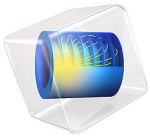

Model of an Argon/Oxygen Capacitively Coupled Plasma Reactor

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Introduction

This tutorial models an argon/oxygen capacitively coupled plasma reactor in 1D. The goal is to show how to prepare a model with a mixture of different elements (in this case Ar and O_2) in which one of the species can dissociate by electron impact (O_2 dissociates into O) and where negative ions exist (the dissociative electron attachment of O_2 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.

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 model presented here is 1D and describes the space- and time-periodic evolution of several macroscopic properties of the plasma sustained within a 4.5 cm gap at 50 mTorr and for an absorbed power of 10 W. The electron mobility and other electron transport properties are automatically computed from the electron impact reactions.

ELECTRIC EXCITATION

The driven electrode has a fixed power. This corresponds to the following expression and constraint on the electric potential:

$$V_s = V_a \cos(2\pi f_p t + \alpha) \tag{1}$$

$$P_{rf} = f_p \int_{\partial t} \int_{\partial \Omega} V_s(\mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e + \mathbf{n} \cdot \mathbf{J}_d) dS dt \,. \tag{2}$$

The constraint in Equation 2 is used to compute the RF potential, V_a such that a fixed amount of power is deposited into the plasma.

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 form Ref. 4).

TABLE 1: ARGON REACTIONS

REACTION	FORMULA	TYPE	$\Delta\varepsilon$(eV)
1	e+Ar=>e+Ar	Elastic	-
2	e+Ar=>e+Ars	Excitation	11.5
3	e+Ars=>e+Ar	Superelastic	-11.5
4	e+Ar=>2e+Ar+	Ionization	15.8
5	e+Ars=>2e+Ar+	Ionization	4.24
6	Ars+Ars=>e+Ar+Ar+	Penning ionization	-
7	Ars+Ar=>Ar+Ar	Metastable quenching	-

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

TABLE 2: OXYGEN ELECTRON IMPACT REACTIONS.

REACTION	FORMULA	TYPE	$\Delta\varepsilon$(eV)
1	e+O_2=>O+O^-	Dissociative attachment	-
2	e+O_2=>e+O_2	Elastic	-
3	e+O_2=>e+O_2	Rotational excitation	0.02
4	e+O_2=>e+O_2	Vibrational excitation	0.19

TABLE 2: OXYGEN ELECTRON IMPACT REACTIONS.

REACTION	FORMULA	TYPE	$\Delta\varepsilon(\mathrm{eV})$
5	$e+O_2=>e+O_2$	Vibrational excitation	0.19
6	$e+O_2=>e+O_2$	Vibrational excitation	0.38
7	$e+O_2=>e+O_2$	Vibrational excitation	0.38
8	$e+O_2=>e+O_2$	Vibrational excitation	0.57
9	$e+O_2=>e+O_2$	Vibrational excitation	0.75
10	$e+O_2=>e+O_2(a^1\Delta_g)$	Excitation	0.977
11	$e+O_2=>e+O_2$	Excitation	1.627
12	$e+O_2=>e+O_2$	Excitation	4.5
13	$e+O_2=>e+O+O$	Dissociative excitation	6.0
14	$e+O_2=>e+O+O(^1D)$	Excitation	8.4
15	$e+O_2=>e+O_2$	Excitation	9.97
16	$e+O_2=>e+O_2^+$	Ionization	12.06
17	$e+O=>e+O$	Elastic	-
18	$e+O=>e+O(^1D)$	Excitation	1.968
19	$e+O=>e+O$	Excitation	4.192
20	$e+O=>e+c$	Ionization	13.618
21	$e+O^-=>O+e+e$	Electron impact detachment	12.00

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

TABLE 3: HEAVY SPECIES REACTIONS INVOLVING IONS.

REACTION	FORMULA	TYPE
1	$O^++O_2=>O+O_2^+$	Charge transfer
2	$O^++O^-=>O+O$	Mutual recombination
3	$O^-+O_2^+=>3O$	Mutual recombination
4	$O^-+O_2^+=>O+O_2$	Mutual recombination
5	$O^-+O_2=>O^2+e$	Detachment
6	$O^-+Ar^+=>O+Ar$	Mutual recombination

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

TABLE 4: SURFACE REACTIONS.

REACTION	FORMULA	STICKING COEFFICIENT	SECONDARY EMISSION COEFFICIENT	MEAN ENERGY OF SECONDARY ELECTRONS (V)
1	Ars=>Ar	1	0	0
2	Ar^+=>Ar	1	0.07	5.8
3	O=>0.5O_2	0.2	0	0
4	O_2^+=>O_2	1	0.05	4
5	O^-=>O	1	0	0
6	$O_2(a^1\Delta_g)$=>O	1	0	0
7	$O(^1D)$=>0.5O_2	0.2	0	0
8	O^+=>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 in the case of the Plasma, Time Periodic interface means that a periodic steady state 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+O_2=>O+O^-). This reaction tends to be very effective at low electron energies and can reduce the electrons in a discharge to a point that an ion-ion discharge is obtained. The transport and volume creation/destruction mechanisms tend to be more complex than electropositive plasmas in many aspects. Here only a few are mentioned with emphasis on the numerical difficulties that they introduce. More information can be found in Ref. 1 section 10.3 and references therein.

In electronegative discharges negative ions are well confined by the ambipolar electric field and losses by transport are very small. This means that to achieve a steady state volume losses need to be included for negative ions. The mechanisms by which negative ions are lost depend on the gas mixture and pressure and they are: mutual recombination with

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

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

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

Negative ions are well confined in the discharge core and can attain negligible densities in the edges. If the density becomes too low it can present a numerical problem. To overcome this difficulty it is necessary to add some artificial creation that can be achieved by enabling the **Reaction source stabilization**.

INFLOW

When solving for plasmas with chemistries that contain more than one element (for example, Ar and O_2) in the Plasma, Time Periodic interface 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 **Inflow** boundary condition fixes the mass fraction or mole fraction of specified species and it is used in this model as a strategy to fix the mass fraction

of O_2 at the left boundary even if no flux exists in the system. An important aspect to remember is that the **Inflow** feature does not apply a constraint to the mass fraction of the species being computed **From mass constraint** and if the other species mass fractions attain important values the mass fraction of the mass constraint species can differ from the value specified. This can be avoided by setting to a small value the mass fraction of the species that attain large values in the inflow region.

Results and Discussion

Figure 1 and Figure 2 show the spatial distribution of period averaged number densities for all charged species and for mole fraction of O_2 of 0.9 and 0.1. In both cases the distribution of charged species is such that in the core of the discharge the dominant charged species are positive and negative ions. Electrons have a number density of two orders of magnitude lower which means that the electronegative is in the 100s. In the discharge edges the negative ion number density drops fast and the plasma becomes electropositive. For $xO_2 = 0.9$ the dominant ion in the edge is O_2^+ and for $xO_2 = 0.1$ the dominant ion in the edge is Ar^+.

The fast drop in the negative ions density can cause numerical issues as explain before. In this model isotropic diffusion was used which smooths the negative ion profile and increase its density in the edges. It is important to not use to much isotropic diffusion so that the negative ion density in the edges becomes important.

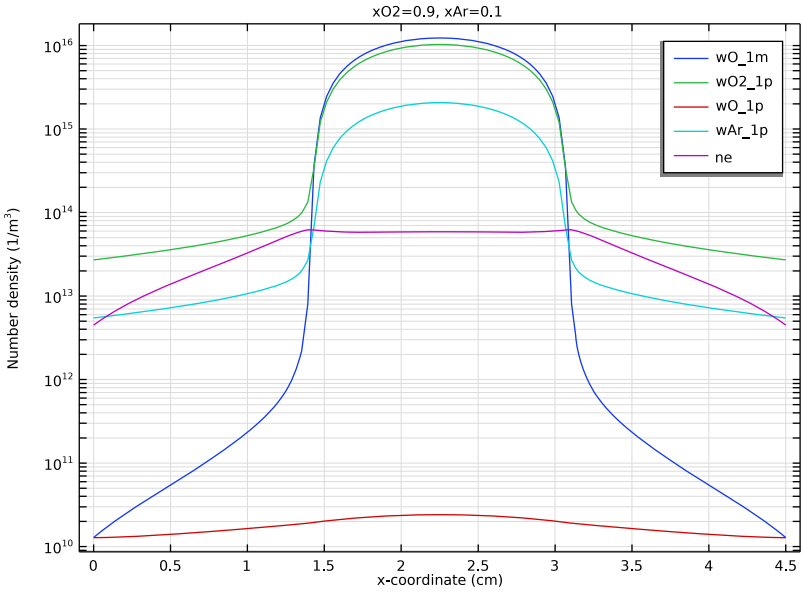

Figure 1: Spatial distribution of period averaged number densities of charged species for an O_2 mole fraction of 0.9.

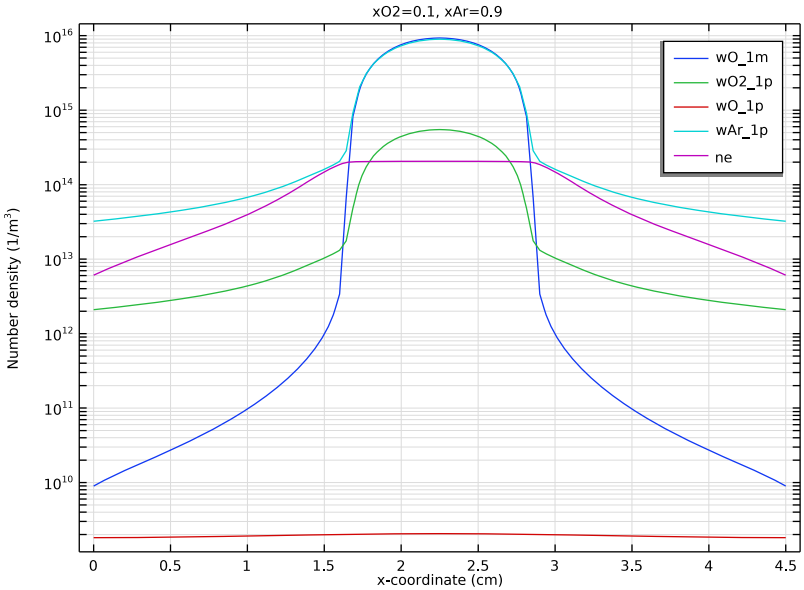

Figure 2: Spatial distribution of period averaged number densities of charged species for an O_2 mole fraction of 0.1.

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/Capacitively_Coupled_Plasmas/ccp_argon_oxygen`

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.

2 In the **Select Physics** tree, select **Plasma>Plasma, Time Periodic (ptp)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Periodic**.

6 Click **Done**.

GEOMETRY 1

Create a 1D domain of length 4.5 cm that corresponds to the distance between plates in the 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**.

Interval 1 (i1)

1 Right-click **Component 1 (comp1)>Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 In the table, enter the following settings:

Coordinates (cm)
0
4.5

Add parameters that represent the mole fractions of O2 and Ar.

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
x02	0.9	0.9	
xAr	1-x02	0.1	

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 1

1 In the **Model Builder** window, under **Global Definitions** click **Plasma Chemistry 1**.

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**.

This model needs stabilization because the density of the negative ions can attain very small values at the reactor edges. The source and reaction source stabilizations add artificial creation to prevent the densities to reach very small values.

6 Click the **Show More Options** button in the **Model Builder** toolbar.

7 In the **Show More Options** dialog box, select **Physics>Stabilization** in the tree.

8 In the tree, select the check box for the node **Physics>Stabilization**.

9 Click **OK**.

PLASMA, TIME PERIODIC (PTP)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Plasma, Time Periodic (ptp)**.

2 In the **Settings** window for **Plasma, Time Periodic**, locate the **Cross-Section Area** section.

3 In the A text field, type `pi*(14.36[cm])^2`.

4 Locate the **Extra Dimension Settings** section. From the **Heavy species selection** list, choose **Base geometry**.

5 Click to expand the **Stabilization** section. Select the **Source stabilization** check box.

6 Click to expand the **Inconsistent Stabilization** section. Select the **Isotropic diffusion for ions** check box.

7 Locate the **Stabilization** section. Select the **Reaction source stabilization** check box.

8 Locate the **Transport Settings** section. Find the **Include** subsection. Select the **Mixture diffusion correction** check box.

9 Locate the **Electron Energy Distribution Function Settings** section. From the **Electron energy distribution function** list, choose **Maxwellian**.

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

Species: O2

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)** click **Species: O2**.

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the x_0 text field, type `x02`.

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: O2+

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

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: 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: 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 **Initial value from electroneutrality constraint** check box.

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

1: Ar+=>Ar

1 In the **Model Builder** window, click **1: Ar+=>Ar**.

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

3 From the **Selection** list, choose **All boundaries**.

2: Ars=>Ar

1 In the **Model Builder** window, click **2: Ars=>Ar**.

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

3 From the **Selection** list, choose **All boundaries**.

3: O=>0.5O2

1 In the **Model Builder** window, click **3: O=>0.5O2**.

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

3 From the **Selection** list, choose **All boundaries**.

4: O2+=>O2

1 In the **Model Builder** window, click **4: O2+=>O2**.

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

3 From the **Selection** list, choose **All boundaries**.

5: O-=>O

1 In the **Model Builder** window, click **5: O-=>O**.

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

3 From the **Selection** list, choose **All boundaries**.

6: O2a1Dg=>O2

1 In the **Model Builder** window, click **6: O2a1Dg=>O2**.

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

3 From the **Selection** list, choose **All boundaries**.

7: O1D=>0.5O2

1 In the **Model Builder** window, click **7: O1D=>0.5O2**.

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

3 From the **Selection** list, choose **All boundaries**.

8: O+=>O

1 In the **Model Builder** window, click **8: O+=>O**.

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

3 From the **Selection** list, choose **All boundaries**.

Set the temperature and pressure of the background neutral gas.

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 In the T text field, type `300[K]`.

4 In the p_A text field, type `0.05[torr]`.

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/m^3]`.

4 From the **Initial electric potential** list, choose **User defined**.

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

10: e+O2=>e+O2a1Dg, 11: e+O2=>e+O2, 12: e+O2=>e+O2, 13: e+O2=>e+O+O, 14: e+O2=>e+O+O1D, 15: e+O2=>e+O2, 16: e+O2=>2e+O2+, 17: e+O=>e+O, 18: e+O=>e+O1D, 19: e+O=>e+O, 1: e+O2=>O+O-, 20: e+O=>2e+O+, 21: e+Ar=>e+Ar, 22: e+Ar=>e+Ars, 23: e+Ars=>e+Ar, 24: e+Ar=>2e+Ar+, 25: e+Ars=>2e+Ar+, 26: e+O-=>O+e+e, 2: e+O2=>e+O2, 3: e+O2=>e+O2, 4: e+O2=>e+O2, 5: e+O2=>e+O2, 6: e+O2=>e+O2, 7: e+O2=>e+O2, 8: e+O2=>e+O2, 9: e+O2=>e+O2, Cross Section Import 1, Cross Section Import 2, Cross Section Import 3

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)**, Ctrl-click to select **Cross Section Import 1**, **Cross Section Import 2**, **Cross Section Import 3**, **1: e+O2=>O+O-**, **2: e+O2=>e+O2**, **3: e+O2=>e+O2**, **4: e+O2=>e+O2**, **5: e+O2=>e+O2**, **6: e+O2=>e+O2**, **7: e+O2=>e+O2**, **8: e+O2=>e+O2**, **9: e+O2=>e+O2**, **10: e+O2=>e+O2a1Dg**, **11: e+O2=>e+O2**, **12: e+O2=>e+O2**, **13: e+O2=>e+O+O**, **14: e+O2=>e+O+O1D**, **15: e+O2=>e+O2**, **16: e+O2=>2e+O2+**, **17: e+O=>e+O**, **18: e+O=>e+O1D**, **19: e+O=>e+O**, **20: e+O=>2e+O+**, **21: e+Ar=>e+Ar**, **22: e+Ar=>e+Ars**, **23: e+Ars=>e+Ar**, **24: e+Ar=>2e+Ar+**, **25: e+Ars=>2e+Ar+**, and **26: e+O-=>O+e+e**.

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

Electron Impact Reactions

In the **Settings** window for **Group**, type `Electron Impact Reactions` in the **Label** text field.

27: O++O2=>O+O2+, 28: O-+O+=>O+O, 29: O-+O2+=>O+O+O, 30: O-+O2+=>O+O2, 31: O-+O=>O2+e, 32: O-+Ar+=>O+Ar

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)**, Ctrl-click to select **27: O++O2=>O+O2+**, **28: O-+O+=>O+O**, **29: O-+O2+=>O+O+O**, **30: O-+O2+=>O+O2**, **31: O-+O=>O2+e**, and **32: O-+Ar+=>O+Ar**.

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

Heavy Species Reactions

In the **Settings** window for **Group**, type `Heavy Species Reactions` in the **Label** text field.

Species: Ar, Species: Ar+, Species: Ars, Species: O, Species: O+, Species: O-, Species: O1D, Species: O2, Species: O2+, Species: O2a1Dg, Species: e

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)**, Ctrl-click to select **Species: e**, **Species: O2**, **Species: O**, **Species: O-**, **Species: O2a1Dg**, **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: Ar+=>Ar, 2: Ars=>Ar, 3: O=>0.5O2, 4: O2+=>O2, 5: O-=>O, 6: O2a1Dg=>O2, 7: O1D=>0.5O2, 8: O+=>O

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)**, Ctrl-click to select **1: Ar+=>Ar**, **2: Ars=>Ar**, **3: O=>0.5O2**, **4: O2+=>O2**, **5: O-=>O**, **6: O2a1Dg=>O2**, **7: O1D=>0.5O2**, and **8: O+=>O**.

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

Surface Reactions

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

Add a **Metal Contact** node to provide electric excitation to the system.

Metal Contact 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 From the **Source** list, choose **RF**.

5 Locate the **RF Source** section. In the P_{rf} text field, type `10[W]`.

Wall 1

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 **All boundaries**.

Ground 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Ground**.

2 Select Boundary 2 only.

The **Inflow** node is used here to fix the mass fraction of O2 at the boundary even if there is no flow going into the reactor.

In the **Plasma, Time Periodic** interface with more than one species types are present, it is difficult to preserve mass among each species type. By fixing the mass fraction of one species at a point that problem does not occur.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Inflow**, locate the **Inflow** section.

4 Click **Add**.

5 In the table, enter the following settings:

Species names	Mole fraction (1)
O2	xO2

6 Click **Add**.

7 In the table, enter the following settings:

Species names	Mole fraction (1)
Ar	xAr

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 2 only.

In electronegative plasmas the negative ions density tends to have very steep gradients at the transition of the electronegative core and electropositive edges. On this transition, a fine mesh is required to prevent oscillations in the negative ion density.

MESH 1

Edge 1

In the **Mesh** toolbar, click **Edge**.

Distribution 1

1 Right-click **Edge 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type 150.

5 In the **Element ratio** text field, type 5.

6 Select the **Symmetric distribution** check box.

Solve for three molar fractions of O2 using the **Auxiliary sweep**.

STUDY 1

Step 1: Time Periodic

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Periodic**.

2 In the **Settings** window for **Time Periodic**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xO2	0.9 0.5 0.1	

6 In the **Home** toolbar, click = **Compute**.

RESULTS

Neutral Species Number Density, Period Averaged (ptp)

1 In the **Model Builder** window, under **Results** click **Neutral Species Number Density, Period Averaged (ptp)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Parameter selection (xO2)** list, choose **From list**.

4 In the **Parameter values (xO2)** list, select **0.9**.

5 In the **Neutral Species Number Density, Period Averaged (ptp)** toolbar, click **Plot**.

Create plots of charged species for molar fractions of O2 equal to 0.1 and 0.9.

Charged Species Number Density, Period Averaged, xO2=0.9

1 In the **Model Builder** window, click **Charged Species Number Density, Period Averaged (ptp)**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 In the **Title** text area, type xO2=0.9, xAr=0.1.

4 Locate the **Data** section. From the **Parameter selection (xO2)** list, choose **From list**.

5 In the **Parameter values (xO2)** list, select **0.9**.

6 In the **Charged Species Number Density, Period Averaged (ptp)** toolbar, click **Plot**.

7 In the **Label** text field, type `Charged Species Number Density, Period Averaged, xO2=0.9`.

Charged Species Number Density, Period Averaged, xO2=0.1

1 Right-click **Charged Species Number Density, Period Averaged, xO2=0.9** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, locate the **Title** section.

3 In the **Title** text area, type `xO2=0.1, xAr=0.9`.

4 In the **Label** text field, type `Charged Species Number Density, Period Averaged, xO2=0.1`.

5 Locate the **Data** section. In the **Parameter values (xO2)** list, select **0.1**.

6 In the **Charged Species Number Density, Period Averaged, xO2=0.1** toolbar, click **Plot**.

7 Right-click **Charged Species Number Density, Period Averaged, xO2=0.1** and choose **Move Up**.