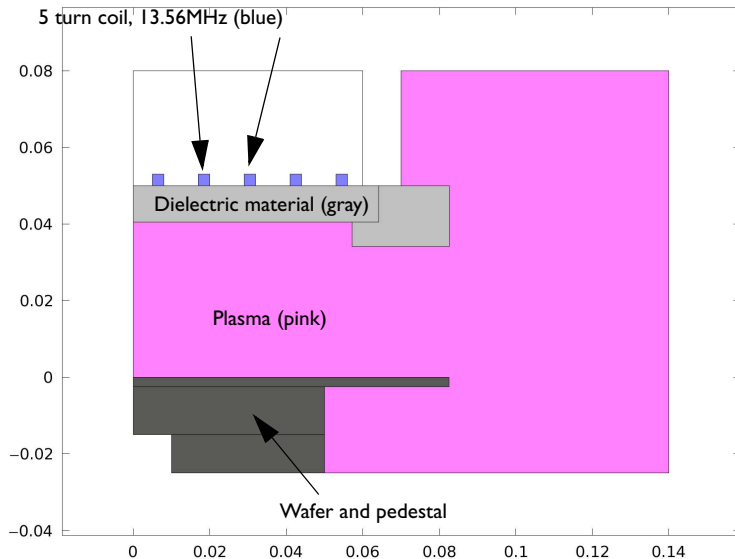


# GEC ICP Reactor, Argon/Oxygen Chemistry

## *Introduction*

Electronegative discharges exhibit very different characteristics to electropositive discharges due to the presence of negative ions. Examples of electronegative gases include oxygen, nitrogen trifluoride ( $\text{NF}_3$ ) and sulfur hexafluoride ( $\text{SF}_6$ ). Details on electron gas interactions for electronegative gases can be found in [Ref. 2](#).

The GEC cell was introduced by NIST in order to provide a standardized platform for experimental and modeling studies of discharges in different laboratories. The plasma is sustained via inductive heating. The Reference Cell operates as an inductively-coupled plasma in this model.



*Figure 1: GEC ICP reactor geometry consisting of a 5 turn copper coil, plasma volume, dielectrics, and wafer with pedestal.*

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**Note:** This model requires the Plasma and AC/DC Modules.

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### *Model Definition*

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Inductively coupled discharges typically operate at low pressures (<10 Pa) and high charge density (>10<sup>17</sup> m<sup>-3</sup>). High density plasma sources are popular because low pressure ion bombardment can provide a greater degree of anisotropy on the surface of the wafer.

#### **DOMAIN EQUATIONS**

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected. For detailed information on electron transport see [Theory for the Drift Diffusion User Interface](#) in the *Plasma Module User's Guide*.

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

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

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

$$\mathbf{D}_e = \boldsymbol{\mu}_e T_e, \boldsymbol{\mu}_\varepsilon = \left(\frac{5}{3}\right)\boldsymbol{\mu}_e, \mathbf{D}_\varepsilon = \boldsymbol{\mu}_\varepsilon T_e$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are  $M$  reactions that contribute to the growth or decay of electron density and  $P$  inelastic electron-neutral collisions. In general  $P \gg M$ . In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^M x_j k_j N_n n_e$$

where  $x_j$  is the mole fraction of the target species for reaction  $j$ ,  $k_j$  is the rate coefficient for reaction  $j$  (SI unit:  $\text{m}^3/\text{s}$ ), 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:

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

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),  $\varepsilon$  is energy (SI unit: V),  $\sigma_k$  is the collision cross section (SI unit:  $\text{m}^2$ ), and  $f$  is the electron energy distribution function. In this case a Maxwellian EEDF is assumed.

For non-electron species, the following equation is solved for the mass fraction of each species. For detailed information on the transport of the non-electron species see [Theory for the Heavy Species Transport User Interface](#) in the *Plasma Module User's Guide*.

$$\rho \frac{\partial}{\partial t} (w_k) + \rho (\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

The electrostatic field is computed using the following equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

The space charge density  $\rho$  is automatically computed based on the plasma chemistry specified in the model using the formula:

$$\rho = q \left( \sum_{k=1}^N Z_k n_k - n_e \right)$$

For detailed information about electrostatics see [Theory for the Electrostatics User Interface](#) in the *Plasma Module User's Guide*.

For a nonmagnetized, nonpolarized plasma, the induction currents are computed in the frequency domain using the following equation:

$$(j\omega\sigma - \omega^2\epsilon_0)\mathbf{A} + \nabla \times (\mu_0^{-1}\nabla \times \mathbf{A}) = \mathbf{J}^e \quad (1)$$

The plasma conductivity needs to be specified as a material property, usually from the cold plasma approximation:

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

where  $n_e$  is the electron density,  $q$  is the electron charge,  $m_e$  is the electron mass,  $\nu_e$  is the collision frequency, and  $\omega$  is the angular frequency.

### 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:

$$-\mathbf{n} \cdot \Gamma_e = \left( \frac{1}{2} \nu_e, \text{th} n_e \right) \quad (3)$$

and the electron energy flux:

$$-\mathbf{n} \cdot \Gamma_\epsilon = \left( \frac{5}{6} \nu_e, \text{th} n_\epsilon \right) \quad (4)$$

The second term on the right hand side of [Equation 3](#) is the gain of electrons due to secondary emission effects,  $\gamma_p$  being the secondary emission coefficient. The second term in [Equation 4](#) is the secondary emission energy flux,  $\epsilon_p$  being the mean energy of the secondary electrons. For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed towards the wall:

$$-\mathbf{n} \cdot \mathbf{j}_k = M_w R_k + M_w c_k Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) [Z_k \mu_k (\mathbf{E} \cdot \mathbf{n}) > 0] \quad (5)$$

The walls of the reactor are grounded.

**PLASMA CHEMISTRY**

A mixture of argon and oxygen is studied. There are 62 reactions and 15 species in the model:

TABLE I: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\epsilon(\text{eV})$
1	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Elastic	0
2	$e+\text{O}_2\Rightarrow\text{O}+\text{O}^-$	Attachment	-
3	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Excitation	0.02
4	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Excitation	0.19
5	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Excitation	0.19
6	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Excitation	0.38
7	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Excitation	0.38
8	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Excitation	0.57
9	$e+\text{O}_2\Rightarrow e+\text{O}_2$	Excitation	0.75
10	$e+\text{O}_2\Rightarrow e+\text{O}_2\text{a} \text{d}$	Excitation	0.977
11	$e+\text{O}_2\text{a} \text{d}\Rightarrow e+\text{O}_2$	Excitation	-0.977
12	$e+\text{O}_2\Rightarrow e+\text{O}_2\text{b} \text{s}$	Excitation	1.627
13	$e+\text{O}_2\text{b} \text{s}\Rightarrow e+\text{O}_2$	Excitation	-1.627
14	$e+\text{O}_2\Rightarrow e+\text{O}_2(45)$	Excitation	4.5
15	$e+\text{O}_2(45)\Rightarrow e+\text{O}_2$	Excitation	-4.5
16	$e+\text{O}_2\Rightarrow e+\text{O}+\text{O}$	Excitation	6.0
17	$e+\text{O}_2\Rightarrow e+\text{O}+\text{O} \text{d}$	Excitation	8.4
18	$e+\text{O}_2\Rightarrow e+\text{O}+\text{O} \text{s}$	Excitation	9.97
19	$e+\text{O}_2\Rightarrow 2e+\text{O}_2^+$	Ionization	12.06
20	$e+\text{O}_2\text{a} \text{d}\Rightarrow e+\text{O}_2\text{a} \text{d}$	Elastic	0
21	$e+\text{O}_2\text{a} \text{d}\Rightarrow e+\text{O}+\text{O}$	Excitation	5.02
22	$e+\text{O}_2\text{a} \text{d}\Rightarrow 2e+\text{O}_2^+$	Ionization	11.09
23	$e+\text{O}_2\text{b} \text{s}\Rightarrow e+\text{O}_2\text{b} \text{s}$	Elastic	0
24	$e+\text{O}_2\text{b} \text{s}\Rightarrow e+\text{O}+\text{O}$	Excitation	4.38
25	$e+\text{O}_2\text{b} \text{s}\Rightarrow 2e+\text{O}_2^+$	Ionization	10.39
26	$e+\text{O}_2(45)\Rightarrow e+\text{O}+\text{O}$	Excitation	1.5
27	$e+\text{O}_2(45)\Rightarrow 2e+\text{O}_2^+$	Ionization	7.58
28	$e+\text{O}\Rightarrow e+\text{O}$	Elastic	0

TABLE I: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\epsilon(\text{eV})$
29	$e+O \Rightarrow e+O\text{I}d$	Excitation	1.968
30	$e+O\text{I}d \Rightarrow e+O$	Excitation	-1.968
31	$e+O \Rightarrow e+O\text{I}s$	Excitation	4.192
32	$e+O\text{I}s \Rightarrow e+O$	Excitation	-4.192
33	$e+O \Rightarrow 2e+O^+$	Ionization	13.192
34	$e+O\text{I}d \Rightarrow e+O\text{I}s$	Excitation	2.224
35	$e+O\text{I}d \Rightarrow 2e+O^+$	Ionization	11.224
36	$e+O\text{I}s \Rightarrow 2e+O^+$	Ionization	9.00
37	$e+\text{Ar} \Rightarrow e+\text{Ar}$	Elastic	0
38	$e+\text{Ar} \Rightarrow e+\text{Ar}s$	Excitation	11.5
39	$e+\text{Ar}s \Rightarrow e+\text{Ar}$	Excitation	-11.5
40	$e+\text{Ar} \Rightarrow 2e+\text{Ar}^+$	Ionization	15.8
41	$e+\text{Ar}s \Rightarrow 2e+\text{Ar}^+$	Ionization	4.427
42	$e+O_2+O_2 \Rightarrow O_2+O_2^-$	Attachment	0
43	$e+O_2^+ \Rightarrow O+O$	Recombination	
44	$e+O_2^+ \Rightarrow O+O\text{I}d$	Recombination	
45	$O_2a\text{I}d+O_2 \Rightarrow O_2+O_2$	Metastable quenching	
46	$O_2a\text{I}d+O \Rightarrow O_2+O$	Metastable quenching	
47	$O_2b\text{I}s+O_2 \Rightarrow O_2+O_2$	Metastable quenching	
48	$O_2b\text{I}s+O \Rightarrow O_2+O$	Metastable quenching	
49	$O_2(45)+O_2 \Rightarrow O_2+O_2$	Metastable quenching	
50	$O\text{I}d+O_2 \Rightarrow O+O_2$	Metastable quenching	
51	$O\text{I}d+O \Rightarrow O+O_2$	Metastable quenching	
52	$O\text{I}s+O_2 \Rightarrow O+O_2$	Metastable quenching	
53	$O\text{I}s+O \Rightarrow O+O$	Metastable quenching	
54	$O+O+O_2 \Rightarrow O_2+O_2$	Recombination	
55	$O+O+O \Rightarrow O+O_2$	Recombination	
56	$O^++O_2 \Rightarrow O+O_2^+$	Charge exchange	
57	$O^-+O \Rightarrow O_2+e$	Detachment	
58	$O^-+O_2 \Rightarrow O_2^-+O$	Charge exchange	
59	$O^-+O^+ \Rightarrow 2O$	Recombination	

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED

REACTION	FORMULA	TYPE	$\Delta\epsilon$ (eV)
60	$O^- + O_2^+ \Rightarrow 3O$	Recombination	
61	$O_2^- + O_2^+ \Rightarrow 2O_2$	Recombination	
62	$O_2^- + O^+ \Rightarrow O_2 + O$	Recombination	

Negative ions cannot escape the ambipolar field, so they do not reach the reactor walls. The only way the negative ions are removed from the plasma is via recombination with positive ions. For this reason, no surface reactions need to be specified for the negative ions. The following surface reactions are included in the model:

TABLE 2: TABLE OF SURFACE REACTIONS

REACTION	FORMULA	STICKING COEFFICIENT
1	$O_2 a   d \Rightarrow O_2$	1
2	$O_2 b   s \Rightarrow O_2$	1
3	$O_2(45) \Rightarrow O_2$	1
4	$O_2^+ \Rightarrow O_2$	1
5	$O   d \Rightarrow O$	1
6	$O   s \Rightarrow O$	1
7	$O^+ \Rightarrow O$	1
8	$O + O \Rightarrow O_2$	$1E-3$
9	$Ar^+ \Rightarrow Ar$	1
10	$Ar_s \Rightarrow Ar$	1

## ELECTRICAL EXCITATION

From an electrical point of view, the GEC reactor behaves as a transformer. A current is applied to the driving coil (the primary) and this induces a current in the plasma (the secondary). The plasma then induces an opposing current back in the coil, increasing its impedance. The current flowing in the plasma depends on the current applied to the coil and the reaction kinetics. The total plasma current can vary from no current (plasma not sustained) to the same current as the primary which corresponds to perfect coupling between the coil and the plasma.

In this case, the total power absorbed by both the coil and the plasma is fixed at 2000 W. When modeling inductively coupled plasmas it is generally best to specify the total power as a setting for the coil rather than the coil current or voltage.

## Results and Discussion

The peak electron density occurs at the center of the reactor, underneath the RF coil. The electron density in this case is high enough to cause some shielding of the azimuthal electric field.

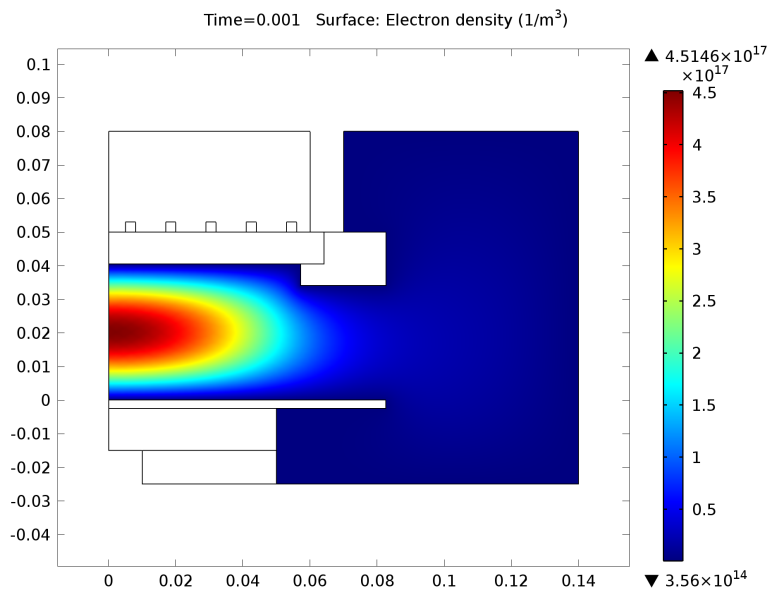


Figure 2: Electron density inside the GEC ICP reactor.

The electron “temperature” is highest directly underneath the coil, which is where the bulk of the power deposition occurs. The plasma potential, [Figure 4](#), peaks at around 28 V which is in line with the expected potential for the computed electron temperature.



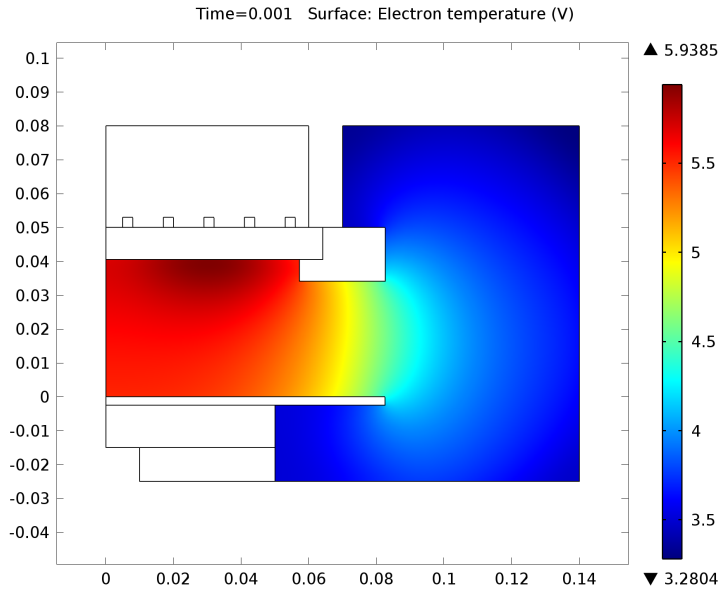


Figure 3: Electron “temperature” inside the GEC ICP reactor.

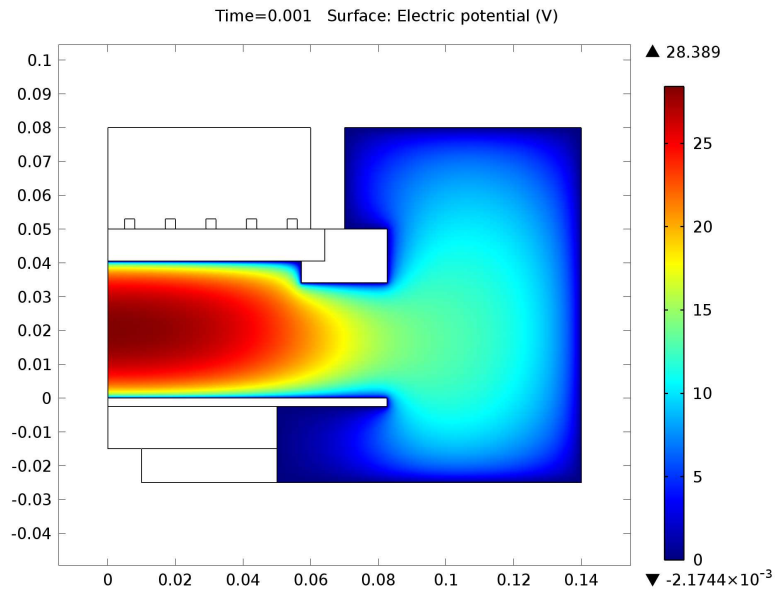
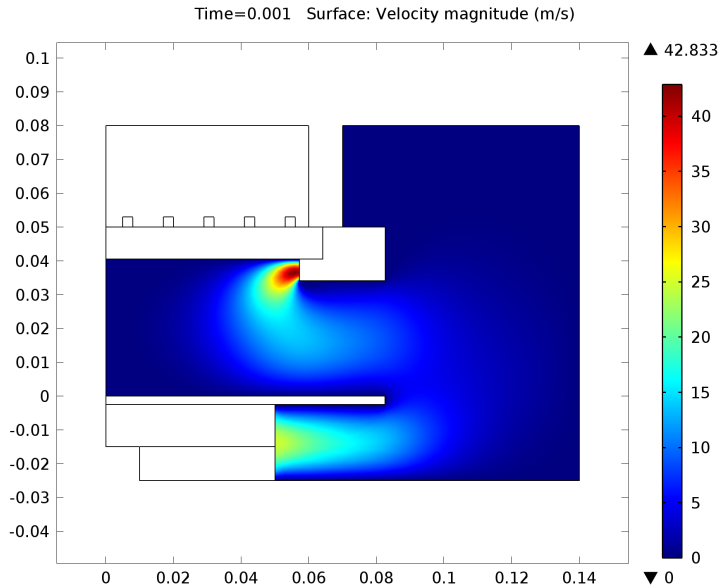


Figure 4: Electric potential inside the GEC ICP reactor.

The velocity field is plotted in [Figure 5](#). At these flow rates the gas does not penetrate deep into the core of the plasma. The pump causes flow of the gas down towards the wafer, then around it and out to the pump. Since inductively coupled plasmas generally operate at very low pressures, the gas flow tends to only have a small effect on the results.



*Figure 5: Velocity field in the GEC ICP reactor.*

The mole fraction of atomic oxygen is plotted in [Figure 6](#). Since the incoming gas mixture is argon and molecular oxygen, the mole fraction is lowest near the gas injector. The molecular oxygen is quickly dissociated into atomic oxygen and other electronically excited states, resulting in a higher mole fraction closer to the axis of symmetry.

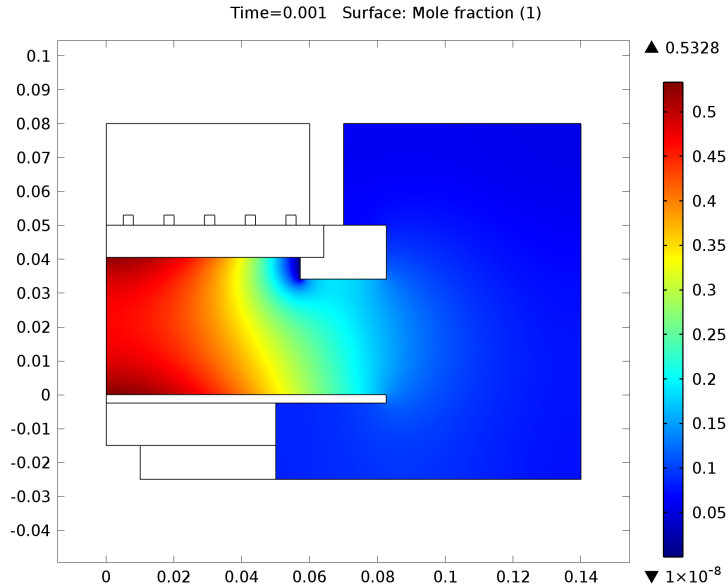


Figure 6: Mole fraction of atomic oxygen inside the GEC ICP reactor.

The number density of negative ions are plotted in [Figure 7](#) and [Figure 8](#). The number density of  $O^-$  ions is higher than  $O_2^-$  due to the fact that the dissociative attachment reaction rate (reaction number 2) is much greater than that of the 3 body attachment reaction (reaction number 42) which is the primary producer of  $O_2^-$ .

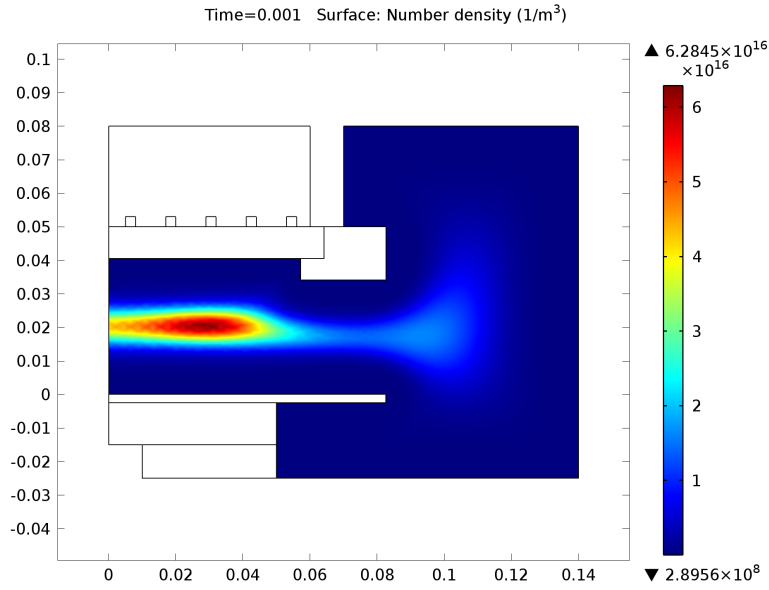


Figure 7: Number density of  $O^-$  ions in the GEC ICP reactor.

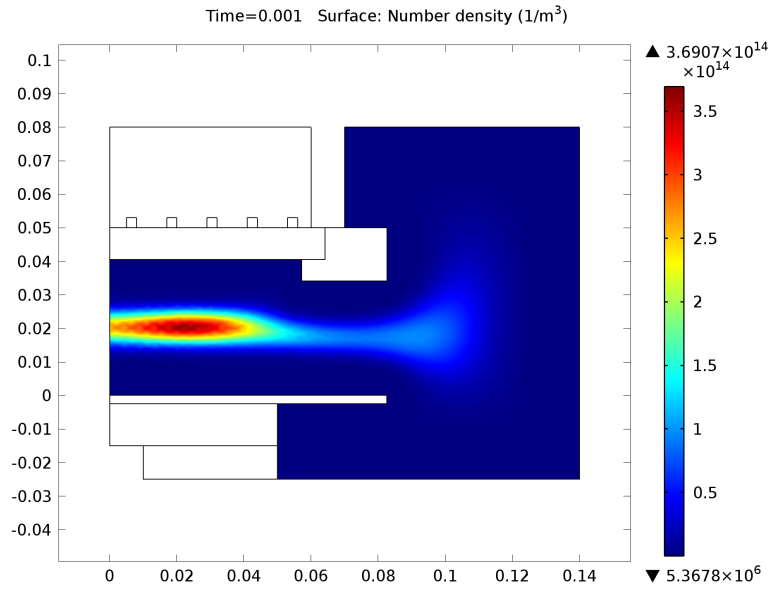


Figure 8: Number density of  $O_2^-$  ions in the GEC ICP reactor.

## *Notes About the COMSOL Implementation*

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The mobility and diffusivity of the negative ions are computed assuming that the negative ion temperature is 0.3 eV. This is a reasonable assumption, since the ions are held in the core of the plasma, where they can acquire energy from the high frequency electromagnetic field.

Due to the large number of reactions and species in the model, it requires a 64 bit machine with at least 4 GB of memory to solve.

### **LIMITATIONS OF THE MODEL**

The plasma chemical mechanism used in the model has not been rigorously validated against experimental measurements. If some of the reactions are removed, or additional reactions added, the results will likely change, possibly significantly. It should also be noted that the mechanism used here does not include ozone or any ionic species with a molecular mass of 48 or 64. At higher pressures (above several torr), the chemical mechanism for an oxygen plasma changes dramatically. Ozone should be included, as should more exotic ionic species like  $O_3^-$  and  $O_4^+$ .

## *References*

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1. G.J.M. Hagelaar, and L.C. Pitchford, "Solving the Boltzmann Equation to Obtain Electron Transport Coefficients and Rate Coefficients for Fluid Models," *Plasma Sources Sci. Technol.*, vol. 14, pp. 722–733, 2005.
2. Loucas G. Christophorou, James K. Olthoff, "Fundamental Electron Interactions with Plasma Processing Gases", Springer, 2003.

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**Model Library path:** Plasma\_Module/Inductively\_Coupled\_Plasmas/  
oxygen\_gec\_icp

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## *Modeling Instructions*

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### **MODEL WIZARD**

- 1 Go to the **Model Wizard** window.
- 2 Click the **2D axisymmetric** button.
- 3 Click **Next**.

- 4 In the **Add physics** tree, select **Plasma>Inductively Coupled Plasma (icp)**.
- 5 Click **Add Selected**.
- 6 In the **Add physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.
- 7 Click **Add Selected**.
- 8 Click **Next**.
- 9 Find the **Studies** subsection. In the tree, select **Preset Studies for Selected Physics>Frequency-Transient**.
- 10 Click **Finish**.
- 11 In the **Model Builder** window's toolbar, click the **Show** button and select **Stabilization** in the menu.
- 12 In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

## GEOMETRY I

### *Import I*

- 1 In the **Model Builder** window, under **Model I** right-click **Geometry I** and choose **Import**.
- 2 In the **Import** settings window, locate the **Import** section.
- 3 Click the **Browse** button.
- 4 Browse to the model's Model Library folder and double-click the file `oxygen_gec_icp.mphbin`.
- 5 Click the **Import** button.

## DEFINITIONS

### *Explicit I*

- 1 In the **Model Builder** window, under **Model I** right-click **Definitions** and choose **Selections>Explicit**.
- 2 Right-click **Explicit I** and choose **Rename**.
- 3 Go to the **Rename Explicit** dialog box and type `Walls` in the **New name** edit field.
- 4 Click **OK**.
- 5 In the **Explicit** settings window, locate the **Input Entities** section.
- 6 From the **Geometric entity level** list, choose **Boundary**.
- 7 Select Boundaries 6, 8, 35–38, 44, 45, and 51–56 only.

**DEFINITIONS***Explicit 2*

- 1 In the **Model Builder** window, under **Model 1** right-click **Definitions** and choose **Selections>Explicit**.
- 2 Right-click **Explicit 2** and choose **Rename**.
- 3 Go to the **Rename Explicit** dialog box and type Coils in the **New name** edit field.
- 4 Click **OK**.
- 5 Select Domains 6 and 8–11 only.

**DEFINITIONS***Explicit 3*

- 1 In the **Model Builder** window, under **Model 1** right-click **Definitions** and choose **Selections>Explicit**.
- 2 Right-click **Explicit 3** and choose **Rename**.
- 3 Go to the **Rename Explicit** dialog box and type Coil Boundaries in the **New name** edit field.
- 4 Click **OK**.
- 5 Select Domains 6 and 8–11 only.
- 6 In the **Explicit** settings window, locate the **Output Entities** section.
- 7 From the **Output entities** list, choose **Adjacent boundaries**.

*Explicit 4*

- 1 In the **Model Builder** window, right-click **Definitions** and choose **Selections>Explicit**.
- 2 In the **Explicit** settings window, locate the **Input Entities** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 Right-click **Model 1>Definitions>Explicit 4** and choose **Rename**.
- 5 Go to the **Rename Explicit** dialog box and type Inlet in the **New name** edit field.
- 6 Click **OK**.
- 7 Select Boundary 44 only.

*Explicit 5*

- 1 In the **Model Builder** window, right-click **Definitions** and choose **Selections>Explicit**.
- 2 In the **Explicit** settings window, locate the **Input Entities** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.

- 4 Right-click **Model 1>Definitions>Explicit 5** and choose **Rename**.
- 5 Go to the **Rename Explicit** dialog box and type **Outlet** in the **New name** edit field.
- 6 Click **OK**.
- 7 Select Boundaries 35 and 37 only.

## DEFINITIONS

### *Variables 1*

- 1 In the **Model Builder** window, under **Model 1** right-click **Definitions** and choose **Variables**.
- 2 In the **Variables** settings window, locate the **Variables** section.
- 3 In the table, enter the following settings:

NAME	EXPRESSION	DESCRIPTION
Qin	100*tanh(1E5*t[1/s])	Inlet flow rate (sccm)
p0	0.02[Torr]	Outlet pressure

## INDUCTIVELY COUPLED PLASMA

- 1 In the **Model Builder** window, under **Model 1** click **Inductively Coupled Plasma**.
- 2 Select Domains 3–6 and 8–12 only.
- 3 In the **Model Builder** window, click **Inductively Coupled Plasma**.
- 4 In the **Inductively Coupled Plasma** settings window, locate the **Transport Settings** section.
- 5 Select the **Convection** check box.
- 6 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** check box.
- 7 Click to expand the **Discretization** section. Find the **Value types when using splitting of complex variables** subsection. In the table, enter the following settings:

Dependent variable	Value type
Electric potential	real

### *Cross Section Import 1*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Cross Section Import**.
- 2 In the **Cross Section Import** settings window, locate the **Cross Section Import** section.
- 3 Click the **Browse** button.



- 4 Browse to the model's Model Library folder and double-click the file `All_O2_xsecs.txt`.

#### *Cross Section Import 2*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Cross Section Import**.
- 2 In the **Cross Section Import** settings window, locate the **Cross Section Import** section.
- 3 Click the **Browse** button.
- 4 Browse to the model's Model Library folder and double-click the file `Ar_xsecs.txt`.

#### *Reaction 1*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $e+02+02=>02-+02$ .
- 4 In the **Reaction** settings window, locate the **Kinetics Expressions** section.
- 5 In the  $k^f$  edit field, type  $3.6e-40*(icp.Te^{-0.5})*N\_A\_const^2$ .

#### *Reaction 2*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $e+02+=>0+0$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*1.95E-13*(300/icp.T)^{0.7}$ .

#### *Reaction 3*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $e+02+=>0+01d$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*1.95E-13*(300/icp.T)^{0.7}$ .

#### *Reaction 4*

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

- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0.2 \times 10^2 \Rightarrow 0.2 + 0.2$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 3e-24 * \exp(-200 / i_{cp} \cdot T)$ .

#### Reaction 5

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport > Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0.2 \times 10^0 \Rightarrow 0.2 + 0$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 2E-22$ .

#### Reaction 6

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport > Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0.2 \times 10^2 \Rightarrow 0.2 + 0.2$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 2.317e-28 * i_{cp} \cdot T^{0.5}$ .

#### Reaction 7

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport > Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0.2 \times 10^0 \Rightarrow 0.2 + 0$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 4.634e-22 * i_{cp} \cdot T^{0.5}$ .

#### Reaction 8

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport > Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0.2 \times 10^2 \Rightarrow 0.2 + 0.2$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 2E-19$ .

*Reaction 9*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $01d+02=>0+02$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*3.2e-17*\exp(67/icp.T)$ .

*Reaction 10*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $01d+0=>0+0$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*8.0E-18$ .

*Reaction 11*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $01s+02=>0+02$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*4.8e-18*\exp(67/icp.T)$ .

*Reaction 12*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $01s+0=>0+0$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*3.33E-17*\exp(-300/icp.T)$ .

*Reaction 13*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0+0+02=>02+02$ .

- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const^{*2*9.268e-42*(icp.T^{-0.63})}$ .

#### Reaction 14

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0+0+0=>0+02$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const^{*2*3.334e-41*(icp.T^{-0.63})}$ .

#### Reaction 15

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0++02=>0+02+$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*1.9E-18*icp.T^{-0.4}$ .

#### Reaction 16

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0-+0=>02+e$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*5.0E-16$ .

#### Reaction 17

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0-+02=>02-+0$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const*1.0E-20$ .

#### Reaction 18

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

- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0 + 0 + \Rightarrow 20$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 2.3E-13 * (i_{cp}.T/300)^{-0.5}$ .

#### *Reaction 19*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0 + 02 + \Rightarrow 30$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 2.3E-13 * (i_{cp}.T/300)^{-0.5}$ .

#### *Reaction 20*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $02 + 02 + \Rightarrow 202$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 2.3E-13 * (i_{cp}.T/300)^{-0.5}$ .

#### *Reaction 21*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Heavy Species Transport>Reaction**.
- 2 In the **Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $02 + 0 + \Rightarrow 02 + 0$ .
- 4 Locate the **Kinetics Expressions** section. In the  $k^f$  edit field, type  $N\_A\_const * 2.3E-13 * (i_{cp}.T/300)^{-0.5}$ .

#### *Plasma Model 1*

- 1 In the **Model Builder** window, under **Model 1>Inductively Coupled Plasma** click **Plasma Model 1**.
- 2 In the **Plasma Model** settings window, locate the **Model Inputs** section.
- 3 From the **u** list, choose **Velocity field (spf/fp1)**.
- 4 In the  $T$  edit field, type  $500 [K]$ .
- 5 From the  $p_A$  list, choose **Pressure (spf/fp1)**.

- 6 Clear the **Reference pressure** check box.
- 7 Locate the **Electron Density and Energy** section. In the  $\mu_e N_n$  edit field, type 4E24.

#### *Initial Values 1*

- 1 In the **Model Builder** window, under **Model 1>Inductively Coupled Plasma** click **Initial Values 1**.
- 2 In the **Initial Values** settings window, locate the **Initial Values** section.
- 3 In the  $n_{e,0}$  edit field, type 1E15.
- 4 In the  $\epsilon_0$  edit field, type 5.

#### *Surface Reaction 1*

- 1 In the **Model Builder** window, right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type 02a1d=>02.
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

#### *Surface Reaction 2*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type 02b1s=>02.
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

#### *Surface Reaction 3*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type 0245=>02.
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

#### *Surface Reaction 4*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type 02+=>02.
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

*Surface Reaction 5*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $01d=>0$ .
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

*Surface Reaction 6*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $01s=>0$ .
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

*Surface Reaction 7*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0+=>0$ .
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

*Surface Reaction 8*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $0+0=>0.502$ .
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.
- 5 Locate the **Kinetics Expressions** section. In the  $\gamma_f$  edit field, type  $1E-3$ .

*Surface Reaction 9*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $Ar+=>Ar$ .
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

*Surface Reaction 10*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Heavy Species Transport>Surface Reaction**.
- 2 In the **Surface Reaction** settings window, locate the **Reaction Formula** section.
- 3 In the **Formula** edit field, type  $Ar_s \Rightarrow Ar$ .
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

*Ampère's Law 1*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Magnetic Fields>Ampère's Law**.
- 2 Select Domains 4–6 and 8–12 only.

*Wall 1*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Drift Diffusion>Wall**.
- 2 In the **Wall** settings window, locate the **General Wall Settings** section.
- 3 In the  $r_e$  edit field, type 0.
- 4 Select Boundaries 6, 8, 35–38, 44, 45, and 51–56 only.
- 5 Locate the **Boundary Selection** section. From the **Selection** list, choose **Walls**.

*Ground 1*

- 1 Right-click **Inductively Coupled Plasma** and choose the boundary condition **Electrostatics>Ground**.
- 2 Select Boundaries 6, 8, 35–38, 44, 45, and 51–56 only.

*Coil Group Domain 1*

- 1 Right-click **Inductively Coupled Plasma** and choose the domain setting **Magnetic Fields>Coil Group Domain**.
- 2 Select Domains 6 and 8–11 only.
- 3 In the **Coil Group Domain** settings window, locate the **Coil Group Domain** section.
- 4 From the **Coil excitation** list, choose **Power**.
- 5 In the  $P_{\text{coil}}$  edit field, type 2000[W].

*Species: O2*

- 1 In the **Model Builder** window, under **Model 1>Inductively Coupled Plasma** click **Species: O2**.
- 2 In the **Species** settings window, locate the **Species Formula** section.



- 3 Select the **From mass constraint** check box.
- 4 Locate the **General Parameters** section. From the **Preset species data** list, choose **O2**.

*Species: O*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O**.

*Inlet 1*

- 1 In the **Model Builder** window, right-click **Species: O** and choose **Inlet**.
- 2 In the **Inlet** settings window, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlet**.
- 4 Locate the **Inlet** section. From the **Mixture specification** list, choose **Mole fraction**.
- 5 In the  $x_0$  edit field, type 1E-8.

*Outflow 1*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** right-click **Species: O** and choose **Outflow**.
- 2 In the **Outflow** settings window, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Outlet**.

*Species: O-*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O-**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O**.
- 4 Click to expand the **Mobility and Diffusivity Expressions** section. From the **Ion temperature** list, choose **Specify ion temperature**.
- 5 In the  $T_{ion}$  edit field, type  $0.3[V]*e\_const/k\_B\_const$ .

*Species: O2a1d*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O2a1d**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O2**.

*Species: O2b1s*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O2b1s**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O2**.

*Species: O245*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O245**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O2**.

*Species: O1d*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O1d**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O**.

*Species: O1s*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O1s**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O**.

*Species: O2+*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O2+**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O2**.
- 4 Locate the **Species Formula** section. Select the **Initial value from electroneutrality constraint** check box.

*Species: O+*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O+**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O**.

*Species: Ar*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: Ar**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **Ar**.
- 4 In the  $x_0$  edit field, type 0.3.

*Inlet 1*

- 1 In the **Model Builder** window, right-click **Species: Ar** and choose **Inlet**.
- 2 In the **Inlet** settings window, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlet**.
- 4 Locate the **Inlet** section. From the **Mixture specification** list, choose **Mole fraction**.
- 5 In the  $x_0$  edit field, type 0.3.

*Outflow 1*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** right-click **Species: Ar** and choose **Outflow**.
- 2 In the **Outflow** settings window, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Outlet**.

*Species: Ars*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: Ars**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **Ar**.

*Species: Ar+*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: Ar+**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **Ar**.

*Species: O2-*

- 1 In the **Model Builder** window, under **Model 1 > Inductively Coupled Plasma** click **Species: O2-**.
- 2 In the **Species** settings window, locate the **General Parameters** section.
- 3 From the **Preset species data** list, choose **O2**.

4 Click to expand the **Mobility and Diffusivity Expressions** section. From the **Ion temperature** list, choose **Specify ion temperature**.

5 In the  $T_{ion}$  edit field, type  $0.3[V]*e\_const/k\_B\_const$ .

#### LAMINAR FLOW

1 In the **Model Builder** window, under **Model 1** click **Laminar Flow**.

2 In the **Laminar Flow** settings window, locate the **Consistent Stabilization** section.

3 Find the **Navier-Stokes equations** subsection. Clear the **Crosswind diffusion** check box.

4 Locate the **Domain Selection** section. Click **Clear Selection**.

5 Select Domain 3 only.

6 Click to expand the **Equation** section. From the **Equation form** list, choose **Stationary**.

#### *Fluid Properties 1*

1 In the **Model Builder** window, under **Model 1>Laminar Flow** click **Fluid Properties 1**.

2 In the **Fluid Properties** settings window, locate the **Fluid Properties** section.

3 From the  $\rho$  list, choose **Density (icp/pem1)**.

4 From the  $\mu$  list, choose **Dynamic viscosity (icp/pem1)**.

#### *Initial Values 1*

1 In the **Model Builder** window, under **Model 1>Laminar Flow** click **Initial Values 1**.

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

3 In the  $p$  edit field, type  $p0$ .

#### *Inlet 1*

1 In the **Model Builder** window, right-click **Laminar Flow** and choose **Inlet**.

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

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

4 In the **Inlet** settings window, locate the **Boundary Condition** section.

5 From the **Boundary condition** list, choose **Mass flow**.

6 Locate the **Mass Flow Rate** section. From the **Mass flow type** list, choose **Standard flow rate (SCCM)**.

7 In the  $Q_{sccm}$  edit field, type  $Q_{in}$ .

8 From the  $M_n$  list, choose **Mean molar mass (icp/pem1)**.

#### *Outlet 1*

1 Right-click **Laminar Flow** and choose **Outlet**.

- 2 In the **Outlet** settings window, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Outlet**.
- 4 Locate the **Boundary Condition** section. In the  $p_0$  edit field, type  $p_0$ .

#### *Inlet 1*

Now you assign material properties to the plasma, air, coil and dielectric domains.

### **MATERIALS**

#### *Material 1*

- 1 In the **Model Builder** window, under **Model 1** right-click **Materials** and choose **Material**.
- 2 In the **Material** settings window, locate the **Geometric Entity Selection** section.
- 3 From the **Selection** list, choose **Coils**.
- 4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Name	Value
Electrical conductivity	sigma	6e7
Relative permittivity	epsilon <sub>r</sub>	1
Relative permeability	mu <sub>r</sub>	1

#### *Material 2*

- 1 In the **Model Builder** window, right-click **Materials** and choose **Material**.
- 2 Select Domains 4, 5, and 12 only.
- 3 In the **Material** settings window, locate the **Material Contents** section.
- 4 In the table, enter the following settings:

Property	Name	Value
Electrical conductivity	sigma	0
Relative permittivity	epsilon <sub>r</sub>	1
Relative permeability	mu <sub>r</sub>	1

### **MESH 1**

Meshing is a critical step in any plasma model. Boundary layer meshing on the reactor walls is nearly always necessary. This is needed to capture the separation of space charge between the electrons and ions close to the wall. You also add a fine mesh in the coil domains since the skin effect needs to be resolved.

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

- 2 In the **Mesh** settings window, locate the **Mesh Settings** section.
- 3 From the **Element size** list, choose **Finer**.

#### *Edge 1*

- 1 Right-click **Mesh 1** and choose **Edge**.
- 2 Select Boundaries 6, 8, 44, 45, and 54 only.

#### *Size 1*

- 1 Right-click **Model 1>Mesh 1>Edge 1** and choose **Size**.
- 2 In the **Size** settings window, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Entire geometry**.
- 4 Locate the **Element Size** section. Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.
- 6 In the associated edit field, type 1E-3.

#### *Free Triangular 1*

- 1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.
- 2 In the **Free Triangular** settings window, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domain 3 only.

#### *Size 1*

- 1 Right-click **Model 1>Mesh 1>Free Triangular 1** and choose **Size**.
- 2 In the **Size** settings window, locate the **Element Size** section.
- 3 From the **Predefined** list, choose **Extra fine**.

#### *Boundary Layers 1*

- 1 In the **Model Builder** window, right-click **Mesh 1** and choose **Boundary Layers**.
- 2 In the **Boundary Layers** settings window, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domain 3 only.

#### *Boundary Layer Properties*

- 1 In the **Model Builder** window, under **Model 1>Mesh 1>Boundary Layers 1** click **Boundary Layer Properties**.

- 2 In the **Boundary Layer Properties** settings window, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Walls**.
- 4 Locate the **Boundary Layer Properties** section. In the **Number of boundary layers** edit field, type 5.
- 5 In the **Boundary layer stretching factor** edit field, type 1.4.

#### *Mapped 1*

- 1 In the **Model Builder** window, right-click **Mesh 1** and choose **Mapped**.
- 2 In the **Mapped** settings window, 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 **Model 1**>**Mesh 1**>**Mapped 1** and choose **Distribution**.
- 2 In the **Distribution** settings window, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Coil Boundaries**.
- 4 In the **Distribution** settings window, locate the **Distribution** section.
- 5 From the **Distribution properties** list, choose **Predefined distribution type**.
- 6 In the **Number of elements** edit field, type 30.
- 7 In the **Element ratio** edit field, type 10.
- 8 From the **Distribution method** list, choose **Geometric sequence**.
- 9 Select the **Symmetric distribution** check box.

#### *Free Triangular 2*

- 1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.
- 2 Right-click **Mesh 1** and choose **Build All**.
- 3 Click the **Zoom Extents** button on the Graphics toolbar.

### **STUDY 1**

The model is now ready to be solved. You just need to enter the list of output times and the frequency for the induction currents.

#### *Step 1: Frequency-Transient*

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

- 2 In the **Frequency-Transient** settings window, locate the **Study Settings** section.
- 3 In the **Times** edit field, type 0.
- 4 Click the **Range** button.
- 5 Go to the **Range** dialog box.
- 6 From the **Entry method** list, choose **Number of values**.
- 7 In the **Start** edit field, type -8.
- 8 In the **Stop** edit field, type -3.
- 9 In the **Number of values** edit field, type 11.
- 10 From the **Function to apply to all values** list, choose **exp10**.
- 11 Click the **Add** button.
- 12 In the **Frequency-Transient** settings window, locate the **Study Settings** section.
- 13 In the **Frequency** edit field, type 13.56E6.

#### *Solver 1*

- 1 In the **Model Builder** window, right-click **Study 1** and choose **Show Default Solver**.
- 2 Expand the **Solver 1** node.
- 3 In the **Model Builder** window, under **Study 1>Solver Configurations>Solver 1** click **Time-Dependent Solver 1**.
- 4 In the **Time-Dependent Solver** settings window, click to expand the **Absolute Tolerance** section.
- 5 From the **Global method** list, choose **Unscaled**.
- 6 Right-click **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1** and choose **Segregated**.
- 7 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1>Segregated 1** node, then click **Segregated Step**.
- 8 In the **Segregated Step** settings window, locate the **General** section.
- 9 In the **Variables** list, choose **Velocity field (mod1.u)**, **Pressure (mod1.p)**, and **mod1.spf.Pmfin11**.
- 10 Under **Variables**, click **Delete**.
- 11 Click to expand the **Method and Termination** section. From the **Jacobian update** list, choose **On every iteration**.
- 12 In the **Model Builder** window, under **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1** right-click **Segregated 1** and choose **Segregated Step**.



- 13 In the **Segregated Step** settings window, locate the **General** section.
- 14 Under **Variables**, click **Add**.
- 15 Go to the **Add** dialog box.
- 16 In the **Variables** list, choose **Velocity field (mod1.u)**, **Pressure (mod1.p)**, and **mod1.spf.Pmfin11**.
- 17 Click the **OK** button.
- 18 In the **Segregated Step** settings window, locate the **Method and Termination** section.
- 19 From the **Jacobian update** list, choose **Once per time step**.
- 20 In the **Model Builder** window, right-click **Study 1** and choose **Compute**.
- 21 Click the **Zoom Extents** button on the Graphics toolbar.

## RESULTS

### *Velocity (spf) 1*

- 1 In the **Model Builder** window, under **Results** right-click **Velocity (spf)** and choose **Duplicate**.
- 2 Right-click **Velocity (spf) 1** and choose **Rename**.
- 3 Go to the **Rename 2D Plot Group** dialog box and type **Atomic Oxygen** in the **New name** edit field.
- 4 Click **OK**.

### *Atomic Oxygen*

- 1 In the **Model Builder** window, expand the **Results>Atomic Oxygen** node, then click **Surface 1**.
- 2 In the **Surface** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Inductively Coupled Plasma (Heavy Species Transport)>Mole fractions>Mole fraction (icp.x\_w0)**.
- 3 Click the **Plot** button.

### *2D Plot Group 8*

- 1 In the **Model Builder** window, right-click **Results** and choose **2D Plot Group**.
- 2 Right-click **2D Plot Group 8** and choose **Surface**.
- 3 In the **Surface** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Inductively Coupled Plasma (Heavy Species Transport)>Number densities>Number density (icp.n\_w0\_1m)**.
- 4 Click the **Plot** button.

*2D Plot Group 9*

- 1** In the **Model Builder** window, right-click **2D Plot Group 8** and choose **Duplicate**.
- 2** In the **Model Builder** window, expand the **2D Plot Group 9** node, then click **Surface 1**.
- 3** In the **Surface** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Inductively Coupled Plasma (Heavy Species Transport)>Number densities>Number density (icp.n\_wO2\_1m)**.
- 4** Click the **Plot** button.