



Model of an Argon/Oxygen Inductively Coupled Plasma Reactor

Introduction

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 O₂) in which one of the species can dissociate by electron impact (O₂ 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 parameterization 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 drift-diffusion 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*.

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

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

The electron source R_e and the energy loss due to inelastic collisions R_ϵ are defined later. The electron diffusivity, energy mobility, and energy diffusivity are computed from the electron mobility using:

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

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_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: $1/\text{m}^3$). The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^P x_j k_j N_n n_e \Delta \varepsilon_j$$

where $\Delta \varepsilon_j$ is the energy loss from reaction j (SI unit: V). The rate coefficients can be computed from cross section data by the following integral:

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

where $\gamma = (2q/m_e)^{1/2}$ (SI unit: $\text{C}^{1/2}/\text{kg}^{1/2}$), m_e is the electron mass (SI unit: kg), ε is energy (SI unit: V), σ_k is the collision cross section (SI unit: m^2), and f is the electron energy distribution function.

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:

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

where n_e is the electron density, q is the electron charge, m_e is the electron mass, ν_e 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:

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

and the electron energy flux:

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

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:

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

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 an 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 from [Ref. 4](#)).

TABLE 1: ARGON REACTIONS

REACTION	FORMULA	TYPE	$\Delta\epsilon(\text{eV})$
1	$\text{e} + \text{Ar} \Rightarrow \text{e} + \text{Ar}$	Elastic	-
2	$\text{e} + \text{Ar} \Rightarrow \text{e} + \text{Ar}^*$	Excitation	11.5
3	$\text{e} + \text{Ar}^* \Rightarrow \text{e} + \text{Ar}$	Superelastic	-11.5
4	$\text{e} + \text{Ar} \Rightarrow 2\text{e} + \text{Ar}^+$	Ionization	15.8
5	$\text{e} + \text{Ar}^* \Rightarrow 2\text{e} + \text{Ar}^+$	Ionization	4.24
6	$\text{Ar}^* + \text{Ar}^* \Rightarrow \text{e} + \text{Ar} + \text{Ar}^+$	Penning ionization	-
7	$\text{Ar}^* + \text{Ar} \Rightarrow \text{Ar} + \text{Ar}$	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 O_2 are from [Ref. 5](#) and electron impact reaction with O are from [Ref. 6](#) except for $\text{e} + \text{O} \Rightarrow \text{O} + \text{e}$, 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 O_2 and O excited states. The only oxygen excited states that are solved explicitly are the singlet delta metastable of molecular oxygen $\text{O}_2(a^1\Delta_g)$ and the metastable state $\text{O}(^1D)$.

TABLE 2: OXYGEN ELECTRON IMPACT REACTIONS

REACTION	FORMULA	TYPE	$\Delta\epsilon(\text{eV})$
1	$\text{e} + \text{O}_2 \Rightarrow \text{O} + \text{O}^-$	Dissociative attachment	-
2	$\text{e} + \text{O}_2 \Rightarrow \text{e} + \text{O}_2$	Elastic	-
3	$\text{e} + \text{O}_2 \Rightarrow \text{e} + \text{O}_2^*$	Rotational excitation	0.02
4	$\text{e} + \text{O}_2 \Rightarrow \text{e} + \text{O}_2^*$	Vibrational excitation	0.19

TABLE 2: OXYGEN ELECTRON IMPACT REACTIONS

REACTION	FORMULA	TYPE	$\Delta\epsilon(\text{eV})$
5	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Vibrational excitation	0.19
6	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Vibrational excitation	0.38
7	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Vibrational excitation	0.38
8	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Vibrational excitation	0.57
9	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Vibrational excitation	0.75
10	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2(\text{a}^1\Delta_g)$	Excitation	0.977
11	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Excitation	1.627
12	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Excitation	4.5
13	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}+\text{O}$	Dissociative excitation	6.0
14	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}+\text{O}(\text{}^1\text{D})$	Excitation	8.4
15	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2$	Excitation	9.97
16	$\text{e}+\text{O}_2\Rightarrow\text{e}+\text{O}_2^+$	Ionization	12.06
17	$\text{e}+\text{O}\Rightarrow\text{e}+\text{O}$	Elastic	-
18	$\text{e}+\text{O}\Rightarrow\text{e}+\text{O}(\text{}^1\text{D})$	Excitation	1.968
19	$\text{e}+\text{O}\Rightarrow\text{e}+\text{O}$	Excitation	4.192
20	$\text{e}+\text{O}\Rightarrow\text{e}+\text{c}$	Ionization	13.618
21	$\text{e}+\text{O}^-\Rightarrow\text{O}+\text{e}+\text{e}$	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	$\text{O}^++\text{O}_2\Rightarrow\text{O}+\text{O}_2^+$	Charge transfer
2	$\text{O}^++\text{O}^-\Rightarrow\text{O}+\text{O}$	Mutual recombination
3	$\text{O}^++\text{O}_2^+\Rightarrow3\text{O}$	Mutual recombination
4	$\text{O}^++\text{O}_2^+\Rightarrow\text{O}+\text{O}_2$	Mutual recombination
5	$\text{O}^++\text{O}_2\Rightarrow\text{O}_2+\text{e}$	Detachment
6	$\text{O}^++\text{Ar}^+\Rightarrow\text{O}+\text{Ar}$	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)
1	$\text{Ar s} \Rightarrow \text{Ar}$	1	0	0
2	$\text{Ar}^+ \Rightarrow \text{Ar}$	1	0.07	5.8
3	$\text{O} \Rightarrow 0.5\text{O}_2$	0.2	0	0
4	$\text{O}_2^+ \Rightarrow \text{O}_2$	1	0.05	4
5	$\text{O}^- \Rightarrow \text{O}$	1	0	0
6	$\text{O}_2(\text{a}^1\Delta_g) \Rightarrow \text{O}$	1	0	0
7	$\text{O}(\text{D}) \Rightarrow 0.5\text{O}_2$	0.2	0	0
8	$\text{O}^+ \Rightarrow \text{O}$	1	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, $e + \text{O}_2 \Rightarrow \text{O} + \text{O}^-$). 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, $\text{O}^- + \text{O}^+ \Rightarrow \text{O} + \text{O}$ or $\text{O}^- + \text{Ar}^+ \Rightarrow \text{O} + \text{Ar}$), detachment in collisions

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

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 an **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 O₂ 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 an electronegative core (where the electrons have a flat profile) and electropositive edges (where the negative ion density drops fast toward 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^+ .

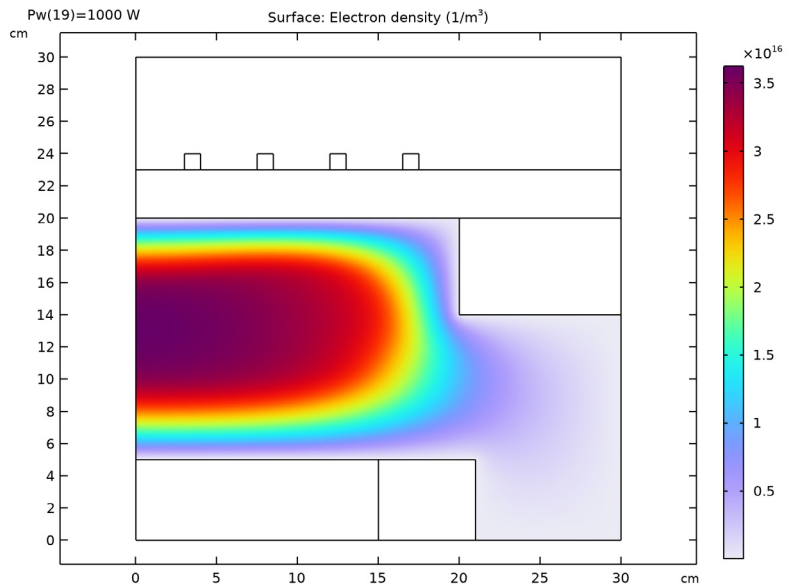


Figure 1: Electron density spatial distribution at 1000 W.

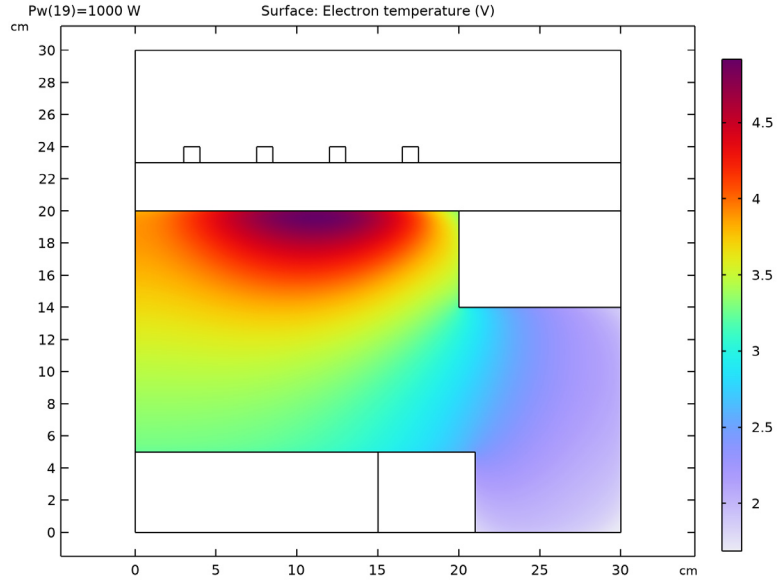


Figure 2: Electron temperature spatial distribution at 1000 W.

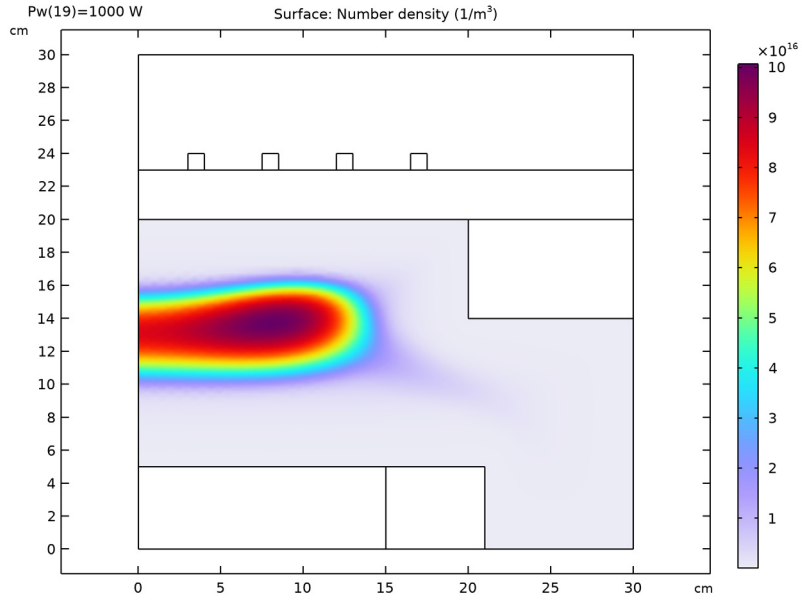


Figure 3: Negative ions density spatial distribution at 1000 W.

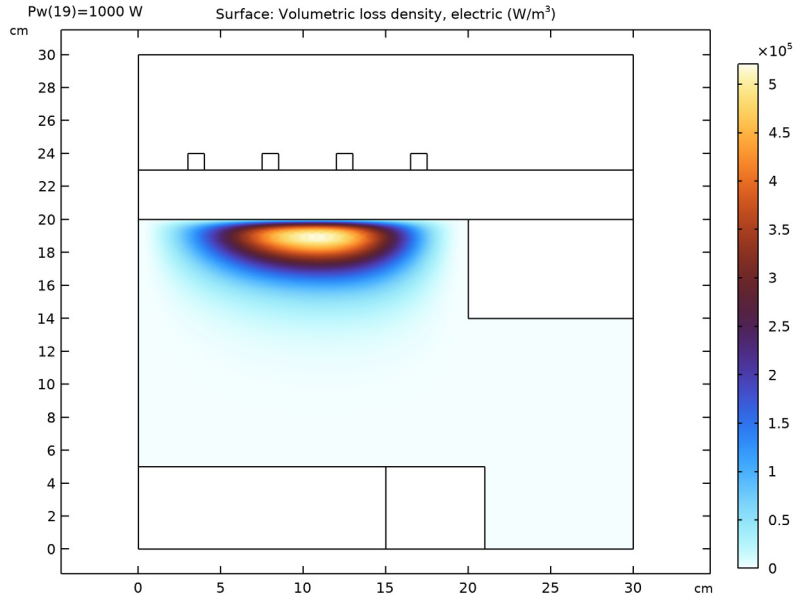


Figure 4: Power absorbed by the electrons at 1000 W.

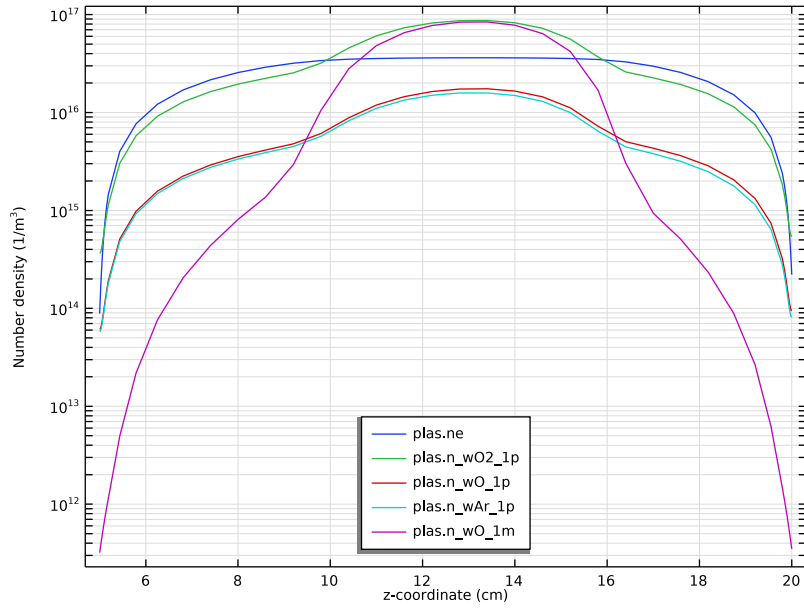


Figure 5: Charged species distribution along the axis-of-symmetry at 1000 W.

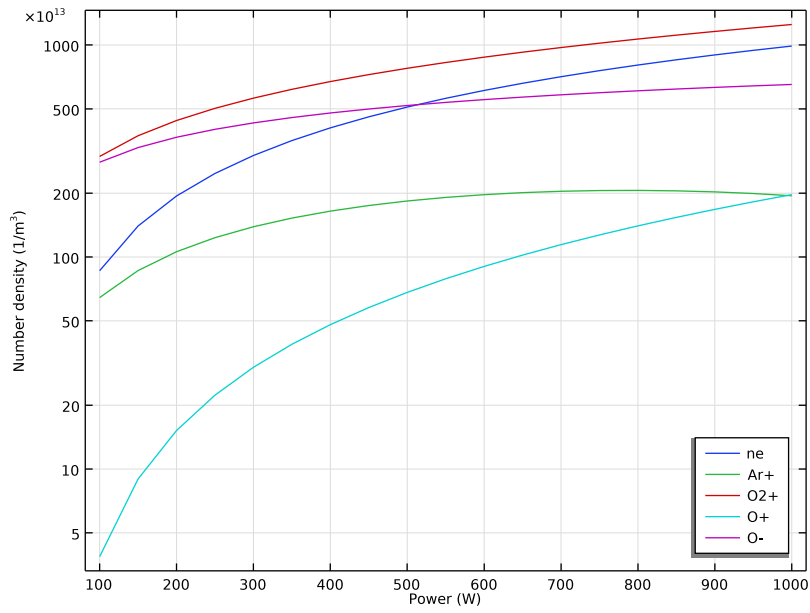


Figure 6: Spatial averaged number density of the charged species as a function of power.

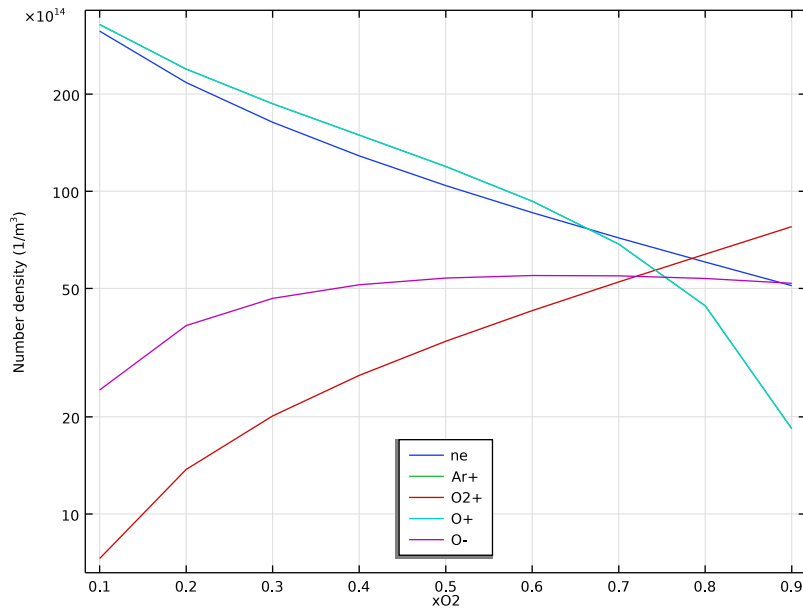


Figure 7: Spatial averaged number density of the charged species as a function of oxygen mole fraction.

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




Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click  **Model Wizard**.

MODEL WIZARD


- 1 In the **Model Wizard** window, click  **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 an ICP reactor.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
- 2 In the **Settings** window for **Geometry**, locate the **Units** section.
- 3 From the **Length unit** list, choose **cm**.

Rectangle 1 (r1)


- 1 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)


- 1 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)

- 1 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 1 (arr1)

- 1 In the **Geometry** toolbar, click  **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)

- 1 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)

- 1 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)

- 1 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 1 (ls1)

- 1 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


- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 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	1E-4	
p0	0.02[torr]	2.6664 Pa	

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


DEFINITIONS

Walls

- 1 In the **Definitions** toolbar, click  **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

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

Coil Boundaries

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

Average I (aveopI)

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

Assign material properties to the different regions of the modeling domain. The domain where the plasma exists is automatically assigned a relative permittivity of 1.


DEFINITIONS

In the **Model Builder** window, collapse the **Component 1 (comp1)>Definitions** node.

GEOMETRY 1

In the **Model Builder** window, collapse the **Component 1 (comp1)>Geometry 1** node.


ADD MATERIAL

- 1 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  **Add Material** to close the **Add Material** window.

MATERIALS

Air (mat1)

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Air (mat1)**.
- 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)

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

Copper (mat3)

- 1 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

- 1 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** (if it is not already selected).



- 3 Click  **Done** 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

- 1 In the **Model Builder** window, under **Global Definitions** click **Plasma Chemistry I**.
- 2 In the **Settings** window for **Plasma Chemistry**, locate the **Plasma Chemistry Import** section.
- 3 Click **Browse**.
- 4 Browse to the model's Application Libraries folder and double-click the file `Ar_O2_plasma_chemistry.txt`.
- 5 Click **Import**.

PLASMA (PLAS)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** 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.
- 11 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: $e+O_2 \Rightarrow e+O_2aIDg$, 11: $e+O_2 \Rightarrow e+O_2$, 12: $e+O_2 \Rightarrow e+O_2$, 13: $e+O_2 \Rightarrow e+O+O$, 14: $e+O_2 \Rightarrow e+O+O1D$, 15: $e+O_2 \Rightarrow e+O_2$, 16: $e+O_2 \Rightarrow 2e+O_2+$, 17: $e+O \Rightarrow e+O$, 18: $e+O \Rightarrow e+O1D$, 19: $e+O \Rightarrow e+O$, 1: $e+O_2 \Rightarrow O+O-$, 20: $e+O \Rightarrow 2e+O+$, 21: $e+Ar \Rightarrow e+Ar$, 22: $e+Ar \Rightarrow e+Ar$, 23: $e+Ar \Rightarrow e+Ar$, 24: $e+Ar \Rightarrow 2e+Ar+$, 25: $e+Ar \Rightarrow 2e+Ar+$, 26: $e+O \Rightarrow O+e+e$, 2: $e+O_2 \Rightarrow e+O_2$, 3: $e+O_2 \Rightarrow e+O_2$, 4: $e+O_2 \Rightarrow e+O_2$, 5: $e+O_2 \Rightarrow e+O_2$, 6: $e+O_2 \Rightarrow e+O_2$, 7: $e+O_2 \Rightarrow e+O_2$, 8: $e+O_2 \Rightarrow e+O_2$, 9: $e+O_2 \Rightarrow e+O_2$, Cross Section Import 1, Cross Section Import 2, Cross Section Import 3

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)**, Ctrl-click to select **Cross Section Import 1, Cross Section Import 2, Cross Section Import 3, 1: $e+O_2 \Rightarrow O+O-$, 2: $e+O_2 \Rightarrow e+O_2$, 3: $e+O_2 \Rightarrow e+O_2$, 4: $e+O_2 \Rightarrow e+O_2$, 5: $e+O_2 \Rightarrow e+O_2$, 6: $e+O_2 \Rightarrow e+O_2$, 7: $e+O_2 \Rightarrow e+O_2$, 8: $e+O_2 \Rightarrow e+O_2$, 9: $e+O_2 \Rightarrow e+O_2$, 10: $e+O_2 \Rightarrow e+O_2aIDg$, 11: $e+O_2 \Rightarrow e+O_2$, 12: $e+O_2 \Rightarrow e+O_2$, 13: $e+O_2 \Rightarrow e+O+O$, 14: $e+O_2 \Rightarrow e+O+O1D$, 15: $e+O_2 \Rightarrow e+O_2$, 16: $e+O_2 \Rightarrow 2e+O_2+$, 17: $e+O \Rightarrow e+O$, 18: $e+O \Rightarrow e+O1D$, 19: $e+O \Rightarrow e+O$, 20: $e+O \Rightarrow 2e+O+$, 21: $e+Ar \Rightarrow e+Ar$, 22: $e+Ar \Rightarrow e+Ar$, 23: $e+Ar \Rightarrow e+Ar$, 24: $e+Ar \Rightarrow 2e+Ar+$, 25: $e+Ar \Rightarrow 2e+Ar+$, and 26: $e+O \Rightarrow O+e+e$.**

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

Electron Impact Cross Sections

1 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: $O++O_2 \Rightarrow O+O_2+$, 28: $O-+O+ \Rightarrow O+O$, 29: $O-+O_2+ \Rightarrow O+O+O$, 30: $O-+O_2+ \Rightarrow O+O_2$, 31: $O-+O \Rightarrow O_2+e$, 32: $O-+Ar+ \Rightarrow O+Ar$

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)**, Ctrl-click to select **27: $O++O_2 \Rightarrow O+O_2+$, 28: $O-+O+ \Rightarrow O+O$, 29: $O-+O_2+ \Rightarrow O+O+O$, 30: $O-+O_2+ \Rightarrow O+O_2$, 31: $O-+O \Rightarrow O_2+e$, and 32: $O-+Ar+ \Rightarrow O+Ar$.**

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

Heavy Species Reactions

1 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: O1D, Species: O2, Species: O2+, Species: O2aIDg, Species: e

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)**, Ctrl-click to select **Species: e, Species: O2, Species: O, Species: O-, Species: O2aIDg, Species: O1D, Species: O2+, Species: O+, 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: $\text{Ar}+ \Rightarrow \text{Ar}$, 2: $\text{Ar}s \Rightarrow \text{Ar}$, 3: $\text{O} \Rightarrow 0.5\text{O}_2$, 4: $\text{O}_2+ \Rightarrow \text{O}_2$, 5: $\text{O}- \Rightarrow \text{O}$, 6: $\text{O}_2a\text{IDg} \Rightarrow \text{O}_2$, 7: $\text{O}\text{ID} \Rightarrow 0.5\text{O}_2$, 8: $\text{O}+ \Rightarrow \text{O}$

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)**, Ctrl-click to select **1: $\text{Ar}+ \Rightarrow \text{Ar}$** , **2: $\text{Ar}s \Rightarrow \text{Ar}$** , **3: $\text{O} \Rightarrow 0.5\text{O}_2$** , **4: $\text{O}_2+ \Rightarrow \text{O}_2$** , **5: $\text{O}- \Rightarrow \text{O}$** , **6: $\text{O}_2a\text{IDg} \Rightarrow \text{O}_2$** , **7: $\text{O}\text{ID} \Rightarrow 0.5\text{O}_2$** , and **8: $\text{O}+ \Rightarrow \text{O}$** .

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 the boundaries where they take place.

On the outlet boundary, it is assumed that ions are neutralized but nothing happens to neutrals. For this reason, neutral species do not have a **Surface Reaction** defined at the outlet.

1: $\text{Ar}+ \Rightarrow \text{Ar}$

1 In the **Model Builder** window, click **1: $\text{Ar}+ \Rightarrow \text{Ar}$** .

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

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

2: $\text{Ar}s \Rightarrow \text{Ar}$

1 In the **Model Builder** window, click **2: $\text{Ar}s \Rightarrow \text{Ar}$** .

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: $\text{O} \Rightarrow 0.5\text{O}_2$

1 In the **Model Builder** window, click **3: $\text{O} \Rightarrow 0.5\text{O}_2$** .

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: $\text{O}_2+ \Rightarrow \text{O}_2$

1 In the **Model Builder** window, click **4: $\text{O}_2+ \Rightarrow \text{O}_2$** .

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

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

5: $O \Rightarrow O$

1 In the **Model Builder** window, click **5: $O \Rightarrow O$** .

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

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

6: $O_2 aIDg \Rightarrow O_2$

1 In the **Model Builder** window, click **6: $O_2 aIDg \Rightarrow O_2$** .

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: $OID \Rightarrow 0.5O_2$

1 In the **Model Builder** window, click **7: $OID \Rightarrow 0.5O_2$** .

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: $O+ \Rightarrow O$

1 In the **Model Builder** window, click **8: $O+ \Rightarrow O$** .

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 O_2 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 O_2 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 condition. It is assumed that ions are neutralized at the outlet.

PLASMA (PLAS)



Surface Reactions

In the **Model Builder** window, collapse the **Component 1 (comp1)>Plasma (plas)>Surface Reactions** node.

Species: O2

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)>Species** click **Species: O2**.
- 2 In the **Settings** window for **Species**, locate the **General Parameters** section.
- 3 In the x_0 text field, type x_{O2} .



Inlet 1

- 1 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 x_{O2} .
- 5 Locate the **Boundary Selection** section. Click  **Clear Selection**.
- 6 Select Boundary 35 only.

Species: O2

In the **Model Builder** window, click **Species: O2**.



Outflow 1

- 1 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

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)>Species** click **Species: O**.
- 2 In the **Settings** window for **Species**, locate the **General Parameters** section.
- 3 In the x_0 text field, type x_O .

Outflow 1

- 1 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-



- 1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)>Species** click **Species: O-**.

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

Species: O2aIDg

In the **Model Builder** window, click **Species: O2aIDg**.



Outflow I

- 1 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 1 (comp1)>Plasma (plas)>Species** click **Species: OID**.

Outflow I

- 1 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: O2+

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma (plas)>Species** click **Species: O2+**.
- 2 In the **Settings** window for **Species**, locate the **Species Formula** section.
- 3 Select the **Initial value from electroneutrality constraint** check box.

Species: O+

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



Species: Ar

- 1 In the **Model Builder** window, click **Species: Ar**.
- 2 In the **Settings** window for **Species**, locate the **Species Formula** section.
- 3 Select the **From mass constraint** check box.

Species: Ars

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

Outflow 1

- 1 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+

- 1 In the **Model Builder** window, under **Component 1 (comp1)>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 $1E10[1/m^3]$.

Set the **Additional enthalpy contribution** field for species with internal energy so that the reaction enthalpy is correctly computed.

Species: O2a1Dg

- 1 In the **Model Builder** window, click **Species: O2a1Dg**.
- 2 In the **Settings** window for **Species**, click to expand the **Species Thermodynamic Parameters** section.
- 3 In the Δh text field, type $9.77e-1$.

Species: O1D

- 1 In the **Model Builder** window, click **Species: O1D**.
- 2 In the **Settings** window for **Species**, locate the **Species Thermodynamic Parameters** section.
- 3 In the Δh text field, type 1.968 .

Species: O2+

- 1 In the **Model Builder** window, click **Species: O2+**.
- 2 In the **Settings** window for **Species**, locate the **Species Thermodynamic Parameters** section.
- 3 In the Δh text field, type 12.06 .

Species: O+

- 1 In the **Model Builder** window, click **Species: O+**.
- 2 In the **Settings** window for **Species**, locate the **Species Thermodynamic Parameters** section.
- 3 In the Δh text field, type 13.618 .

Species: Ars

- 1 In the **Model Builder** window, click **Species: Ars**.
- 2 In the **Settings** window for **Species**, locate the **Species Thermodynamic Parameters** section.
- 3 In the Δh text field, type 11.5.

Species: Ar+

- 1 In the **Model Builder** window, click **Species: Ar+**.
- 2 In the **Settings** window for **Species**, locate the **Species Thermodynamic Parameters** section.
- 3 In the Δh text field, type 15.8.

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 1 (comp1)>Plasma (plas)>Species** node.


Plasma Model 1

- 1 In the **Model Builder** window, click **Plasma Model 1**.
- 2 In the **Settings** window for **Plasma Model**, locate the **Model Inputs** section.
- 3 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

- 1 In the **Model Builder** window, click **Initial Values 1**.
- 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

- 1 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

- 1 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 for exciting the plasma.


PLASMA (PLAS)

In the **Model Builder** window, collapse the **Component 1 (comp1)>Plasma (plas)** node.

MAGNETIC FIELDS (MF)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Magnetic Fields (mf)**.
- 2 Select Domains 2–7 and 9 only.


Coil

- 1 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 P_w .

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

Set the wall temperature to 300 K.


HEAT TRANSFER IN FLUIDS (HT)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** 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

- 1 In the **Model Builder** window, under **Component 1 (comp1)**>**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 \mathbf{u} list, choose **Velocity field (spf)**.
- 5 Locate the **Heat Conduction, Fluid** section. From the k list, choose **Thermal conductivity (plas/pes1)**.
- 6 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.
- 7 From the ρ list, choose **Density (plas/pes1)**.
- 8 From the C_p list, choose **Heat capacity at constant pressure (plas/pes1)**.
- 9 From the γ list, choose **User defined**.

Temperature 1


- 1 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

- 1 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)


- 1 In the **Model Builder** window, under **Component 1 (comp1)** 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 I

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Laminar Flow (spf)** click **Fluid Properties I**.
- 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/pes1)**.

Inlet I

- 1 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_{sccm} text field, type Qf.
- 7 From the M_n list, choose **Mean molar mass (plas/pes1)**.

Outlet I

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

MESH I

Size I

- 1 In the **Model Builder** window, under **Component 1 (comp1)** 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


- 1 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

- 1 In the **Model Builder** window, right-click **Mesh 1** 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 1

- 1 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 1

- 1 Right-click **Mapped 1** and choose **Distribution**.
- 2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Coil 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 1


- In the **Mesh** toolbar, click  **Free Triangular**.

Boundary Layers 1

- 1 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

- 1 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 $x_{O_2}=0.9$. The solution of this study will be used in the subsequent study.

BASE CASE

- 1 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  **Get Initial Value**.

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

RESULTS

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

- 1 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 (ht)**, **Velocity (spf)**, **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

Step 1: Frequency-Stationary

- 1 In the **Model Builder** window, expand the **Base Case>Solver Configurations** node, then click **Base Case>Step 1: 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 1 (sol1)

- 1 In the **Model Builder** window, expand the **Base Case>Solver Configurations>Solution 1 (sol1)>Stationary Solver 1** node, then click **Fully Coupled 1**.
- 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

- 1 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

- 1 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.
- 11 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  **Get Initial Value**.

RESULTS

Electric Potential (plas) 1, Electron Density (plas) 1, Electron Temperature (plas) 1, Magnetic Flux Density Norm (mf) 1, Magnetic Flux Density Norm, Revolved Geometry (mf) 1, Pressure (spf) 1, Temperature (ht) 1, Velocity (spf) 1, Velocity, 3D (spf) 1

- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Electron Density (plas) 1**, **Electron Temperature (plas) 1**, **Electric Potential (plas) 1**, **Magnetic Flux Density Norm (mf) 1**, **Magnetic Flux Density Norm, Revolved Geometry (mf) 1**, **Temperature (ht) 1**, **Pressure (spf) 1**, **Velocity (spf) 1**, **Pressure (spf) 1**, and **Velocity, 3D (spf) 1**.
- 2 Right-click and choose **Group**.

RESULTS


Power Sweep

- 1 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)

- 1 In the **Model Builder** window, expand the **Power Sweep>Solver Configurations>Solution 2 (sol2)>Stationary Solver 1** node, then click **Fully Coupled 1**.
- 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) I**.
- 6 In the **Study** toolbar, click  **Compute**.



RESULTS

Electron Density (plas) I

Add a study to do an 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

- 1 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


- 1 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.
- 11 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.
- 14 In the **Step** text field, type -0.1.
- 15 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 xO2 Sweep in the **Label** text field.
- 22 In the **Study** toolbar, click  **Get Initial Value**.

RESULTS

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

- 1 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 (ht) 2**, **Velocity, 3D (spf) 2**, **Velocity (spf) 2**, **Pressure (spf) 2**, and **Velocity, 3D (spf) 2**.
- 2 Right-click and choose **Group**.


RESULTS

xO2 Sweep

- 1 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 xO2 Sweep in the **Label** text field.


XO2 SWEEP

Solution 3 (sol3)


- 1 In the **Model Builder** window, expand the **xO2 Sweep>Solver Configurations>Solution 3 (sol3)>Stationary Solver 1** node, then click **Fully Coupled 1**.
- 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

- 1 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 symmetry axis, and for averaged densities of the charged species as functions 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

- 1 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

- 1 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

1 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

1 Right-click **Surface 1** and choose **Selection**.

2 Select Domain 2 only.

3 In the **Absorbed Power** toolbar, click  **Plot**.

Charged Species Along Axis-of-Symmetry

1 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 ($1/m^{>3</sup>}$).

8 Locate the **Legend** section. From the **Position** list, choose **Lower middle**.

Line Graph 1

1 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

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `plas.n_w02_1p`.

Line Graph 3

1 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 Graph 4

1 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

1 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

1 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 ($1/m^{>3}$)**.

8 Locate the **Legend** section. From the **Position** list, choose **Lower right**.


Global 1

- 1 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_wO2_1p)	1 / m ³	O2+
aveop1(plas.n_w0_1p)	1 / m ³	O+
aveop1(plas.n_w0_1m)	1 / m ³	O-

- 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



- 1 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. xO2 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 xO2.
- 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 1

- 1 Right-click **Space Averaged Charged Species vs. xO2** 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_wO2_1p)	1/m^3	O2+
aveop1(plas.n_wAr_1p)	1/m^3	O+
aveop1(plas.n_wO_1m)	1/m^3	O-

- 4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **xO2**.
- 5 Locate the **Legends** section. Find the **Include** subsection. Clear the **Solution** check box.
- 6 In the **Space Averaged Charged Species vs. xO2** toolbar, click  **Plot**.
- 7 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

