# 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.

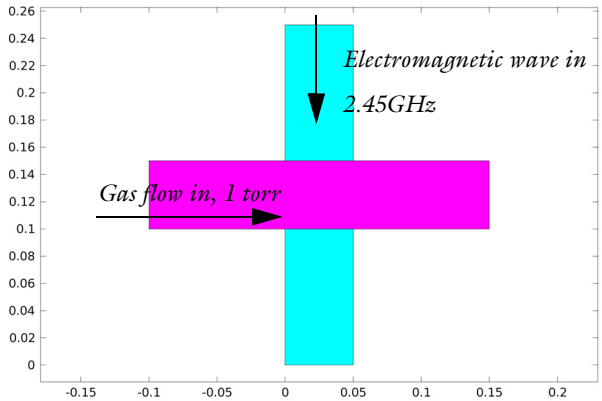


*Figure 1: Diagram of geometry modeled. A TE mode wave enters from the top port and intersects the gas flow leading to the formation of a plasma.*

**Note:** The model requires the Plasma and RF modules.

## *Model Definition*

### 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 User 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 $R_\varepsilon$ 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:

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

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $C^{1/2}/kg^{1/2}$), $m_e$ is the electron mass (SI unit: kg), $\varepsilon$ is energy (SI unit: V), $\sigma_k$ 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 User 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 $\rho$ 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 User 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:

$$\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) - k_0^2 \left(\varepsilon_r - \frac{j\boldsymbol{\sigma}}{\omega \varepsilon_0}\right) \mathbf{E} = 0 \qquad (1)$$

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:

$$\boldsymbol{\sigma}^{-1} \bullet \mathbf{J} = \mathbf{E} \qquad (2)$$

Here, $\sigma$ is the plasma conductivity tensor, which is a function of the electron density, collision frequency, and magnetic flux density. Using the definitions:

$$\alpha = \frac{q}{m_e(\nu_e + j\omega)}, \beta = n_e q \alpha \tag{3}$$

where $q$ is the electron charge, $m_e$ is the electron mass, $n_e$ is the collision frequency, and $\omega$ 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:

$$\boldsymbol{\sigma}^{-1} = \begin{bmatrix} \frac{1}{\beta} & 0 & 0 \\ 0 & \frac{1}{\beta} & 0 \\ 0 & 0 & \frac{1}{\beta} \end{bmatrix}. \tag{4}$$

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

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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 will revert 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 power of 500 W is fed into the port and a certain amount of this power is absorbed and a certain amount is reflected. The amount of power absorbed depends on the plasma conductivity which is a function of the electron density and collision frequency.

## *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.

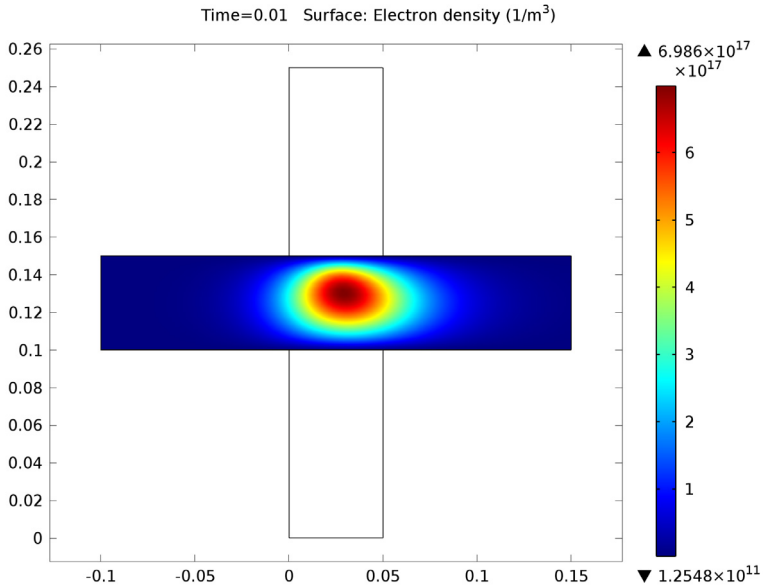


*Figure 2: Plot of the electron density.*

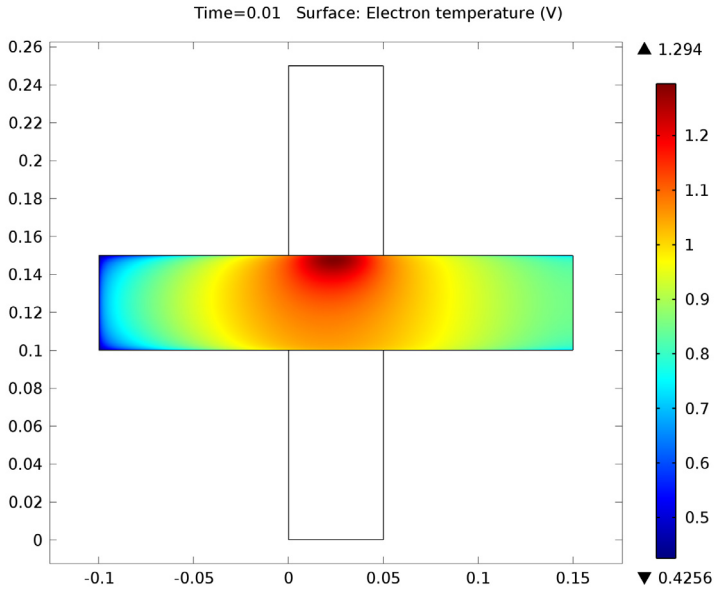


*Figure 3: Plot of the electron temperature in the reactor.*



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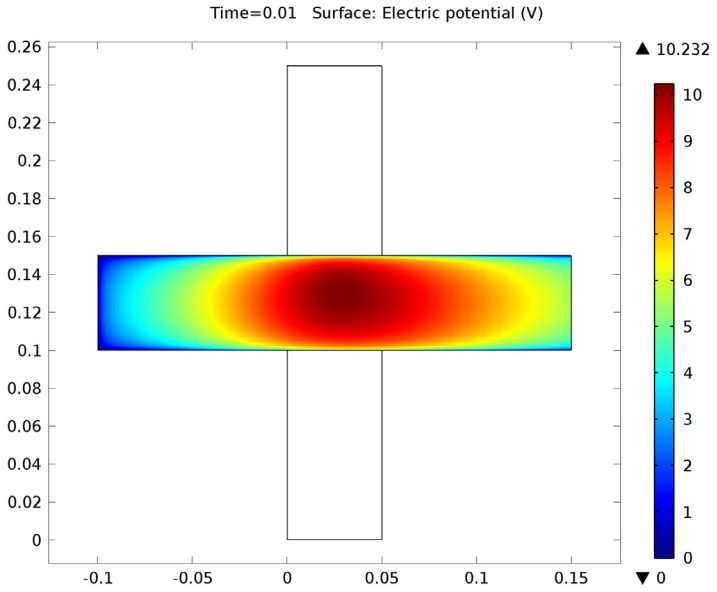


*Figure 4: Plot of the plasma potential in the reactor.*

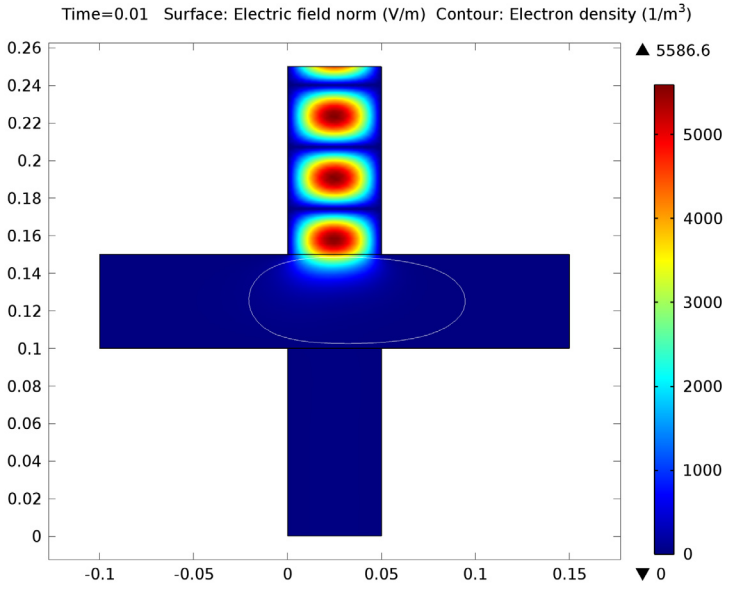


*Figure 5: Plot of the electric field norm. The white contour represents the critical plasma*

*density, where the electron density is equal to 7.6E16[1/m$^3$].*

## *Reference*

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

**Model Library path:** `Plasma_Module/Wave-Heated_Discharges/inplane_microwave_plasma`

## *Modeling Instructions*

### MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Click the **2D** button.

3 Click **Next**.

4 In the **Add physics** tree, select **Plasma>Microwave Plasma (mwp)**.

5 Click **Add Selected**.

6 Click **Next**.

7 Find the **Studies** subsection. In the tree, select **Preset Studies>Frequency-Transient**.

8 Click **Finish**.

### GEOMETRY 1

*Rectangle 1*

1 In the **Model Builder** window, under **Model 1** right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `0.05`.

4 In the **Height** edit field, type `0.1`.

5 Click the **Build All** button.

*Rectangle 2*

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Rectangle**.

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2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `0.25`.

4 In the **Height** edit field, type `0.05`.

5 Locate the **Position** section. In the **x** edit field, type `-0.1`.

6 In the **y** edit field, type `0.1`.

*Rectangle 3*

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `0.05`.

4 In the **Height** edit field, type `0.1`.

5 Locate the **Position** section. In the **y** edit field, type `0.15`.

6 Click the **Build All** button.

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

## DEFINITIONS

*Explicit 1*

1 In the **Model Builder** window, under **Model 1** right-click **Definitions** and choose **Selections>Explicit**.

2 In the **Explicit** settings window, 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 **Model 1>Definitions>Explicit 1** and choose **Rename**.

6 Go to the **Rename Explicit** dialog box and type `Walls` in the **New name** edit field.

7 Click **OK**.

## MICROWAVE PLASMA

1 In the **Microwave Plasma** settings window, locate the **Settings** section.

2 From the **Electric field components solved for** list, choose **Out-of-plane vector**.

*Cross Section Import 1*

1 Right-click **Model 1>Microwave Plasma** and choose the domain setting **Heavy Species Transport>Cross Section Import**.

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

3 Click the **Browse** button.

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

*Reaction 1*

1 In the **Model Builder** window, right-click **Microwave Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.

2 In the **Reaction** settings window, locate the **Reaction Formula** section.

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

4 Locate the **Kinetics Expressions** section. In the $k^{\mathrm{f}}$ edit field, type `3.734E8`.

*Reaction 2*

1 Right-click **Microwave Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.

2 In the **Reaction** settings window, locate the **Reaction Formula** section.

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

4 In the **Reaction** settings window, locate the **Kinetics Expressions** section.

5 In the $k^{\mathrm{f}}$ edit field, type `1807`.

*Species: Ar*

1 In the **Model Builder** window, under **Model 1>Microwave Plasma** click **Species: Ar**.

2 In the **Species** settings window, locate the **Species Formula** section.

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

*Species: Ar+*

1 In the **Model Builder** window, under **Model 1>Microwave Plasma** click **Species: Ar+**.

2 In the **Species** settings window, 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 **Microwave Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.

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

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

4 In the **Surface Reaction** settings window, locate the **Boundary Selection** section.

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

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*Surface Reaction 2*

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

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

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

4 In the **Surface Reaction** settings window, locate the **Boundary Selection** section.

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

6 In the **Model Builder** window, click **Microwave Plasma**.

7 In the **Microwave Plasma** settings window, locate the **Transport Settings** section.

8 Select the **Convection** check box.

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

*Plasma Model 1*

1 In the **Model Builder** window, under **Model 1>Microwave Plasma** click **Plasma Model 1**.

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

3 In the **u** table, enter the following settings:

| | |
|---|---|
| 10 | x |
| 0 | y |

4 In the $T$ edit field, type `350`.

5 In the $p_A$ edit field, type `1[torr]`.

6 Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ edit field, type `4E24`.

*Wave Equation, Electric 1*

1 In the **Model Builder** window, right-click **Microwave Plasma** and choose the domain setting **Electromagnetic Waves>Wave Equation, Electric**.

2 Select Domains 2 and 3 only.

*Initial Values 1*

1 In the **Model Builder** window, under **Model 1>Microwave Plasma** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the $n_{e,0}$ edit field, type `1E17`.

*Wall 1*

1 In the **Model Builder** window, right-click **Microwave Plasma** and choose the boundary condition **Drift Diffusion>Wall**.

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

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

*Ground 1*

1 Right-click **Microwave Plasma** and choose the boundary condition **Electrostatics>Ground**.

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

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

*Electron Outlet 1*

1 Right-click **Microwave Plasma** and choose the boundary condition **Drift Diffusion>Electron Outlet**.

2 Select Boundary 14 only.

*Port 1*

1 Right-click **Microwave Plasma** and choose the boundary condition **Electromagnetic Waves>Port**.

2 Select Boundary 9 only.

3 In the **Port** settings window, 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 In the $P_{\text{in}}$ edit field, type 500.

*Port 2*

1 Right-click **Microwave Plasma** and choose the boundary condition **Electromagnetic Waves>Port**.

2 Select Boundary 5 only.

3 In the **Port** settings window, locate the **Port Properties** section.

4 From the **Type of port** list, choose **Rectangular**.

*Outflow 1*

1 In the **Model Builder** window, under **Model 1>Microwave Plasma** right-click **Species: Ars** and choose **Outflow**.

2 In the **Outflow** settings window, locate the **Boundary Selection** section.

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3 Click **Clear Selection**.

4 Select Boundary 14 only.

*Outflow 1*

1 In the **Model Builder** window, under **Model 1>Microwave Plasma** right-click **Species: Ar+** and choose **Outflow**.

2 In the **Outflow** settings window, locate the **Boundary Selection** section.

3 Click **Clear Selection**.

4 Select Boundary 14 only.

## MATERIALS

*Material 1*

1 In the **Model Builder** window, under **Model 1** right-click **Materials** and choose **Material**.

2 Select Domains 2 and 3 only.

3 In the **Material** settings window, locate the **Material Contents** section.

4 In the table, enter the following settings:

| Property | Name | Value |
|---|---|---|
| Electrical conductivity | sigma | 0 |
| Relative permittivity | epsilonr | 5 |
| Relative permeability | mur | 1 |

## MESH 1

*Boundary Layers 1*

1 In the **Model Builder** window, under **Model 1** right-click **Mesh 1** and choose **Boundary Layers**.

2 In the **Boundary Layers** settings window, 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 **Model 1>Mesh 1>Boundary Layers 1** click **Boundary Layer Properties**.

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

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

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

*Size*

1 In the **Model Builder** window, under **Model 1>Mesh 1** click **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Calibrate for** list, choose **Plasma**.

4 From the **Predefined** list, choose **Fine**.

5 Click the **Build All** button.

## STUDY 1

*Step 1: Frequency-Transient*

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Frequency-Transient**.

2 In the **Frequency-Transient** settings window, locate the **Study Settings** section.

3 In the **Times** edit field, type `0`.

4 Click the **Range** button.

5 Go to the **Range** dialog box.

6 From the **Entry method** list, choose **Number of values**.

7 In the **Start** edit field, type `-8`.

8 In the **Stop** edit field, type `-2`.

9 In the **Number of values** edit field, type `31`.

10 From the **Function to apply to all values** list, choose **exp10**.

11 Click the **Add** button.

12 In the **Frequency-Transient** settings window, locate the **Study Settings** section.

13 In the **Frequency** edit field, type `2.45E9`.

14 In the **Model Builder** window, right-click **Study 1** and choose **Show Default Solver**.

15 Expand the **Study 1>Solver Configurations** node.

*Solver 1*

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

2 Right-click **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1** and choose **Segregated**.

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3 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1>Segregated 1** node, then click **Segregated Step**.

4 In the **Segregated Step** settings window, locate the **General** section.

5 In the **Variables** list, choose **Electric field (mod1.E)**, **mod1.Sparam1**, and **mod1.Sparam2**.

6 Under **Variables**, click **Delete**.

7 In the **Model Builder** window, under **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1** right-click **Segregated 1** and choose **Segregated Step**.

8 In the **Segregated Step** settings window, locate the **General** section.

9 Under **Variables**, click **Add**.

10 Go to the **Add** dialog box.

11 In the **Variables** list, choose **Electric field (mod1.E)**, **mod1.Sparam1**, and **mod1.Sparam2**.

12 Click the **OK** button.

13 In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

## RESULTS

### *2D Plot Group 4*

1 In the **Model Builder** window, right-click **Results** and choose **2D Plot Group**.

2 Right-click **2D Plot Group 4** and choose **Surface**.

3 In the **Surface** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Microwave Plasma (Electromagnetic Waves)>Electric>Electric field norm (mwp.normE)**.

4 Click to expand the **Quality** section. From the **Resolution** list, choose **Extra fine**.

5 In the **Model Builder** window, right-click **2D Plot Group 4** and choose **Contour**.

6 In the **Contour** settings window, locate the **Levels** section.

7 From the **Entry method** list, choose **Levels**.

8 In the **Levels** edit field, type `7.6E16`.

9 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

10 From the **Coloring** list, choose **Uniform**.

11 From the **Color** list, choose **White**.

12 Click the **Plot** button.

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