

Model of an Argon/Oxygen Inductively Coupled Plasma Reactor

This tutorial models an argon/oxygen inductively coupled plasma reactor. The main goal is to show how to prepare a model with a mixture of different elements (in this case Ar and O_2) in which one of the species can dissociate by electron impact (O_2 dissociates into O) and where negative ions exist (the dissociative electron attachment of O₂ creates O⁻).

A simplified plasma chemistry is used to discuss the main aspects of such discharges. It is important to keep in mind that a benchmark is not attempted and the idea is to provide a base case that can be used to develop more complex chemistries. In fact, it might be necessary to modify the data used and add more reactions to achieve experimental verification.

The plasma model is solved self-consistently with the Laminar Flow and Heat Transfer in Fluids interfaces. A Frequency-Stationary study step is used to do fast parametrization in the input power and oxygen mole fraction.

In this model the many features used to setup the plasma chemistry are created automatically from a text file by using the Plasma Chemistry add-in.

Model Definition

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.

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

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

The electron source R_e and the energy loss due to inelastic collisions R_e 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 $\Delta \epsilon_j$ 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.

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 electromagnetic wave "sees" a plasma defined by the plasma conductivity in the cold plasma approximation that is set in the **Plasma Conductivity Coupling** multiphysics feature:

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

where n_{ρ} is the electron density, q is the electron charge, m_{ρ} is the electron mass, v_{ρ} is the collision frequency, and ω is the angular frequency. The Joule heating term that is responsible to heat the electrons is set in the Electron Heat Source multiphysics feature.

BOUNDARY CONDITIONS

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

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

and the electron energy flux:

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

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:

$$\mathbf{n} \cdot \mathbf{j}_{b} = M_{m}R_{b} + M_{m}c_{b}Z\mu_{b}(\mathbf{E} \cdot \mathbf{n})[Z_{b}\mu_{b}(\mathbf{E} \cdot \mathbf{n}) > 0]$$

The walls of the reactor are grounded.

PLASMA CHEMISTRY

Negative ions are created in certain molecular gaseous discharges (like chlorine, oxygen, hydrogen, fluorocarbons, and so on) and these discharges tend to have complex plasma chemistries with many ions, dissociative products, and excited states. Here a simple plasma chemistry is used and no benchmark is attempted. In fact, it might be necessary to modify the data used and add more reactions to achieve experimental verification. Nevertheless,

this plasma chemistry allows to show the main aspects of an electronegative discharge. The plasma chemistry for oxygen is based on the one presented in Ref. 1 (from the section "A Data Set for Oxygen," page 270) but the electron impact reactions are mostly retrieved from Ref. 2 in the form of electron impact cross sections. A good discussion of the chemistry of a oxygen/argon plasma at low pressures can be found in Ref. 3.

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 presented in Table 1 (electron impact cross sections are obtained form Ref. 4).

TABLE I: ARGON REACTIONS

REACTION	FORMULA	ТҮРЕ	$\Delta\epsilon(eV)$
1	e+Ar=>e+Ar	Elastic	-
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	-

Oxygen has a much more rich reaction set that includes vibrational and rotational excitations, excitation of several electronic excited states, electron impact dissociation, dissociative attachment, and many others. Electron impact reactions with O2 are from Ref. 5 and electron impact reaction with O are from Ref. 6 except for e+O-=>O+e+e, which is from Ref. 1. The electron impact reactions used in this model are presented in Table 2. The following simplifications were made: 3-body attachment is not included, rotational and vibrational states are not treated explicitly but energy losses are considered, the dissociative excitation reaction at 14.7 eV is not included, polar dissociation is not included, reverse reaction by detailed balance are not included for O2 and O excited states. The only oxygen excited states that are solved explicitly are the singlet delta metastable of molecular oxygen $O_2(a^1\Delta_g)$ and the metastable state $O(^1D)$.

TABLE 2: OXYGEN ELECTRON IMPACT REACTIONS

REACTION	FORMULA	TYPE	$\Delta\epsilon(eV)$
1	e+O ₂ =>O+O	Dissociative attachment	-
2	e+O ₂ =>e+O ₂	Elastic	-
3	e+O ₂ =>e+O ₂	Rotational excitation	0.02
4	e+O ₂ =>e+O ₂	Vibrational excitation	0.19

TABLE 2: OXYGEN ELECTRON IMPACT REACTIONS

REACTION	FORMULA	ТҮРЕ	$\Delta\epsilon(eV)$
5	e+O ₂ =>e+O ₂	Vibrational excitation	0.19
6	e+O ₂ =>e+O ₂	Vibrational excitation	0.38
7	e+O ₂ =>e+O ₂	Vibrational excitation	0.38
8	e+O ₂ =>e+O ₂	Vibrational excitation	0.57
9	e+O ₂ =>e+O ₂	Vibrational excitation	0.75
10	$e+O_2=>e+O_2(a^{\dagger}\Delta_g)$	Excitation	0.977
П	e+O ₂ =>e+O ₂	Excitation	1.627
12	e+O ₂ =>e+O ₂	Excitation	4.5
13	e+O ₂ =>e+O+O	Dissociative excitation	6.0
14	e+O ₂ =>e+O+O(¹ D)	Excitation	8.4
15	e+O ₂ =>e+O ₂	Excitation	9.97
16	e+O ₂ =>e+O ₂ +	Ionization	12.06
17	e+O=>e+O	Elastic	-
18	e+O=>e+O(¹ D)	Excitation	1.968
19	e+O=>e+O	Excitation	4.192
20	e+O=>e+c	Ionization	13.618
21	e+O ⁻ =>O+e+e	Electron impact detachment	12.00

On Table 3 are presented heavy species reaction involving ions. For reaction 6 it is used the same rate constant as for reaction 2.

TABLE 3: HEAVY SPECIES REACTIONS INVOLVING IONS

REACTION	FORMULA	TYPE
1	O ⁺ +O ₂ =>O+O ₂ ⁺	Charge transfer
2	O ⁺ +O ⁻ =>O+O	Mutual recombination
3	O ⁻ +O ₂ ⁺ =>3O	Mutual recombination
4	$O^{-}+O_{2}^{+}=>O+O_{2}$	Mutual recombination
5	O-+O ₂ =>O ₂ +e	Detachment
6	$O^-+Ar^+=>O+Ar$	Mutual recombination

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

TABLE 4: SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT	SECONDARY EMISSION COEFFICIENT	MEAN ENERGY OF SECONDARY ELECTRONS (V)
I	Ars=>Ar	I	0	0
2	Ar ⁺ =>Ar	I	0.07	5.8
3	O=>0.5O ₂	0.2	0	0
4	O ₂ ⁺ =>O ₂	I	0.05	4
5	O-=>O	I	0	0
6	$O_2(a^{\dagger}\Delta_g) => O$	I	0	0
7	$O(^{1}D) = > 0.5O_{2}$	0.2	0	0
8	O ⁺ =>O	I	0.05	4

It is by using surface reactions that boundary conditions for heavy species are introduced in the model. If no surface reactions that leads to the lost of a given species at a surface are introduced in the model, that species will not have losses by transport. This can lead to the unbounded growth of a given species and a steady state solution might not be possible.

Atomic recombination (reaction 3 in Table 4) at a surface is an important aspect of plasma discharges with molecular species since it influences the dissociation degree in the discharge. The sticking coefficient for atomic recombination is a function of the surface type and temperature.

ELECTRONEGATIVE PLASMAS

Electronegative plasmas are plasmas that contain negative ions. Negative ions are mainly created by electron dissociative attachment (for example, e+O₂=>O+O⁻). This reaction tends to be very effective at low electron energies and can reduce the electrons in a discharge to a point that an ion-ion discharge is obtained. The transport and volume creation/destruction mechanisms tend to be more complex than electropositive plasmas in many aspects. Here only a few are mentioned with emphasis on the numerical difficulties that they introduce. More information can be found in Ref. 1 section 10.3 and references therein.

In electronegative discharges negative ions are well confined by the ambipolar electric field and losses by transport are very small. This means that to achieve a steady state volume losses need to be included for negative ions. The mechanisms by which negative ions are lost depend on the gas mixture and pressure and they are: mutual recombination with positive ions (for example, O+O+O+O+O+O+O+O+Ar+=>O+Ar), detachment in collisions

with excited or neutral atoms or molecules (for example, O +O=>O2+e or O +O2=>O+ O_2+e), and electron-impact detachment (for example, $e+O^-=>O+2e$).

In electronegative discharges it is often possible to identify two spatial regions using the electronegativity (ratio of the negative ion density to the electron density): (i) one in the core of the discharge (the electronegative core) with high electronegativity where the dominant charge species are positive and negative ions; (ii) and the other close to the boundaries (electropositive edges) where the dominant charged species are electron and positive ions. In the transition between these two regions the negative ion density drops abruptly causing a chock-like phenomena. This transition needs to be well resolved spatially. If not, oscillations can be seen in the negative ion density and the model might not converge. Some strategies to deal with this are:

- Increase the negative ion temperature of about 0.3 eV. An higher ion temperature makes the transport numerical easier. The ion temperature is defined in the section Mobility and Diffusivity Expressions in the species Settings. By default the ion temperature is the gas temperature.
- Enable Isotropic diffusion for ions in the Inconsistent Stabilization section (the stabilization sections are visible when **Stabilization** is selected in **Show More Options**). This option adds artificial diffusion to all ions and helps smoothing the sharp transition of the negative ion density between the electropositive edge and the electronegative core, and also increase the density of the negative ions in the electropositive edge effectively increasing its losses by transport. This option should be used very carefully since completely wrong results can be obtained if too much diffusion is used (the tuning parameter for ions should not be larger than 0.1). A useful strategy is to start with a large Tuning parameter for ions (for example, 0.5) and ramp it down using a Auxiliary sweep.

INLET AND OUTFLOW

When solving for plasmas with chemistries that contain more than one element (for example, Ar and O2) with a stationary solver the mass fraction of each element is not conserved if no constraint is used. This problem is similar in nature to the one found when solving for Navier-Stokes equations in steady state without fixing the pressure somewhere. The Inlet boundary condition fixes the mass fraction or mole fraction of specified species and it is used in this model as a real inlet for O_2 and as a strategy to fix its mass fraction. An important aspect to remember is that no **Inlet** is used for Ar since this species is being computed From mass constraint. It is assumed that ions are neutralized at the outlet boundary and as such no Outflow boundary condition is applied. For the species to which an Outflow boundary condition is applied no surface reaction is applied at the same

boundary to represent a species that flows out of the system without interacting with a surface.

Results and Discussion

Figure 1 to Figure 4 show spatial distributions of the electron density, electron temperature, negative ion density, and power absorbed by the electrons at 1000 W. The power absorbed by the electrons and electron temperature profiles are typical of an ICP discharge. Most of the power deposition occurs below the coil and is shielded by the high dense plasma, and the electron temperature is relatively flat in the plasma region. The electron and negative ion density have a typical distribution of electronegative plasmas with a electronegative core (where the electrons have a flat profile) and electropositive edges (where the negative ion density drops fast towards the surface). These regions can be better observed in Figure 5 that shows the distribution of the charged species along the axis-of-symmetry.

Figure 6 presents the space average number density of charged species as a function of power. At 100 W the negative ions are the dominant negatively charged species. As power increases the discharge electronegativity decreases; at 1000 W, the averaged electronegativity is slightly smaller than one, with the electrons now being the dominant negative charged species. However, the electronegative core is always present, as shown in Figure 5.

Figure 7 presents the space average number density of charged species as a function of the mole fraction of oxygen. With low oxygen content the discharge has low electronegativity and O⁺ is the dominant positive ion. Increasing the oxygen content leads to higher electronegativity and a progressive change of the dominant positive ion to be O_2^+ .

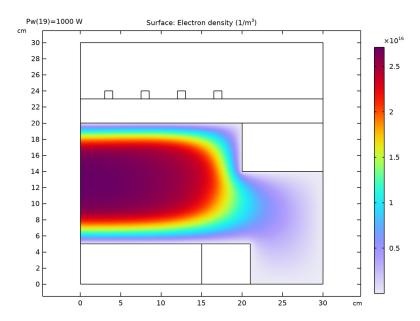


Figure 1: Electron density spatial distribution at 1000 W.

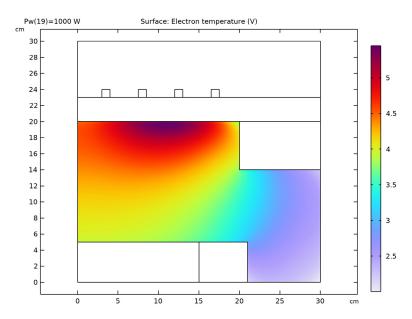


Figure 2: Electron temperature spatial distribution at 1000 W.

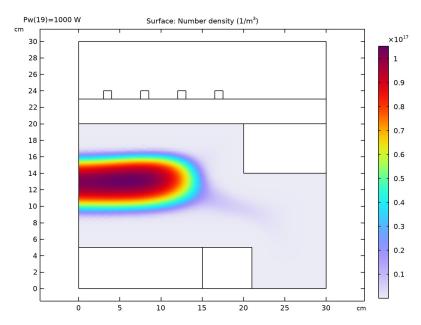


Figure 3: Negative ions density spatial distribution at 1000 W.

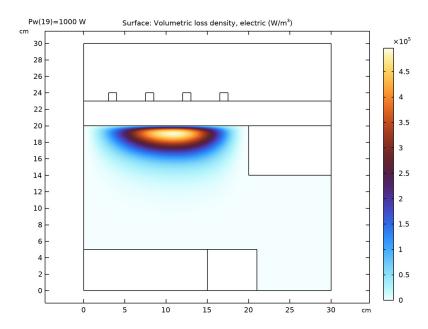


Figure 4: Power absorbed by the electrons at 1000 W.

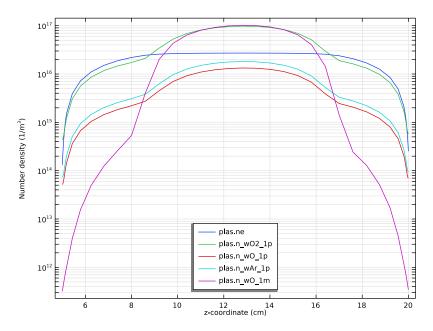


Figure 5: Charged species distribution along the axis-of-symmetry at 1000 W.

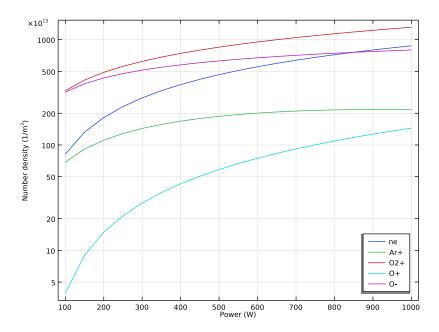


Figure 6: Spatial averaged number density of the charged species as a function of power.

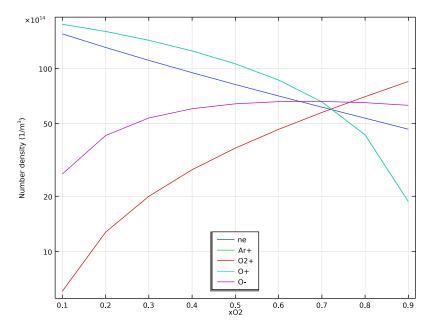


Figure 7: Spatial averaged number density of the charged species as a function of oxygen mole fraction.

References

- 1. M.A. Lieberman and A.J. Lichtenberg, Principles of Plasma Discharges and Materials Processing, John Wiley & Sons, 2005.
- 2. www.lxcat.net
- 3. J.T. Gudmundsson and E.G. Thorsteinsson, "Oxygen discharges diluted with argon: dissociation process," Plasma Sources Sci. Technol., vol. 16, pp. 399-412, 2007.
- 4. Phelps database, www.lxcat.net, retrieved 2017.
- 5. Phelps database, www.lxcat.net, retrieved 2022.
- 6. Morgan database, www.lxcat.net, retrieved 2022.

Application Library path: Plasma_Module/Inductively_Coupled_Plasmas/ icp_argon_oxygen

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 2D Axisymmetric.
- 2 In the Select Physics tree, select Plasma>Inductively Coupled Plasma.
- 3 Click Add.
- 4 In the Select Physics tree, select Heat Transfer>Heat Transfer in Fluids (ht).
- 5 Click Add.
- 6 In the Select Physics tree, select Fluid Flow>Single-Phase Flow>Laminar Flow (spf).
- 7 Click Add.
- 8 Click 🔵 Study.
- 9 In the Select Study tree, select Preset Studies for Selected Multiphysics>Frequency-Stationary.
- 10 Click Done.

GEOMETRY I

Create the geometry for a ICP reactor.

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 2 In the Settings window for Geometry, locate the Units section.
- 3 From the Length unit list, choose cm.

Rectangle I (rI)

- I In the Geometry toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type 30.
- 4 In the Height text field, type 30.

Rectangle 2 (r2)

- I In the Geometry toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type 30.

- 4 In the Height text field, type 3. **5** Locate the **Position** section. In the **z** text field, type 20.
- Rectangle 3 (r3)
- I In the Geometry toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Position section.
- 3 In the r text field, type 3.
- 4 In the z text field, type 23.

Array I (arrI)

- I In the Geometry toolbar, click \(\sum_{\text{in}} \) Transforms and choose Array.
- 2 Select the object **r3** only.
- 3 In the Settings window for Array, locate the Size section.
- 4 In the r size text field, type 4.
- **5** Locate the **Displacement** section. In the **r** text field, type **4.5**.

Rectangle 4 (r4)

- I In the Geometry toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type 15.
- 4 In the Height text field, type 5.

Rectangle 5 (r5)

- I In the Geometry toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type 6.
- **4** In the **Height** text field, type **5**.
- 5 Locate the **Position** section. In the r text field, type 15.

Rectangle 6 (r6)

- I In the Geometry toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type 10.
- 4 In the **Height** text field, type 6.
- 5 Locate the Position section. In the r text field, type 20.
- 6 In the z text field, type 14.

Line Segment I (Is I)

- I In the Geometry toolbar, click * More Primitives and choose Line Segment.
- 2 In the Settings window for Line Segment, locate the Starting Point section.
- **3** From the **Specify** list, choose **Coordinates**.
- 4 In the r text field, type 20.
- 5 In the z text field, type 17.
- 6 Locate the Endpoint section. From the Specify list, choose Coordinates.
- 7 In the r text field, type 20.
- 8 In the z text field, type 18.
- 9 Click Build All Objects.

Add some parameters to be used in the model.

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
Pw	100[W]	100 W	
Qf	250	250	
x02	0.9	0.9	
x0	1e-4	IE-4	
p0	0.02[torr]	2.6664 Pa	

Create explicitly selections to be used later in the model when defining selections of different features.

DEFINITIONS

Walls

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

4 Locate the Output Entities section. From the Output entities list, choose Adjacent boundaries.

Coils

- I In the **Definitions** toolbar, click **\(\frac{1}{2} \) Explicit**.
- 2 In the Settings window for Explicit, type Coils in the Label text field.
- **3** Select Domains 5–7 and 9 only.

Coils boundaries

- I Right-click Coils and choose Duplicate.
- 2 In the Settings window for Explicit, type Coils boundaries in the Label text field.
- 3 Locate the Output Entities section. From the Output entities list, choose Adjacent boundaries.

Average I (aveob I)

- I In the Definitions toolbar, click Monlocal Couplings and choose Average. Add an average operator to evaluate space averages of several quantities in the results section.
- 2 Select Domain 2 only.

Set material properties to different regions of the domain. The domain where the plasma exist is assigned automatically a relative permittivity of 1.

DEFINITIONS

In the Model Builder window, collapse the Component I (compl)>Definitions node.

GEOMETRY I

In the Model Builder window, collapse the Component I (compl)>Geometry I node.

ADD MATERIAL

- I In the Home toolbar, click **Add Material** to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select Built-in>Air.
- 4 Click Add to Component in the window toolbar.
- 5 In the tree, select Built-in>Glass (quartz).
- **6** Click **Add to Component** in the window toolbar.
- 7 In the tree, select Built-in>Copper.
- **8** Click **Add to Component** in the window toolbar.

9 In the Home toolbar, click Radd Material to close the Add Material window.

MATERIALS

Air (mat1)

- I In the Model Builder window, under Component I (compl)>Materials click Air (matl).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 Click Clear Selection.
- 4 Select Domain 4 only.

Glass (quartz) (mat2)

- I In the Model Builder window, click Glass (quartz) (mat2).
- **2** Select Domain 3 only.

Copper (mat3)

- I In the Model Builder window, click Copper (mat3).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- **3** From the **Selection** list, choose **Coils**.

THE PLASMA CHEMISTRY ADD-IN

The next steps have instructions to first import the **Plasma Chemistry** add-in and then to use this add-in to import a file that automatically creates the argon-oxygen plasma chemistry.

The following is set or created automatically:

- a Species properties using Preset species data
- **b** Electron impact reactions for argon and oxygen
- c Heavy species reactions
- **d** Surface reactions

The documentation accompanying the **Plasma Chemistry** add-in contains more information about the file structure and what can be set automatically.

In the **Home** toolbar, click Windows and choose **Add-in Libraries**.

ADD-IN LIBRARIES

- I In the Add-in Libraries window, select Plasma Module>plasma_chemistry in the tree.
- 2 In the tree, select the check box for the node Plasma Module>plasma_chemistry.
- **3** Click **One** to load the add-in and close the **Add-in Libraries** window.

4 In the Developer toolbar, click Add-ins and choose Plasma Chemistry> Plasma Chemistry.

GLOBAL DEFINITIONS

Plasma Chemistry I

- I In the Model Builder window, under Global Definitions click Plasma Chemistry I.
- 2 In the Settings window for Plasma Chemistry, click Browse.
- **3** Browse to the model's Application Libraries folder and double-click the file Ar 02 plasma chemistry.txt.
- 4 Click Import.

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 2 only.
- 5 Click the Show More Options button in the Model Builder toolbar.
- 6 In the Show More Options dialog box, select Physics>Stabilization in the tree.
- 7 In the tree, select the check box for the node **Physics>Stabilization**.
- 8 Click OK.

This model needs stabilization because the density of the negative ions can drop sharply when approaching the reactor edges.

- 9 In the Settings window for Plasma, click to expand the Inconsistent Stabilization section.
- **10** Select the **Isotropic diffusion for ions** check box.
- II In the $\delta_{id.i}$ text field, type 0.1.
- 12 Locate the Transport Settings section. Find the Include subsection. Select the Calculate thermodynamic properties check box.
- 13 Select the Mixture diffusion correction check box.
- 14 Select the Convection check box.

In the following, the different types of features are grouped to make the **Model Builder** tree easier to navigate.

```
10: e+O2=>e+O2a1Dg, 11: e+O2=>e+O2, 12: e+O2=>e+O2, 13: e+O2=>e+O+O.
14: e+O2=>e+O+O1D, 15: e+O2=>e+O2, 16: e+O2=>2e+O2+, 17: e+O=>e+O, 18:
```

- e+O=>e+OID, 19: e+O=>e+O, 1: e+O2=>O+O, 20: e+O=>2e+O+, 21: e+Ar=>e+O+O+Ar, 22: e+Ar=>e+Ars, 23: e+Ars=>e+Ar, 24: e+Ar=>2e+Ar+, 25: e+Ars=>2e+Ar+, 26: e+O-=>O+e+e, 2: e+O2=>e+O2, 3: e+O2=>e+O2, 4: e+O2=>e+O2, 5: e+O2=>e+O202, 6: e+02 = e+02, 7: e+02 = e+02, 8: e+02 = e+02, 9: e+02 = e+02, Cross Section Import 1, Cross Section Import 2, Cross Section Import 3
- I In the Model Builder window, under Component I (compl)>Plasma (plas), Ctrl-click to select Cross Section Import 1, Cross Section Import 2, Cross Section Import 3, 1: e+02=> 0+0-, 2: e+02=>e+02, 3: e+02=>e+02, 4: e+02=>e+02, 5: e+02=>e+02, 6: e+02=>e+0202, 7: e+02=>e+02, 8: e+02=>e+02, 9: e+02=>e+02, 10: e+02=>e+02alDg, 11: e+02=>e+02, 12: e+02=>e+02, 13: e+02=>e+0+0, 14: e+02=>e+0+01D, 15: e+02=>e+ 02, 16: e+02=>2e+02+, 17: e+0=>e+0, 18: e+0=>e+01D, 19: e+0=>e+0, 20: e+0=> 2e+O+, 21: e+Ar=>e+Ar, 22: e+Ar=>e+Ars, 23: e+Ars=>e+Ar, 24: e+Ar=>2e+Ar+, 25: e+ Ars=>2e+Ar+, and 26: e+0-=>0+e+e.
- 2 Right-click and choose **Group**.

Electron Impact Cross Sections

- I In the Settings window for Group, type Electron Impact Cross Sections in the Label text field.
- 2 In the Model Builder window, collapse the Electron Impact Cross Sections node.

```
27: 0++02=>0+02+, 28: 0-+0+=>0+0, 29: 0-+02+=>0+0+0, 30: 0-+02+=>0+
02. 31: 0-+0=>02+e, 32: 0-+Ar+=>0+Ar
```

- I In the Model Builder window, under Component I (compl)>Plasma (plas), Ctrl-click to select 27: 0++02=>0+02+, 28: 0-+0+=>0+0, 29: 0-+02+=>0+0+0, 30: 0-+02+=>0+ 02, 31: 0-+0=>02+e, and 32: 0-+Ar+=>0+Ar.
- 2 Right-click and choose **Group**.

Heavy Species Reactions

- I In the Settings window for Group, type Heavy Species Reactions in the Label text field.
- 2 In the Model Builder window, collapse the Heavy Species Reactions node.

Species: Ar, Species: Ar+, Species: Ars, Species: O, Species: O+, Species: O-, Species: OID, Species: O2, Species: O2+, Species: O2aIDg, Species: e

- I In the Model Builder window, under Component I (compl)>Plasma (plas), Ctrl-click to select Species: e, Species: O2, Species: O, Species: O-, Species: O2alDg, Species: O1D, Species: 02+, Species: 0+, Species: Ar, Species: Ars, and Species: Ar+.
- 2 Right-click and choose **Group**.

Species

In the Settings window for Group, type Species in the Label text field.

```
1: Ar+=>Ar, 2: Ars=>Ar, 3: O=>0.502, 4: O2+=>02, 5: O-=>0, 6: O2alDg=>02, 7:
OID=>0.502, 8: O+=>0
```

- I In the Model Builder window, under Component I (compl)>Plasma (plas), Ctrl-click to select 1: Ar+=>Ar, 2: Ars=>Ar, 3: 0=>0.502, 4: 02+=>02, 5: 0-=>0, 6: 02a1Dg=>02, 7: OID=>0.502, and 8: O+=>0.
- **2** Right-click and choose **Group**.

Surface Reactions

In the Settings window for Group, type Surface Reactions in the Label text field.

The surface reactions used in the model were created automatically but it is still necessary to specify at which boundary they are going to exist.

In the outlet boundary, it is assumed that ions are neutralized but nothing happens to neutrals. As such, neutral species don't have a Surface Reaction defined in the outlet.

$$I: Ar+=>Ar$$

- I In the Model Builder window, click I: Ar+=>Ar.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- 2: Ars => Ar
- I In the Model Builder window, click 2: Ars=>Ar.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- **4** Select Boundaries 3, 4, 6, 27, 33–36, 38, and 40 only.
- 3: 0=>0.502
- I In the Model Builder window, click 3: 0=>0.502.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- **4** Select Boundaries 3, 4, 6, 27, 33–36, 38, and 40 only.
- 4: 02+=>02
- I In the Model Builder window, click 4: 02+=>02.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.

- 5: O-=>O
- I In the Model Builder window, click 5: 0-=>0.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- 6: O2a1Dg=>O2
- I In the Model Builder window, click 6: 02a1Dg=>02.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- **4** Select Boundaries 3, 4, 6, 27, 33–36, 38, and 40 only.
- 7: OID=>0.502
- I In the Model Builder window, click 7: 01D=>0.502.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- **4** Select Boundaries 3, 4, 6, 27, 33–36, 38, and 40 only.
- 8: 0+=>0
- I In the Model Builder window, click 8: 0+=>0.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.

In the following, the initial mole fraction for O2 and the initial number density for ions are specified. The mass fraction of Ar is found from a mass constraint and the initial density of Ar+ is found by requiring electroneutrality.

The mole fraction of O2 is set at the inlet. Since the mass fraction of Ar is found from mass constraint nothing needs to be done to it.

Only neutral species have an **Outflow** boundary conditions. It is assumed that ions are neutralized at that boundary.

PLASMA (PLAS)

Surface Reactions

In the Model Builder window, collapse the Component I (compl)>Plasma (plas)> Surface Reactions node.

Species: 02

- I In the Model Builder window, under Component I (compl)>Plasma (plas)>Species click Species: 02.
- 2 In the Settings window for Species, locate the General Parameters section.
- **3** In the x_0 text field, type x02.

Inlet I

- I In the **Physics** toolbar, click **Attributes** and choose **Inlet**.
- 2 In the Settings window for Inlet, locate the Inlet section.
- 3 From the Mixture specification list, choose Mole fraction.
- **4** In the x_0 text field, type x02.
- 5 Locate the Boundary Selection section. Click Clear Selection.
- 6 Select Boundary 35 only.

Species: 02

In the Model Builder window, click Species: 02.

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 Click Clear Selection.
- 4 Select Boundary 39 only.

Species: O

- I In the Model Builder window, under Component I (compl)>Plasma (plas)>Species click Species: 0.
- 2 In the Settings window for Species, locate the General Parameters section.
- **3** In the x_0 text field, type x0.

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 Click Clear Selection.
- 4 Select Boundary 39 only.

Species: O-

I In the Model Builder window, under Component I (compl)>Plasma (plas)>Species click Species: 0-.

- 2 In the Settings window for Species, locate the General Parameters section.
- **3** In the n_0 text field, type 1E10[1/m³].

Species: O2aIDg

In the Model Builder window, click Species: 02al Dg.

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 Click Clear Selection.
- 4 Select Boundary 39 only.

Species: OID

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

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 Click Clear Selection.
- 4 Select Boundary 39 only.

Species: 02+

- I In the Model Builder window, under Component I (compl)>Plasma (plas)>Species click Species: 02+.
- 2 In the Settings window for Species, locate the Species Formula section.
- 3 Select the Initial value from electroneutrality constraint check box.

Species: O+

- I In the Model Builder window, click Species: 0+.
- 2 In the Settings window for Species, locate the General Parameters section.
- **3** In the n_0 text field, type 1E10[1/m³].

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: Ars

In the Model Builder window, click Species: Ars.

- I In the Physics toolbar, click Attributes and choose Outflow.
- 2 In the Settings window for Outflow, locate the Boundary Selection section.
- 3 Click Clear Selection.
- 4 Select Boundary 39 only.

Species: Ar+

- I In the Model Builder window, under Component I (compl)>Plasma (plas)>Species click Species: Ar+.
- 2 In the Settings window for Species, locate the General Parameters section.
- **3** In the n_0 text field, type 1E10[1/m³].

Set the plasma model to use the temperature, fluid velocity, and pressure computed by the Heat Transfer in Fluids and Laminar Flow interfaces.

PLASMA (PLAS)

Species

In the Model Builder window, collapse the Component I (compl)>Plasma (plas)>Species node.

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 From the **u** list, choose **Velocity field (spf)**.
- 4 From the T list, choose Temperature (ht).
- **5** From the p_A list, choose **Absolute pressure (spf)**.
- 6 Locate the Electron Density and Energy section. From the Electron transport properties list, choose From electron impact reactions.

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 1E15[1/m³].
- **4** In the ε_0 text field, type 2[V].

Ground 1

- 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 Walls.
- **4** Select Boundaries 4, 6, 27, 33–36, and 38–40 only.

The **Wall** node sets boundary conditions for the electron transport equations.

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 Walls.

Add the coil that is responsible to excite the plasma.

PLASMA (PLAS)

In the Model Builder window, collapse the Component I (compl)>Plasma (plas) node.

MAGNETIC FIELDS (MF)

- I In the Model Builder window, under Component I (compl) click Magnetic Fields (mf).
- 2 Select Domains 2–7 and 9 only.

Coil I

- I In the Physics toolbar, click **Domains** and choose **Coil**.
- 2 In the Settings window for Coil, locate the Domain Selection section.
- **3** From the **Selection** list, choose **Coils**.
- **4** Locate the **Coil** section. Select the **Coil** group check box.
- 5 From the Coil excitation list, choose Power.
- **6** In the P_{coil} text field, type Pw.

Set the thermodynamic properties and a heat source to use values computed in the Plasma interface.

Set the wall temperature to be 300 K.

HEAT TRANSFER IN FLUIDS (HT)

- I In the Model Builder window, under Component I (compl) click Heat Transfer in Fluids (ht).
- 2 In the Settings window for Heat Transfer in Fluids, locate the Domain Selection section.

- 3 Click Clear Selection.
- 4 Select Domain 2 only.

Fluid 1

- I In the Model Builder window, under Component I (compl)>Heat Transfer in Fluids (ht) click Fluid 1.
- 2 In the Settings window for Fluid, locate the Model Input section.
- **3** From the p_A list, choose **Absolute pressure (spf)**.
- 4 Locate the Heat Convection section. From the u list, choose Velocity field (spf).
- **5** Locate the **Heat Conduction, Fluid** section. From the k list, choose Thermal conductivity (plas/pes I).
- 6 Locate the Thermodynamics, Fluid section. From the Fluid type list, choose Gas/Liquid.
- 7 From the ρ list, choose **Density** (plas/pes I).
- 8 From the C_p list, choose Heat capacity at constant pressure (plas/pes1).
- **9** From the γ list, choose User defined.

Temperature I

- I In the Physics toolbar, click Boundaries and choose Temperature.
- 2 In the Settings window for Temperature, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- **4** Locate the **Temperature** section. In the T_0 text field, type 300[K].

Heat Source 1

- I In the Physics toolbar, click **Domains** and choose **Heat Source**.
- 2 In the Settings window for Heat Source, locate the Heat Source section.
- **3** From the Q_0 list, choose Heat source for gas (plas/pes1).
- 4 Select Domain 2 only.

Set the fluid properties to use values computed in the **Plasma** interface. And set the flow inlet and outlet in the system.

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 Domain Selection section.
- 3 Click Clear Selection.
- 4 Select Domain 2 only.

- 5 Locate the Physical Model section. From the Compressibility list, choose Compressible flow (Ma<0.3).
- **6** 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 Model Input section.
- **3** From the T list, choose **Temperature** (ht).
- 4 Locate the Fluid Properties section. From the ρ list, choose Density (plas/pes1).
- 5 From the μ list, choose Dynamic viscosity (plas/pes I).

Inlet I

- I In the Physics toolbar, click Boundaries and choose Inlet.
- 2 Select Boundary 35 only.
- 3 In the Settings window for Inlet, locate the Boundary Condition section.
- 4 From the list, choose Mass flow.
- 5 Locate the Mass Flow section. From the Mass flow type list, choose Standard flow rate (SCCM).
- **6** In the Q_{scem} text field, type Qf.
- 7 From the M_n list, choose Mean molar mass (plas/pes1).

Outlet I

- I In the Physics toolbar, click Boundaries and choose Outlet.
- 2 Select Boundary 39 only.

MESH I

Size 1

- I In the Model Builder window, under Component I (compl) right-click Mesh I and choose Size.
- 2 In the Settings window for Size, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- **4** Select Domain 2 only.
- 5 Locate the Element Size section. From the Calibrate for list, choose Plasma.

Size

- I In the Model Builder window, click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** From the **Predefined** list, choose **Finer**.

Size 2

- I In the Model Builder window, right-click Mesh I and choose Size.
- 2 In the Settings window for Size, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 From the Selection list, choose Walls.
- **5** Select Boundaries 4, 6, 27, 33–36, and 38–40 only.
- 6 Locate the Element Size section. From the Calibrate for list, choose Plasma.
- **7** From the **Predefined** list, choose **Finer**.

Mapped I

- I In the Mesh toolbar, click Mapped.
- 2 In the Settings window for Mapped, locate the Domain Selection section.
- 3 From the Geometric entity level list, choose Domain.
- **4** From the **Selection** list, choose **Coils**.

Distribution I

- I Right-click Mapped I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Boundary Selection section.
- 3 From the Selection list, choose Coils boundaries.
- 4 Locate the Distribution section. From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 25.
- 6 In the Element ratio text field, type 20.
- 7 Select the Symmetric distribution check box.

Free Triangular I

In the Mesh toolbar, click Free Triangular.

Boundary Layers 1

- I In the Mesh toolbar, click Boundary Layers.
- 2 In the Settings window for Boundary Layers, click to expand the Corner Settings section.
- 3 From the Handling of sharp corners list, choose No special handling.

- 4 Click to expand the Transition section. Clear the Smooth transition to interior mesh check box.
- 5 Locate the Domain Selection section. From the Geometric entity level list, choose Domain.
- **6** Select Domain 2 only.

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 Walls.
- **4** Select Boundaries 4, 6, 27, 33, 34, 36, and 38–40 only.
- 5 Click **Build All**.

The first study solves for 100 W and xO2=0.9. The solution of this study is going to be used in the subsequent study.

BASE CASE

- I In the Model Builder window, click Study I.
- 2 In the Settings window for Study, type Base Case in the Label text field.
- 3 In the Study toolbar, click $\underset{=0}{\overset{\cup}{}}$ Get Initial Value.

Organize the results from this study with a **Group** node.

RESULTS

Electric Potential (plas), Electron Density (plas), Electron Temperature (plas), Isothermal Contours (ht), Magnetic Flux Density Norm (mf), Magnetic Flux Density Norm, Revolved Geometry (mf), Pressure (spf), Temperature, 3D (ht), Velocity (spf), Velocity, 3D (spf)

- I In the Model Builder window, under Results, Ctrl-click to select Electron Density (plas), Electron Temperature (plas), Electric Potential (plas), Magnetic Flux Density Norm (mf), Magnetic Flux Density Norm, Revolved Geometry (mf), Temperature, 3D (ht), Isothermal Contours (ht), Velocity (spf), Pressure (spf), and Velocity, 3D (spf).
- 2 Right-click and choose **Group**.

Base Case

In the **Settings** window for **Group**, type Base Case in the **Label** text field.

BASE CASE

Steb 1: Frequency-Stationary

- I In the Model Builder window, expand the Base Case>Solver Configurations node, then click Base Case>Step I: Frequency-Stationary.
- 2 In the Settings window for Frequency-Stationary, locate the Study Settings section.
- **3** In the **Frequency** text field, type 13.56[MHz].

Solution I (soll)

- I In the Model Builder window, expand the Base Case>Solver Configurations> Solution I (soll)>Stationary Solver I node, then click Fully Coupled I.
- 2 In the Settings window for Fully Coupled, click to expand the Results While Solving section.
- **3** Select the **Plot** check box.
- 4 Click **Compute**.

RESULTS

Electron Density (plas)

Add a study to do a power sweep. This study will use the solution of the previous study as initial conditions to save computation time.

The **Initial damping factor** is set to 1 because a solution is used as initial condition and because the next parameter will use the previous solution.

ADD STUDY

- I In the Study toolbar, click Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select Preset Studies for Selected Multiphysics>Frequency-Stationary.
- 4 Click Add Study in the window toolbar.
- 5 In the Study toolbar, click Add Study to close the Add Study window.

STUDY 2

Step 1: Frequency-Stationary

- I In the Settings window for Frequency-Stationary, locate the Study Settings section.
- 2 In the Frequency text field, type 13.56[MHz].

- 3 Click to expand the Values of Dependent Variables section. Find the Initial values of variables solved for subsection. From the Settings list, choose User controlled.
- 4 From the Method list, choose Solution.
- 5 From the Study list, choose Base Case, Frequency-Stationary.
- 6 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.
- 7 Click + Add.
- **8** In the table, click to select the cell at row number 1 and column number 2.
- 9 Click Range.
- 10 In the Range dialog box, type 100 in the Start text field.
- II In the **Step** text field, type 50.
- 12 In the Stop text field, type 1000.
- 13 Click Replace.
- 14 In the Model Builder window, click Study 2.
- 15 In the Settings window for Study, type Power Sweep in the Label text field.
- 16 In the Study toolbar, click $t_{=0}^{U}$ Get Initial Value.

RESULTS

Electric Potential (plas) I, Electron Density (plas) I, Electron Temperature (plas) I, Isothermal Contours (ht) I, Magnetic Flux Density Norm (mf) I, Magnetic Flux Density Norm, Revolved Geometry (mf) I, Pressure (spf) I, Temperature, 3D (ht) I, Velocity (spf) I, Velocity, 3D (spf) I

- I In the Model Builder window, under Results, Ctrl-click to select Electron Density (plas) I, Electron Temperature (plas) I, Electric Potential (plas) I, Magnetic Flux Density Norm (mf) I, Magnetic Flux Density Norm, Revolved Geometry (mf) I, Temperature, 3D (ht) I, Isothermal Contours (ht) I, Velocity (spf) I, Pressure (spf) I, and Velocity, 3D (spf) I.
- 2 Right-click and choose **Group**.

RESULTS

Power Sweep

- I In the Model Builder window, expand the Power Sweep>Solver Configurations node, then click Results>Group 6.
- 2 In the Settings window for Group, type Power Sweep in the Label text field.

POWER SWEEP

Solution 2 (sol2)

- I In the Model Builder window, expand the Power Sweep>Solver Configurations> Solution 2 (sol2)>Stationary Solver I node, then click Fully Coupled I.
- 2 In the Settings window for Fully Coupled, click to expand the Method and Termination section.
- 3 In the Initial damping factor text field, type 1.
- **4** Locate the **Results While Solving** section. Select the **Plot** check box.
- 5 From the Plot group list, choose Electron Density (plas) 1.
- 6 In the Study toolbar, click **Compute**.

RESULTS

Electron Density (plas) I

Add a study to do a O2 mole fraction sweep. This study will use a solution of the previous study as initial conditions to save computation time.

The **Initial damping factor** is again set to 1 because a solution is used as initial condition and because the next parameter will use the previous solution.

ADD STUDY

- I In the Study toolbar, click Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select Preset Studies for Selected Multiphysics>Frequency-Stationary.
- 4 Click Add Study in the window toolbar.
- 5 In the Study toolbar, click Add Study to close the Add Study window.

STUDY 3

Step 1: Frequency-Stationary

- I In the Settings window for Frequency-Stationary, locate the Study Settings section.
- 2 In the Frequency text field, type 13.56[MHz].
- 3 Locate the Values of Dependent Variables section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose User controlled.
- 4 From the Method list, choose Solution.

- 5 From the Study list, choose Power Sweep, Frequency-Stationary.
- 6 From the Parameter value (Pw (W)) list, choose 500 W.
- 7 Locate the Study Extensions section. Select the Auxiliary sweep check box.
- 8 From the Sweep type list, choose All combinations.
- 9 Click + Add.
- **10** In the table, click to select the cell at row number 1 and column number 2.
- II In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xO2		

- 12 Click Range.
- 13 In the Range dialog box, type 0.9 in the Start text field.
- **I4** In the **Step** text field, type -0.1.
- **I5** In the **Stop** text field, type **0.1**.
- 16 Click Replace.
- 17 In the Settings window for Frequency-Stationary, locate the Study Extensions section.
- 18 Click + Add.
- 19 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Pw	500	W

- 20 In the Model Builder window, click Study 3.
- 21 In the Settings window for Study, type x02 Sweep in the Label text field.
- **22** In the Study toolbar, click $\underset{=}{\overset{\cup}{\cup}}$ Get Initial Value.

RESULTS

Electric Potential (plas) 2, Electron Density (plas) 2, Electron Temperature (plas) 2, Isothermal Contours (ht) 2, Magnetic Flux Density Norm (mf) 2, Magnetic Flux Density Norm, Revolved Geometry (mf) 2, Pressure (spf) 2, Temperature, 3D (ht) 2, Velocity (spf) 2, Velocity, 3D (spf) 2

I In the Model Builder window, under Results, Ctrl-click to select Electron Density (plas) 2, Electron Temperature (plas) 2, Electric Potential (plas) 2, Magnetic Flux Density Norm (mf) 2, Magnetic Flux Density Norm,

Revolved Geometry (mf) 2, Temperature, 3D (ht) 2, Isothermal Contours (ht) 2, Velocity (spf) 2, Pressure (spf) 2, and Velocity, 3D (spf) 2.

2 Right-click and choose **Group**.

RESULTS

xO2 Sweep

- I In the Model Builder window, expand the xO2 Sweep>Solver Configurations node, then click Results>Group 7.
- 2 In the Settings window for Group, type x02 Sweep in the Label text field.

XO2 SWEEP

Solution 3 (sol3)

- I In the Model Builder window, expand the xO2 Sweep>Solver Configurations> Solution 3 (sol3)>Stationary Solver I node, then click Fully Coupled I.
- 2 In the Settings window for Fully Coupled, locate the Method and Termination section.
- 3 In the **Initial damping factor** text field, type 1.
- **4** Locate the **Results While Solving** section. Select the **Plot** check box.
- 5 From the Plot group list, choose Electron Density (plas) 2.
- 6 In the Study toolbar, click **Compute**.

RESULTS

Negative Ion Density

- I In the Home toolbar, click Add Plot Group and choose 2D Plot Group. Create plots for the negative ion density, the power absorbed by the electrons, the space distribution of the charged species along the axis-of-symmetry, and for averaged densities of charged species as a function of power and oxygen mole fraction.
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Dataset list, choose Power Sweep/Solution 2 (sol2).
- 4 In the Label text field, type Negative Ion Density.

Surface 1

- I Right-click Negative Ion Density and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- 3 In the Expression text field, type plas.n w0 1m.

4 In the Negative Ion Density toolbar, click Plot.

Absorbed Power

- I In the Home toolbar, click **Add Plot Group** and choose **2D Plot Group**.
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Dataset list, choose Power Sweep/Solution 2 (sol2).
- 4 In the Label text field, type Absorbed Power.

Surface 1

- I Right-click Absorbed Power and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- 3 In the Expression text field, type mf.Qrh.
- 4 Locate the Coloring and Style section. Click Change Color Table.
- 5 In the Color Table dialog box, select Thermal>ThermalWave in the tree.
- 6 Click OK.

Selection 1

- I Right-click Surface I and choose Selection.
- **2** Select Domain 2 only.
- 3 In the Absorbed Power toolbar, click Plot.

Charged Species Along Axis-of-Symmetry

- I In the Home toolbar, click **Add Plot Group** and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Charged Species Along Axis-of-Symmetry in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Power Sweep/Solution 2 (sol2).
- 4 From the Parameter selection (Pw) list, choose Last.
- **5** Click to expand the **Title** section. From the **Title type** list, choose **None**.
- **6** Locate the **Plot Settings** section.
- 7 Select the y-axis label check box. In the associated text field, type Number density (1/ m < sup > 3 < / sup >).
- 8 Locate the Legend section. From the Position list, choose Lower middle.

Line Graph 1

- I Right-click Charged Species Along Axis-of-Symmetry and choose Line Graph.
- **2** Select Boundary 3 only.

- 3 In the Settings window for Line Graph, locate the x-Axis Data section.
- 4 From the Parameter list, choose Expression.
- **5** In the **Expression** text field, type z.
- 6 Click to expand the **Legends** section. Select the **Show legends** check box.
- **7** Find the **Include** subsection. Clear the **Solution** check box.
- 8 Select the Expression check box.

Line Graph 2

- I Right-click Line Graph I 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.n w02 1p.

Line Graph 3

- I Right-click Line Graph 2 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. n w0 1p.

Line Grabh 4

- I Right-click Line Graph 3 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.n wAr 1p.

Line Graph 5

- I Right-click Line Graph 4 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.n w0 1m.
- 4 Click the y-Axis Log Scale button in the Graphics toolbar.

Space Averaged Charged Species vs. Power

- I In the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Space Averaged Charged Species vs. Power in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Power Sweep/Solution 2 (sol2).
- 4 Locate the Title section. From the Title type list, choose None.
- 5 Locate the Plot Settings section.
- 6 Select the x-axis label check box. In the associated text field, type Power (W).

- 7 Select the y-axis label check box. In the associated text field, type Number density (1/m³).
- 8 Locate the Legend section. From the Position list, choose Lower right.

Global I

- I Right-click Space Averaged Charged Species vs. Power and choose Global.
- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
aveop1(plas.ne)	1/m^3	ne
aveop1(plas.n_wAr_1p)	1/m^3	Ar+
aveop1(plas.n_w02_1p)	1/m^3	02+
aveop1(plas.n_w0_1p)	1/m^3	0+
aveop1(plas.n_w0_1m)	1/m^3	0 -

- 4 Click to expand the Legends section. Find the Include subsection. Clear the Solution check box.
- 5 In the Space Averaged Charged Species vs. Power toolbar, click Plot.
- 6 Click the y-Axis Log Scale button in the Graphics toolbar.

Space Averaged Charged Species vs. xO2

- I In the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the **Settings** window for **ID Plot Group**, type Space Averaged Charged Species vs. x02 in the **Label** text field.
- 3 Locate the Data section. From the Dataset list, choose xO2 Sweep/Solution 3 (sol3).
- 4 From the Parameter selection (Pw) list, choose First.
- **5** Locate the **Title** section. From the **Title type** list, choose **None**.
- 6 Locate the Plot Settings section.
- 7 Select the x-axis label check box. In the associated text field, type x02.
- 8 Select the **y-axis label** check box. In the associated text field, type Number density (1/ m³).
- **9** Locate the Legend section. From the Position list, choose Lower middle.

Global I

- I Right-click Space Averaged Charged Species vs. x02 and choose Global.
- 2 In the Settings window for Global, locate the y-Axis Data section.

3 In the table, enter the following settings:

Expression	Unit	Description
aveop1(plas.ne)	1/m^3	ne
aveop1(plas.n_wAr_1p)	1/m^3	Ar+
aveop1(plas.n_w02_1p)	1/m^3	02+
aveop1(plas.n_wAr_1p)	1/m^3	0+
aveop1(plas.n_w0_1m)	1/m^3	0 -

- 4 Locate the x-Axis Data section. From the Axis source data list, choose x02.
- **5** Locate the **Legends** section. Find the **Include** subsection. Clear the **Solution** check box.
- 6 In the Space Averaged Charged Species vs. x02 toolbar, click on Plot.
- 7 Click the y-Axis Log Scale button in the Graphics toolbar.