I In the **Definitions** toolbar, click **a= 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
Mw	0.04[kg/mol]	kg/mol	Molecular weight
T	300[K]	K	Model temperature
p0	0.02[Torr]	Pa	Outlet pressure
rho_stp	101325[Pa]*Mw/ R_const/273.15[K]	kg/m³	Density at standard pressure and temperature
Qin	0.5E-2[m^3/s]	m³/s	Volumetric flow rate
Js0	1E3[A/m]*tanh(1E7* t[1/s])	A/m	Surface current density

PLASMA (PLAS)

I In the Model Builder window, under Component I (compl) click Plasma (plas).

- 2 In the Settings window for Plasma, locate the Domain Selection section.
- 3 Click Clear Selection.
- 4 Select Domain 1 only.

MAGNETIC FIELDS (MF)

- I In the Model Builder window, under Component I (compl) click Magnetic Fields (mf).
- **2** Select Domains 1–3 only.

LAMINAR FLOW (SPF)

Since the density variation is not small, the flow cannot be regarded as incompressible. Therefore set the flow to be compressible.

- I In the Model Builder window, under Component I (compl) 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. Click Clear Selection.
- **5** Select Domain 1 only. Define the pressure reference level in the interface properties.
- **6** Locate the **Physical Model** section. In the p_{ref} text field, type 0.

PLASMA (PLAS)

In the Model Builder window, under Component I (compl) click Plasma (plas).

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 Ar xsecs.txt.
- 5 Click | Import.
- 6 In the Model Builder window, click Plasma (plas).
- 7 In the Settings window for Plasma, locate the Transport Settings section.
- **8** Find the **Include** subsection. Select the **Convection** check box.

Species: Ar

I 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.

Species: Ar+

- I 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.

Species: Ars

- I In the Model Builder window, 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.

Initial Values 1

- I In the Model Builder window, click Initial Values I.
- 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 4.

Plasma Model I

- I In the Model Builder window, click Plasma Model I.
- 2 In the Settings window for Plasma Model, locate the Electron Density and Energy section.
- 3 In the μ_e text field, type 4E24[1/(m*V*s)]/plas.Nn.
- 4 Locate the Model Inputs section. From the **u** list, choose Velocity field (spf).
- **5** In the *T* text field, type T.
- **6** From the p_A list, choose **Absolute pressure (spf)**.

MAGNETIC FIELDS (MF)

In the Model Builder window, under Component I (compl) click Magnetic Fields (mf).

Impedance Boundary Condition I

- In the Physics toolbar, click Boundaries and choose Impedance Boundary Condition.
- 2 In the Settings window for Impedance Boundary Condition, locate the Boundary Selection section.
- 3 From the Selection list, choose Coil boundaries.

Surface Current Density I

I In the Physics toolbar, click **Boundaries** and choose Surface Current Density.

- 2 In the Settings window for Surface Current Density, locate the Boundary Selection section.
- 3 From the Selection list, choose Current density.
- **4** Locate the **Surface Current Density** section. Specify the J_{s0} vector as

Js0	x
0	у
0	z

PLASMA (PLAS)

In the Model Builder window, under Component I (compl) click Plasma (plas).

Ground I

- I In 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 Plasma walls.

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 Plasma walls.

Surface Reaction 1

- I In 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 Plasma walls.
- **4** Locate the **Reaction Formula** section. In the **Formula** text field, type Ar+=>Ar.

Surface Reaction 2

- I In 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 Plasma walls.
- 4 Locate the Reaction Formula section. In the Formula text field, type Ars=>Ar.

Species: Ars

In the Model Builder window, click Species: Ars.

Outflow I

I In the Physics toolbar, click 🖳 Attributes and choose Outflow.

- 2 In the Settings window for Outflow, locate the Boundary Selection section.
- **3** From the **Selection** list, choose **Outlet**.

Species: Ar+

In the Model Builder window, under Component I (compl)>Plasma (plas) click Species: Ar+.

Outflow I

- I In the Physics toolbar, click **Attributes** and choose **Outflow**.
- 2 In the Settings window for Outflow, locate the Boundary Selection section.
- **3** From the **Selection** list, choose **Outlet**.

LAMINAR FLOW (SPF)

- I In the Model Builder window, under Component I (compl) click Laminar Flow (spf).
- 2 In the Settings window for Laminar Flow, locate the Physical Model section.
- 3 In the p_{ref} text field, type p0.

Fluid Properties 1

- I In the Model Builder window, under Component I (compl)>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 (plas/pes I).
- 4 From the μ list, choose Dynamic viscosity (plas/pes I).

Inlet 1

- I In the Physics toolbar, click **Boundaries** and choose Inlet.
- 2 In the Settings window for Inlet, locate the Boundary Selection section.
- **3** From the **Selection** list, choose **Inlets**.
- 4 Locate the Boundary Condition section. From the list, choose Fully developed flow.
- **5** Locate the **Fully Developed Flow** section. Click the **Flow rate** button.
- **6** In the V_0 text field, type Qin.

Outlet I

- I In the Physics toolbar, click **Boundaries** and choose **Outlet**.
- 2 In the Settings window for Outlet, locate the Boundary Selection section.
- 3 From the Selection list, choose Outlet.

MATERIALS

Material I (mat I)

- I In the Model Builder window, under Component I (compl) right-click Materials and choose Blank Material.
- 2 Select Domains 1–3 only.
- 3 In the Settings window for Material, locate the Material Contents section.
- **4** In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permeability	mur_iso; murii = mur_iso, murij = 0	1	I	Basic
Electrical conductivity	sigma_iso; sigmaii = sigma_iso, sigmaij = 0	0	S/m	Basic
Relative permittivity	epsilonr_iso; epsilonrii = epsilonr_iso, epsilonrij = 0	1	I	Basic

Material 2 (mat2)

- I Right-click Materials and choose Blank Material.
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 From the Selection list, choose Coil boundaries.
- **5** Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilonr_iso; epsilonrii = epsilonr_iso, epsilonrij = 0	1	I	Basic

Property	Variable	Value	Unit	Property group
Relative permeability	mur_iso; murii = mur_iso, murij = 0	1	I	Basic
Electrical conductivity	sigma_iso; sigmaii = sigma_iso, sigmaij = 0	6e7	S/m	Basic

MESH I

Free Tetrahedral I

- I In the Mesh toolbar, click A Free Tetrahedral.
- 2 In the Model Builder window, right-click Mesh I and choose Build All.

MESH 2

- I In the Mesh toolbar, click Add Mesh and choose Add Mesh.
- 2 In the Mesh toolbar, click A Free Tetrahedral.

Free Tetrahedral I

- I In the Settings window for Free Tetrahedral, locate the Domain Selection section.
- 2 From the Geometric entity level list, choose Domain.
- **3** Select Domains 2 and 3 only.

Boundary Layers 1

- I In the Mesh toolbar, click Boundary Layers.
- 2 In the Settings window for Boundary Layers, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Plasma.

Boundary Layer Properties

- I In the Model Builder window, click Boundary Layer Properties.
- 2 In the Settings window for Boundary Layer Properties, locate the Boundary Selection section.
- 3 From the Selection list, choose Plasma walls.
- 4 In the Model Builder window, right-click Mesh 2 and choose Build All.

ADD STUDY

- I In the Home toolbar, click Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select Empty Study.
- 4 Click Add Study in the window toolbar.
- 5 In the Home toolbar, click Add Study to close the Add Study window.

STUDY I

Stationary

- I In the Study toolbar, click Study Steps and choose Stationary>Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- 3 In the table, clear the Solve for check boxes for Plasma (plas) and Magnetic Fields (mf).

Frequency-Transient

- I In the Study toolbar, click Study Steps and choose Time Dependent>Frequency-Transient.
- 2 In the Settings window for Frequency-Transient, locate the Study Settings section.
- 3 In the Output times text field, type 0 $10^{\text{nage}(-8,6/10,-3)}$.
- 4 In the Frequency text field, type 13.56[MHz].
- 5 Locate the Physics and Variables Selection section. In the table, clear the Solve for check box for Laminar Flow (spf).
- **6** Click to expand the **Mesh Selection** section. Click to expand the **Values of Dependent Variables** section. In the **Study** toolbar, click **Compute**.

RESULTS

Study I/Solution Store I (3) (sol2)

- I In the Model Builder window, expand the Results>Datasets node.
- 2 Right-click Results>Datasets>Study I/Solution Store I (sol2) and choose Duplicate.
- 3 In the Settings window for Solution, locate the Solution section.
- 4 From the Solution list, choose Solution I (soll).

Selection

- I Right-click Study I/Solution I (3) (soll) and choose 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 Domain 1 only.

Streamline 1

- I In the Model Builder window, right-click Electron Temperature (plas) and choose Streamline.
- 2 In the Settings window for Streamline, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Magnetic Fields>Magnetic>Ax,Ay,Az - Magnetic vector potential.
- 3 Locate the Data section. From the Dataset list, choose Study I/Solution I (1) (soll).
- 4 Locate the Streamline Positioning section. From the Positioning list, choose Startingpoint controlled.
- 5 From the Entry method list, choose Coordinates.
- 6 In the x text field, type range (-0.12, 0.02, 0.12).
- 7 In the y text field, type -0.12.
- 8 In the z text field, type -0.05.
- **9** Locate the Coloring and Style section. Find the Line style subsection. From the Type list, choose Tube.

Color Expression 1

- I Right-click Streamline I and choose Color Expression.
- 2 In the Settings window for Color Expression, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Magnetic Fields>Electric>mf.normE - Electric field norm - V/m.
- 3 Locate the Coloring and Style section. Clear the Color legend check box.
- 4 In the Electron Temperature (plas) toolbar, click Plot.