



# Model of an Argon/Chlorine Inductively Coupled Plasma Reactor with RF Bias

## *Introduction*

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This tutorial uses the **inductively Coupled Plasma with RF Bias** interface to model an argon/chlorine inductively coupled plasma reactor with RF bias (also known as ICP/CCP). The **Inductively Coupled Plasma with RF Bias** interface is used to study discharges that are sustained by induction currents and have an additional time-periodic electric excitation. This interface adds the **Plasma, Time Periodic** and **Magnetic Fields** interfaces. The magnetic field is solved in the frequency domain and the plasma solves for a periodic solution. The multiphysics couplings couple the time-averaged plasma conductivity to the **Magnetic Fields** interface and couple the resulting electron heating due to the induction currents back to the **Plasma, Time Periodic** interface.

It is also shown how to prepare a model with a mixture of different elements (in this case Ar and Cl<sub>2</sub>) in which one of the species can dissociate by electron impact (Cl<sub>2</sub> dissociates into Cl) and where negative ions exist (the dissociative electron attachment of Cl<sub>2</sub> creates Cl<sup>-</sup>).

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 to add more reactions to achieve experimental verification.

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

## *Model Definition*

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The plasma model is solved self-consistently with the **Magnetic Fields**, **Laminar Flow** and **Heat Transfer in Fluids** interfaces. The plasma transport equations coupled with Poisson's equation are solved in a time-periodic fashion, allowing for the description of the different quantities along the period. In this way, electrons exhibit periodic modulation caused by the RF bias. The **Magnetic Fields** interface is solved in the frequency domain. The Joule heating term obtained from the **Magnetic Fields** interface is thus an averaged quantity and is given to the electron mean-energy equation as a constant value along the period. The plasma conductivity used in the magnetic field equations is computed from period-averaged quantities obtained using the **Plasma, Time Periodic** interface.

The **Laminar Flow** and **Heat Transfer in Fluids** interfaces are solved in a stationary form and consequently all period evolution is neglected. The fluid and thermodynamic properties

computed in the plasma model and passed on to the **Laminar Flow** and **Heat Transfer in Fluids** interfaces are period-averaged quantities.

In particular, this model assumes that the heavy species only exist in the **Base geometry**. This means that ions and neutrals do not have a period modulation and only experience a time-averaged electric field.

### ELECTRIC EXCITATION

There are two independent forms of electric excitation present in this model

- The inductively coupled power controlled by the coil
- The capacitively coupled power controlled by the RF bias

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

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

The electromagnetic excitation “sees” a plasma defined by the plasma conductivity in the cold plasma approximation that is set in the **Plasma Conductivity Coupling** multiphysics feature:

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

Here,  $\langle n_e \rangle$  is the period averaged electron density,  $q$  is the electron charge,  $m_e$  is the electron mass,  $\langle \nu_e \rangle$  is the period averaged collision frequency, and  $\omega$  is the angular frequency. The Joule heating term, which represents the heating of the electrons, is set in the **Electron Heat Source** multiphysics feature.

The biased electrode is driven by a sinusoidal excitation at constant voltage amplitude

$$V_s = V_{rf} \cos(2\pi f_p t + \alpha) + V_{dc,b} \quad (1)$$

The DC bias voltage  $V_{dc,b}$  is computed so that the net current over a period is zero.

### PLASMA 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:

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

and the electron energy flux:

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

For the heavy species, ions are lost to the wall due to surface reactions and the fact that the electric field is directed toward the wall:

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

The walls of the reactor are grounded with the exception of the biased electrode.

## 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 should be adapt and improved for specific applications as needed. One aspect that emerges from analyzing model results of the present model is that the dissociation degree is high. Knowing this it might be needed to add more reactions involving Cl.

The plasma chemistry used here includes electron impact reactions from [Ref. 1](#) and [Ref. 2](#), and some reactions are estimated from similar reactions based on data from [Ref. 3](#). A good discussion of plasma chemistry for electronegative gases can be found in [Ref. 4](#). In particular, in the section “A Data Set for Oxygen,” page 270 of [Ref. 4](#) a set of reactions for oxygen discharges is discussed.

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 three species and seven reactions presented in Table 1 (electron impact cross sections are obtained from Ref. 1).

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	-

Chlorine 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  $\text{Cl}_2$  are from Ref. 2 except for  $\text{e} + \text{Cl} \Rightarrow \text{Cl} + \text{e} + \text{e}$  and  $\text{e} + \text{Cl} \Rightarrow \text{Cl} + \text{e} + \text{e}$ , which are estimated from similar reactions from Ref. 3. Electron impact reactions are neglected except for  $\text{e} + \text{Cl} \Rightarrow \text{Cl} + \text{e} + \text{e}$ . For simplicity, rotational, vibrational, and electronic excited states are not treated explicitly but energy losses are considered. The chlorine electron impact reactions used in this model are presented in Table 2.

TABLE 2: CHLORINE ELECTRON IMPACT REACTIONS.

Reaction	Formula	Type	$\Delta\epsilon(\text{eV})$
1	$\text{e} + \text{Cl}_2 \Rightarrow \text{Cl} + \text{Cl}^-$	Dissociative attachment	-
2	$\text{e} + \text{Cl}_2 \Rightarrow \text{e} + \text{Cl}_2$	Elastic	-
3	$\text{e} + \text{Cl}_2 \Rightarrow \text{e} + \text{Cl}_2$	Vibrational excitation	0.069
4	$\text{e} + \text{Cl}_2 \Rightarrow \text{e} + \text{Cl}_2$	Vibrational excitation	0.139
5-9	$\text{e} + \text{Cl}_2 \Rightarrow \text{e} + \text{Cl} + \text{Cl}$	Dissociative excitation	3.36-7.02
10	$\text{e} + \text{Cl}_2 \Rightarrow \text{e} + \text{Cl}_2$	Excitation	10.54
11	$\text{e} + \text{Cl}_2 \Rightarrow \text{e} + \text{Cl}_2$	Excitation	10.7
12	$\text{e} + \text{Cl}_2 \Rightarrow \text{e} + \text{Cl}^- + \text{Cl}^+$	Excitation	11
13	$\text{e} + \text{Cl}_2 \Rightarrow 2\text{e} + \text{Cl}_2^+$	Ionization	11.49
14	$\text{e} + \text{Cl}_2 \Rightarrow 2\text{e} + \text{Cl} + \text{Cl}^+$	Ionization	11.49
15	$\text{e} + \text{Cl} \Rightarrow 2\text{e} + \text{Cl}^+$	Ionization	14.25
16	$\text{e} + \text{Cl}^- \Rightarrow 2\text{e} + \text{Cl}$	Ionization	14.25

Table 3 presents the heavy species reactions involving ions. All these reactions rates are estimated from similar reactions from Ref. 3.

TABLE 3: HEAVY SPECIES REACTIONS INVOLVING IONS.

Reaction	Formula	Type
1	$\text{Cl}^+ + \text{Cl}^- \Rightarrow 2\text{Cl}$	Mutual recombination
2	$\text{Cl}_2^+ + \text{Cl}^- \Rightarrow 3\text{Cl}$	Mutual recombination
3	$\text{Cl}^- + \text{Ar}^+ \Rightarrow \text{Cl} + \text{Ar}$	Mutual recombination

In addition to volumetric reactions, Table 4 lists the surface reactions implemented.

TABLE 4: SURFACE REACTIONS.

Reaction	Formula	Sticking coefficient	Secondary emission coefficient	Mean energy of secondary electrons (V)
1	$\text{Ar} \Rightarrow \text{Ar}$	1	0.07	5.8
2	$\text{Ar}^+ \Rightarrow \text{Ar}$	1	0.07	5.8
3	$\text{Cl} \Rightarrow 0.5\text{Cl}_2$	0.01	0	0
4	$\text{Cl}_2^+ \Rightarrow \text{Cl}_2$	1	0.07	5.8
5	$\text{Cl}^- \Rightarrow \text{Cl}$	1	0	0
6	$\text{Cl}^+ \Rightarrow \text{Cl}$	1	0.07	5.8

Boundary conditions for heavy species are introduced in the model by using surface reactions. If no surface reactions that lead to the loss 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,  $e + \text{Cl}_2 \Rightarrow \text{Cl} + \text{Cl}^-$ ). This reaction tends to be very effective at low electron energies and can reduce the electrons in a discharge to the 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 respects. Here, only a few are mentioned with emphasis on the numerical

difficulties that they introduce. More information can be found in [Ref. 4](#), 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,  $\text{Cl}^- + \text{Cl}^+ \Rightarrow 2\text{Cl}$  or  $\text{Cl}^- + \text{Ar}^+ \Rightarrow \text{Cl} + \text{Ar}$ ), detachment in collisions with excited or neutral atoms or molecules (for example,  $\text{Cl}^- + \text{Cl} \Rightarrow \text{Cl}_2 + e$  or  $\text{Cl}^- + \text{Cl}_2 \Rightarrow \text{Cl} + \text{Cl}_2 + e$ ), and electron-impact detachment (for example,  $e + \text{Cl}^- \Rightarrow \text{Cl} + 2e$ ).

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 diffusion coefficient or decreasing its mobility. When using the option **Compute Mobility and Diffusivity** the mobility is computed using Einstein relation which by default uses the gas temperature. By specifying a higher ion temperature results in a smaller mobility.
- Enable **Isotropic diffusion for ions** in the **Inconsistent Stabilization** section (the stabilization sections are visible when **Stabilization** is selected in **Show More Options**). This option adds artificial diffusion to all ions and helps smoothing the sharp transition of the negative ion density between the electropositive edge and the electronegative core, and also increase the density of the negative ions in the electropositive edge effectively increasing its losses by transport. This option should be used very carefully since completely wrong results can be obtained if too much diffusion is used (the tuning parameter for ions should not be larger than 0.1). A useful strategy is to start with a large **Tuning parameter for ions** (for example, 0.5) and ramp it down using a **Auxiliary sweep**.

## INFLOW AND OUTFLOW

The **Inflow** boundary condition fixes the mass fraction or mole fraction of specified species. It is used in this model to set the mole fraction of the inlet mixture at a boundary. The fluid velocity is computed and set at the same boundary by the **Inlet** feature of the **Laminar Flow** interface. At the **Inflow** boundary condition the model fraction of Cl is set to a small

number so that the mole fraction of Ar/Cl<sub>2</sub> is always respected at the boundary. When dissociation is high, the mole fraction of Ar can be different than specified because the mass fraction of Ar is obtained from a mass constraint and, in fact, no explicit constraint is applied at the boundary.

The **Outflow** boundary condition removes transport by diffusion at the boundary but it still keeps transport by convection and migration in the electric field. The **Outflow** boundary condition only sets boundary conditions for heavy species. To model a net outflow out of the system the **Outlet** boundary condition of the Laminar flow interface should be used.

When solving for plasmas with chemistries that contain more than one element (for example, Ar and Cl<sub>2</sub>) 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. As a strategy to overcome this problem, one can fix the mole fraction of a given species using the **Inflow** boundary condition even if no fluid flow exists in the system.

In the present model, it is assumed that the charged species (electrons and ions) are lost by transport at the inflow and outflow boundaries. This is modeled by applying the surface reactions for ions and the **Wall** feature for electrons. This could represent a metal grid boundary that allows the neutral gas to flow through it, while the plasma “sees” a metal boundary. It is also assumed that Ar and Cl can react at the inflow and outflow boundaries. To adjust the probability of a reaction to occur at a surface, the **Forward sticking coefficient** in the **Surface Reaction** feature can be adjusted. As an example, to model a 50% probability of Ar to react at the outflow grid, the **Forward sticking coefficient** should be set to 0.5.

## SOLUTION STRATEGY

The recommended solution strategy to model an inductively coupled plasma with RF bias is as follows. First solve the problem with inductively coupled plasma only. To speed up this study, set the **Number of elements** in the **Extra Dimension Settings** to 1. Since there is no RF bias applied yet it is not necessary to have resolution along the period. Afterward, add a second study that uses the solution of the previous study as initial conditions. Increase the **Number of elements** to a value in the range 30–50 and use the **Auxiliary sweep** to increase the amplitude of the applied voltage.

For pure CCP problems, it is advised to set the **Terminal type** to **Power** in the **Metal Contact** feature because it makes the numerical problem much easier. For ICP/CCP models, it is advised to set **Terminal type** to **Voltage**.



At the biased electrode, the electrons can exhibit strong period modulation and can attain as high energies as in a pure CCP reactor. For these reasons, the space and period resolutions need to be as high as in a pure CCP reactor model.

## *Results and Discussion*

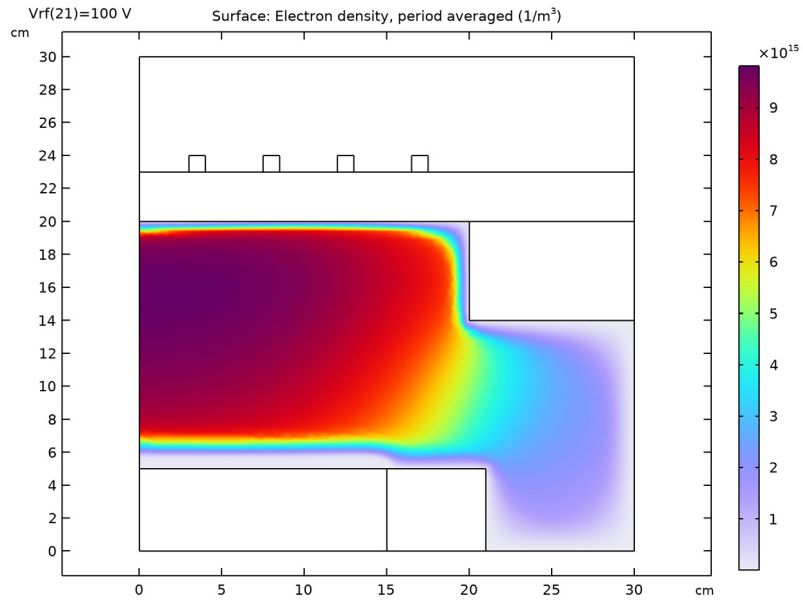
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Figure 1 through Figure 3 show the period-averaged spatial distributions of the electron density, electron temperature, and electric potential for 250 W of coil power and  $V_{rf} = 100$  V. The electron density is relatively low (almost  $10^{16} \text{ m}^{-3}$ ) and has a flat profile in the core of the discharge, where the dominant charged species are the ions of chlorine (not shown) with number densities of the order of  $10^{17} \text{ m}^{-3}$ . This makes the discharge have high electronegativity in most of the reactor. At the edges, the negative ion density decreases fast and the plasma becomes electropositive.

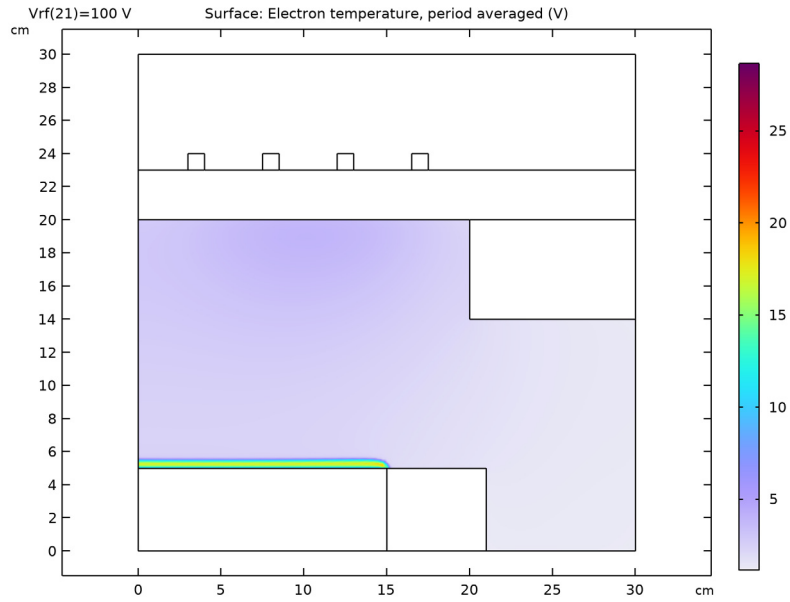
The dominant power coupled to the system is inductive and is responsible for maintaining a high plasma density. The RF bias influences the plasma density significantly but the electron temperature changes from having a maximum just below the coil for  $V_{rf} = 0$  V to a maximum at the biased electrode for higher voltages.

From the period-averaged potential it is possible to see that a DC bias of about  $-75$  V is developed at the biased electrode. This is also possible to see from the period evolution of the applied voltage Figure 4. This figure also shows the current at the electrode, which strongly deviates from a sinusoidal and has a strong contribution from the electron current when the sheath collapses.

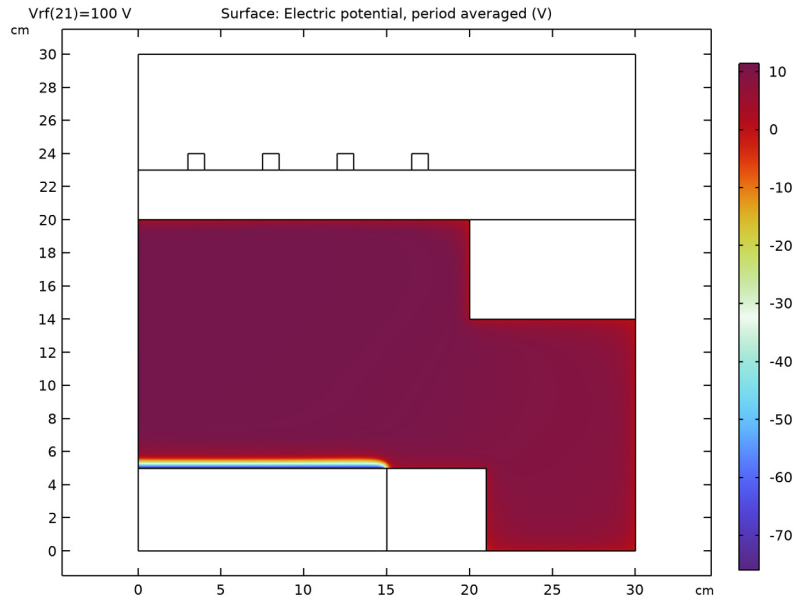
Figure 5 and Figure 6 show the magnitude of the fluid velocity and the gas temperature, respectively. The flow pattern, as expected, has its maximum at the inlet and the trajectory strongly connects to the outlet with the region at the symmetry axis having low fluid velocities. The background gas temperature attains 1000 K with elastic collisions of electrons with the background gas being the main heating mechanism.



*Figure 1: Period averaged electron density for 250 W of coil power and  $V_{rf} = 100$  V.*



*Figure 2: Period averaged electron temperature for 250 W of coil power and  $V_{rf} = 100$  V.*



*Figure 3: Period averaged electric potential for 250 W of coil power and  $V_{rf} = 100$  V.*

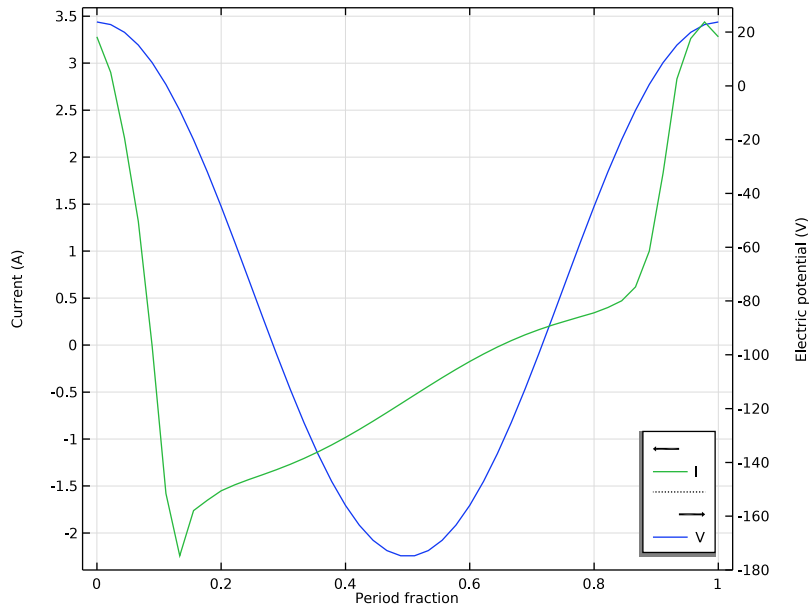
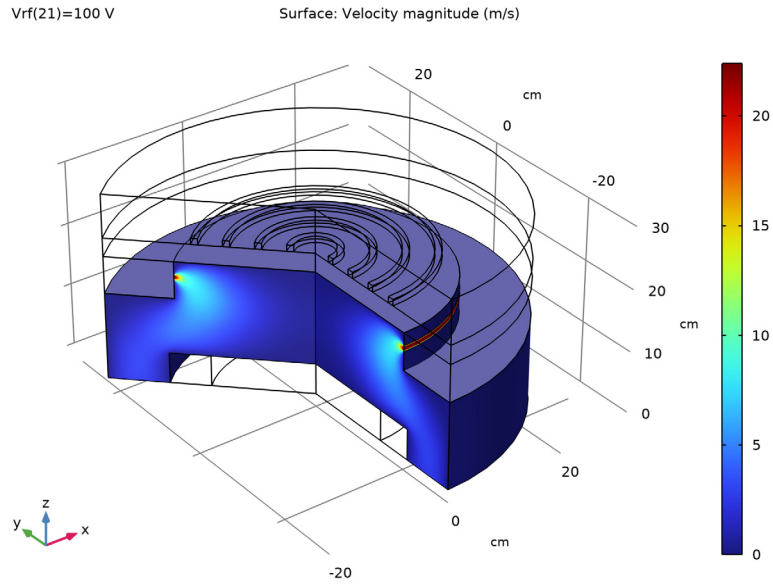


Figure 4: Current and voltage at the biased electrode for 250 W of coil power and  $V_{rf} = 100$  V.



*Figure 5: Magnitude of the fluid velocity for 250 W of coil power and  $V_{\text{rf}} = 100$  V.*

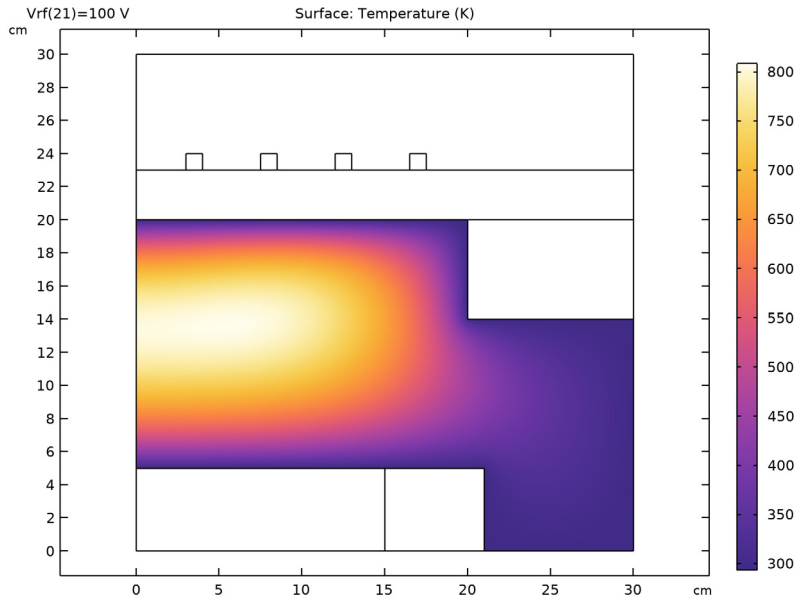


Figure 6: Gas temperature for 250 W of coil power and  $V_{rf} = 100$  V.

## References

1. Phelps database, [www.lxcat.net](http://www.lxcat.net), retrieved 2017.
2. SIGLO database, [www.lxcat.net](http://www.lxcat.net), retrieved 2022.
3. A. Friedman, Plasma Chemistry, *Cambridge University Press*, 2008
4. M.A. Lieberman and A.J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, John Wiley & Sons, 2005.


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**Application Library path:** Plasma\_Module/Inductively\_Coupled\_Plasmas/  
icp\_ccp\_argon\_chlorine




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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 with RF Bias**.
- 3 Click **Add**.
- 4 In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.
- 5 Click **Add**.
- 6 In the **Select Physics** tree, select **Heat Transfer>Heat Transfer in Fluids (ht)**.
- 7 Click **Add**.
- 8 Click  **Study**.
- 9 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Frequency-Time Periodic**.
- 10 Click  **Done**.

## **GEOMETRY I**


Create the geometry of a generic 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 15.
- 4 Locate the **Position** section. In the **z** text field, type 5.

#### *Rectangle 7 (r7)*




- 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 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.
- 5 Locate the **Starting Point** section. In the **r** text field, type 20.
- 6 In the **z** text field, type 17.
- 7 Locate the **Endpoint** section. In the **r** text field, type 20.
- 8 In the **z** text field, type 18.

#### *Mesh Control Edges 1 (mce1)*

- 1 In the **Geometry** toolbar, click  **Virtual Operations** and choose **Mesh Control Edges**.
- 2 On the object **fin**, select Boundaries 6 and 29 only.
- 3 In the **Geometry** toolbar, click  **Build All**.
- 4 Click the  **Zoom Extents** button in the **Graphics** toolbar.

### **GEOMETRY 1**

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

Add parameters for use in the model, such as the mole fractions of Cl<sub>2</sub> and Ar as well as the amplitude of the RF bias  $V_{rf}$ .

### **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
Isopar	0.1	0.1	Ions isotropic diffusion
Picp	250[W]	250 W	Coil power
Qf	250	250	Mass flow in SCCCM
xC12	0.9	0.9	Inflow mole fraction of C12
xAr	1-xC12	0.1	Inflow mole fraction of Ar
Vrf	0[V]	0 V	Voltage amplitude of rf bias

Create explicit selections to simplify the model creation.

## DEFINITIONS (COMPI)


### Coil

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

### Coil Boundaries

- 1 Right-click **Coil** 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**.


### 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**.

Add materials to define the properties of the coil, dielectric window, and air surrounding the coil.


## 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>Copper**.
- 6 Click **Add to Component** in the window toolbar.
- 7 In the tree, select **Built-in>Glass (quartz)**.
- 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.

### *Copper (mat2)*

- 1 In the **Model Builder** window, click **Copper (mat2)**.
- 2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 3 From the **Selection** list, choose **Coil**.


### *Glass (quartz) (mat3)*

- 1 In the **Model Builder** window, click **Glass (quartz) (mat3)**.
- 2 Select Domain 3 only.

## DEFINITIONS (COMP1)

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

## MATERIALS


- 1 In the **Model Builder** window, collapse the **Component 1 (comp1)>Materials** node.
- 2 Click the  **Show More Options** button in the **Model Builder** toolbar.
- 3 In the **Show More Options** dialog box, select **Physics>Stabilization** in the tree.
- 4 In the tree, select the check box for the node **Physics>Stabilization**.
- 5 Click **OK**.

Select some transport settings to couple the plasma model with heat transfer and fluid flow. Also select **Mixture diffusion correction** to add a correction term to the heavy species flux.

This model needs stabilization because the density of the negative ions can drop sharply and attain very small values at the reactor edges. The reaction source stabilizations add artificial creation to prevent the densities to reach very small values, and isotropic diffusion prevents the appearance of instabilities when the negative ion density drops sharply.

Set the **Number of elements** in the extra dimension to 1 because in the first study only the ICP power is added and resolution along the period is not necessary.

### 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**, click to expand the **Stabilization** section.
- 3 Select the **Reaction source stabilization** check box.
- 4 Locate the **Transport Settings** section. Find the **Include** subsection. Select the **Calculate thermodynamic properties** check box.
- 5 Select the **Mixture diffusion correction** check box.
- 6 Select the **Convection** check box.
- 7 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** check box.
- 8 Locate the **Electron Energy Distribution Function Settings** section. From the **Electron energy distribution function** list, choose **Maxwellian**.
- 9 Locate the **Extra Dimension Settings** section. In the  $N$  text field, type 1.
- 10 From the **Heavy species selection** list, choose **Base geometry**.
- 11 Click to expand the **Inconsistent Stabilization** section. Select the **Isotropic diffusion for ions** check box.
- 12 In the  $\delta_{id,i}$  text field, type Isopar.
- 13 Locate the **Domain Selection** section. Click  **Clear Selection**.
- 14 Select Domain 2 only.

### 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_Cl2_plasma_chemistry.txt`.
- 5 Click **Import**.

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

#### PLASMA, TIME PERIODIC (PTP)

*10: e+Cl2=>e+Cl2, 11: e+Cl2=>e+Cl2, 12: e+Cl2=>e+Cl+Cl+, 13: e+Cl2=>2e+Cl2+, 14: e+Cl2=>2e+Cl+Cl+, 15: e+Ar=>e+Ar, 16: e+Ar=>e+Ars, 17: e+Ars=>e+Ar, 18: e+Ar=>2e+Ar+, 19: e+Ars=>2e+Ar+, 1: e+Cl2=>Cl+Cl-, 20: e+Cl=>Cl++2e, 21: e+Cl-=>Cl+2e, 2: e+Cl2=>e+Cl2, 3: e+Cl2=>e+Cl2, 4: e+Cl2=>e+Cl2, 5: e+Cl2=>e+*

$Cl+Cl$ , 6:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 7:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 8:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 9:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , *Cross Section Import 1*, *Cross Section Import 2*

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**, 1:  $e+Cl_2 \Rightarrow Cl+Cl-$ , 2:  $e+Cl_2 \Rightarrow e+Cl_2$ , 3:  $e+Cl_2 \Rightarrow e+Cl_2$ , 4:  $e+Cl_2 \Rightarrow e+Cl_2$ , 5:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 6:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 7:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 8:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 9:  $e+Cl_2 \Rightarrow e+Cl+Cl$ , 10:  $e+Cl_2 \Rightarrow e+Cl_2$ , 11:  $e+Cl_2 \Rightarrow e+Cl_2$ , 12:  $e+Cl_2 \Rightarrow e+Cl+Cl+$ , 13:  $e+Cl_2 \Rightarrow 2e+Cl_2+$ , 14:  $e+Cl_2 \Rightarrow 2e+Cl+Cl+$ , 15:  $e+Ar \Rightarrow e+Ar$ , 16:  $e+Ar \Rightarrow e+Ar$ , 17:  $e+Ar \Rightarrow e+Ar$ , 18:  $e+Ar \Rightarrow 2e+Ar+$ , 19:  $e+Ar \Rightarrow 2e+Ar+$ , 20:  $e+Cl \Rightarrow Cl++2e$ , and 21:  $e+Cl \Rightarrow Cl+2e$ .

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

#### *Electron Impact Reactions*

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

2 In the **Model Builder** window, collapse the **Electron Impact Reactions** node.

22:  $Ar+Ar \Rightarrow Ar++Ar+e$ , 23:  $Cl++Cl \Rightarrow 2Cl$ , 24:  $Cl_2++Cl \Rightarrow 3Cl$ , 25:  $Cl+Ar \Rightarrow Cl+Ar$

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)**, Ctrl-click to select **22:  $Ar+Ar \Rightarrow Ar++Ar+e$** , **23:  $Cl++Cl \Rightarrow 2Cl$** , **24:  $Cl_2++Cl \Rightarrow 3Cl$** , and **25:  $Cl+Ar \Rightarrow Cl+Ar$** .

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: Cl, Species: Cl+, Species: Cl-, Species: Cl2, Species: Cl2+, Species: e*

1 In the **Model Builder** window, under **Component 1 (comp1)>Plasma, Time Periodic (ptp)**, Ctrl-click to select **Species: e**, **Species: Cl2**, **Species: Cl**, **Species: Cl-**, **Species: Cl+**, **Species: Cl2+**, **Species: Ar**, **Species: Ars**, and **Species: Ar+**.

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

#### *Species*

In the following, initial mole fractions and initial number density for ions are specified. The mass fraction of Ar is found from a mass constraint and the initial density of  $Cl_2+$  is found by requiring electroneutrality.

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

*Species: Cl2*

- 1 In the **Model Builder** window, click **Species: Cl2**.
- 2 In the **Settings** window for **Species**, locate the **General Parameters** section.
- 3 In the  $x_0$  text field, type  $xCl2$ .

*Species: Cl*

- 1 In the **Model Builder** window, click **Species: Cl**.
- 2 In the **Settings** window for **Species**, locate the **General Parameters** section.
- 3 In the  $x_0$  text field, type  $1e-4$ .

*Species: Cl-*

- 1 In the **Model Builder** window, click **Species: Cl-**.
- 2 In the **Settings** window for **Species**, locate the **General Parameters** section.
- 3 In the  $n_0$  text field, type  $1e10$ .

*Species: Cl+*

- 1 In the **Model Builder** window, click **Species: Cl+**.
- 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: Cl2+*

- 1 In the **Model Builder** window, click **Species: Cl2+**.
- 2 In the **Settings** window for **Species**, locate the **Species Formula** section.
- 3 Select the **Initial value from electroneutrality 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 **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 **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.



- 4 Click to expand the **Species Thermodynamic Parameters** section. In the  $\Delta h$  text field, type 15.80.

*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  $\Delta h$  text field, type 11.5.

*Species: Cl2+*

- 1 In the **Model Builder** window, click **Species: Cl2+**.
- 2 In the **Settings** window for **Species**, locate the **Species Thermodynamic Parameters** section.
- 3 In the  $\Delta h$  text field, type 11.49.

*Species: Cl+*

- 1 In the **Model Builder** window, click **Species: Cl+**.
- 2 In the **Settings** window for **Species**, locate the **Species Thermodynamic Parameters** section.
- 3 In the  $\Delta h$  text field, type 14.25.

## PLASMA, TIME PERIODIC (PTP)

*Species*

In the **Model Builder** window, collapse the **Component 1 (comp1)>Plasma, Time Periodic (ptp)>Species** node.

*1: Ar+=>Ar, 2: Ars=>Ar, 3: Cl=>0.5Cl2, 4: Cl-=>Cl, 5: Cl2+=>Cl2, 6: Cl+=>Cl*

- 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: Cl=>0.5Cl2, 4: Cl-=>Cl, 5: Cl2+=>Cl2, and 6: Cl+=>Cl**.
- 2 Right-click and choose **Group**.

*Surface Reactions*

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

*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 **Walls**.

2:  $Ars \Rightarrow Ar$

- 1 In the **Model Builder** window, click **2:  $Ars \Rightarrow Ar$** .
- 2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Walls**.

3:  $Cl \Rightarrow 0.5 Cl_2$

- 1 In the **Model Builder** window, click **3:  $Cl \Rightarrow 0.5 Cl_2$** .
- 2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Walls**.

4:  $Cl \Rightarrow Cl$

- 1 In the **Model Builder** window, click **4:  $Cl \Rightarrow Cl$** .
- 2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Walls**.

5:  $Cl_2 \Rightarrow Cl_2$

- 1 In the **Model Builder** window, click **5:  $Cl_2 \Rightarrow Cl_2$** .
- 2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Walls**.

6:  $Cl \Rightarrow Cl$

- 1 In the **Model Builder** window, click **6:  $Cl \Rightarrow Cl$** .
- 2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Walls**.

## **PLASMA, TIME PERIODIC (PTP)**

### *Surface Reactions*

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

In the following, select the fluid velocity, temperature and pressure to come from the **Laminar Flow** and **Heat Transfer in Fluids** interfaces.

Set the electron mobility. All other electron transport properties are computed from the given electron mobility.

### *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<sub>A</sub>** list, choose **Absolute pressure (spf)**.
- 6 Locate the **Electron Density and Energy** section. From the **Electron transport properties** list, choose **Specify mobility only**.
- 7 In the  $\mu_e N_n$  text field, type  $0.7e24[1/V/m/s]*(ptp.Te/1[V])^{-0.6}*exp(1.3[V]/ptp.Te)$ .


#### Initial Values I

- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the  $n_{e,0}$  text field, type  $1E15[1/m^3]$ .
- 4 In the  $\varepsilon_0$  text field, type  $2[V]$ .

#### Wall I

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Wall**.  
The **Wall** node sets boundary conditions for the electron transport equations.
- 2 In the **Settings** window for **Wall**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Walls**.



#### Ground I

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Ground**.
- 2 Select Boundaries 6, 33–36, 39, and 40 only.

The **Inflow** node is used here to fix the mole fraction of Ar, Cl<sub>2</sub>, and Cl at the boundary that represents the inlet.

The mole fraction of xCl is fixed at a low value to prevent it to attain large values due to dissociation of Cl<sub>2</sub>.

#### Inflow I

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inflow**.
- 2 In the **Settings** window for **Inflow**, locate the **Inflow** section.
- 3 Click  **Add**.
- 4 In the table, enter the following settings:

Species names	Mole fraction (I)
Ar	xAr

5 Click  **Add**.

6 In the table, enter the following settings:

Species names	Mole fraction (l)
C12	xCl2

7 Click  **Add**.

8 In the table, enter the following settings:

Species names	Mole fraction (l)
C1	1e-4

9 Select Boundary 35 only.

*Outflow I*

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

2 Select Boundary 39 only.

*Dielectric Contact I*

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

2 Select Boundaries 27 and 38 only.

Add a **Metal Contact** node to set a RF bias.

*Metal Contact I*

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

2 Select Boundary 4 only.

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

4 From the **Terminal type** list, choose **Voltage**.

5 Locate the **RF Source** section. In the  $V_a$  text field, type  $V_{rf}$ .

6 Locate the **DC Source** section. Select the **Compute DC self-bias** check box.

**PLASMA, TIME PERIODIC (PTP)**


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

Select the domains where the magnetic fields are to be solved and add the coil that is responsible for exciting the plasma.

## 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*

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


## MAGNETIC FIELDS (MF)

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

Select the domain where the fluid flow is to be solved and select the fluid properties to come from the **Plasma, Time Periodic** interface and the fluid temperature to come from the **Heat Transfer in Fluids** interface.

Also, set an inlet and outlet for the flow in the system, and set the operation pressure.

## 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  $p_{\text{ref}}$  text field, type  $0.015[\text{torr}]$ .

### *Fluid Properties 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Laminar Flow (spf)** click **Fluid Properties 1**.
- 2 In the **Settings** window for **Fluid Properties**, locate the **Model Input** section.
- 3 From the  $T$  list, choose **Temperature (ht)**.
- 4 Locate the **Fluid Properties** section. From the  $\rho$  list, choose **Density, period averaged (ptp/pes1)**.

- 5 From the  $\mu$  list, choose **Dynamic viscosity, period averaged (ptp/pesI)**.

#### *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  $Q_{\text{sccm}}$  text field, type Qf.
- 7 From the  $M_n$  list, choose **Mean molar mass, period averaged (ptp/pesI)**.

#### *Outlet I*


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

Select the domain where the **Heat Transfer in Fluids** interface is to be solved and select the fluid properties to come from the **Plasma, Time Periodic** interface and the fluid velocity and pressure to come from the **Laminar Flow** interface.

### **LAMINAR FLOW (SPF)**

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

### **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 I*

- 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 **u** list, choose **Velocity field (spf)**.


- 5 Locate the **Heat Conduction, Fluid** section. From the  $k$  list, choose **Thermal conductivity, period averaged (ptp/pesI)**.
- 6 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.
- 7 From the  $\rho$  list, choose **Density, period averaged (ptp/pesI)**.
- 8 From the  $C_p$  list, choose **Heat capacity at constant pressure, period averaged (ptp/pesI)**.
- 9 From the  $\gamma$  list, choose **User defined**.

#### *Temperature I*

- 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**.

Add a heat source term for the gas coming from the plasma volume reactions.

#### *Heat Source I*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Heat Source**.
- 2 Select Domain 2 only.
- 3 In the **Settings** window for **Heat Source**, locate the **Heat Source** section.
- 4 From the  $Q_0$  list, choose **Heat source for gas, period averaged (ptp/pesI)**.

### **HEAT TRANSFER IN FLUIDS (HT)**

In the **Model Builder** window, collapse the **Component 1 (comp1)>Heat Transfer in Fluids (ht)** node.

### **MULTIPHYSICS**

#### *Electron Heat Source I (ehsptpI)*

Add a mesh as it was for an ICP reactor but with more refinement at the biased surface.

### **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 Domains 2, 10, and 11 only.
- 5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Plasma**.

- 6 From the **Predefined** list, choose **Coarse**.

#### *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 3, 4, 6, 27, 33–36, and 38–40 only.
- 6 Locate the **Element Size** section. From the **Calibrate for** list, choose **Plasma**.


#### *Edge 1*

- 1 In the **Mesh** toolbar, click  **Edge**.
- 2 Select Boundary 35 only.

#### *Distribution 1*

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


#### *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 **Coil**.

#### *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.

#### *Mapped 2*

- 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 Select Domain 2 only.



- 5 Click to expand the **Control Entities** section. Clear the **Smooth across removed control entities** check box.

#### *Distribution 1*

- 1 Right-click **Mapped 2** and choose **Distribution**.
- 2 Select Boundaries 4 and 45 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 30.
- 6 In the **Element ratio** text field, type 3.
- 7 Select the **Reverse direction** check box.


#### *Distribution 2*

- 1 In the **Model Builder** window, right-click **Mapped 2** and choose **Distribution**.
- 2 Select Boundaries 3 and 46 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 15.
- 6 In the **Element ratio** text field, type 10.

#### *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**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domains 2 and 11 only.
- 5 Click to expand the **Corner Settings** section. From the **Handling of sharp corners** list, choose **No special handling**.
- 6 Click to expand the **Transition** section. Clear the **Smooth transition to interior mesh** check box.

#### *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 Locate the **Layers** section. In the **Number of layers** text field, type 3.
- 6 In the **Stretching factor** text field, type 1.7.

#### *Free Triangular I*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Free Triangular 1**.
- 2 In the **Settings** window for **Free Triangular**, click to expand the **Control Entities** section.
- 3 Clear the **Smooth across removed control entities** check box.
- 4 Click  **Build All**.

### **MESH 1**

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


In the first study only inductive power is coupled to the system. The amplitude of the bias  $V_{rf}$  is set to 0V. This first study is necessary to provide initial conditions to a subsequent study where  $V_{rf}$  is increased using the **Auxiliary sweep**.

The solver setting of this study need to be changed manually.

### **ICP**

- 1 In the **Model Builder** window, click **Study 1**.
- 2 In the **Settings** window for **Study**, type ICP in the **Label** text field.

#### *Step 1: Frequency-Time Periodic*

- 1 In the **Model Builder** window, under **ICP** click **Step 1: Frequency-Time Periodic**.
- 2 In the **Settings** window for **Frequency-Time Periodic**, locate the **Study Settings** section.
- 3 In the **Frequency** text field, type 13.56[MHz].
- 4 In the **Study** toolbar, click  **Get Initial Value**.

### **RESULTS**

*Capacitive Power Deposition, Period Averaged (ptp), Current and Voltage, Metal Contact 1 (ptp), Electric Potential, Period Averaged (ptp), Electron Density, Period Averaged (ptp), Electron Temperature, Period Averaged (ptp), 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, Period Averaged (ptp), Electron Temperature, Period Averaged (ptp), Electric Potential, Period Averaged (ptp), Capacitive Power Deposition, Period Averaged (ptp), Current and Voltage, Metal Contact I (ptp), Magnetic Flux Density Norm (mf), Magnetic Flux Density Norm, Revolved Geometry (mf), Velocity (spf), Pressure (spf), Velocity, 3D (spf), and Temperature (ht)**.
- 2 Right-click and choose **Group**.

## RESULTS

### ICP

- 1 In the **Model Builder** window, expand the **ICP>Solver Configurations** node, then click **Results>Group 5**.
- 2 In the **Settings** window for **Group**, type ICP in the **Label** text field.


### ICP

#### *Solution I (sol1)*

- 1 In the **Model Builder** window, expand the **ICP>Solver Configurations>Solution I (sol1)>Stationary Solver I** node, then click **Fully Coupled I**.
- 2 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.
- 3 In the **Restriction for step-size increase** text field, type 0.05.
- 4 In the **Recovery damping factor** text field, type 0.01.
- 5 From the **Update automatic scale factors in weights** list, choose **Use threshold for weights**.
- 6 In the **Fraction of current damping factor** text field, type 0.1.
- 7 Click to expand the **Results While Solving** section. Select the **Plot** check box.
- 8 In the **Model Builder** window, under **ICP>Solver Configurations>Solution I (sol1)>Stationary Solver I** click **Direct, heat transfer variables (ht) (Merged)**.
- 9 In the **Settings** window for **Direct**, locate the **General** section.
- 10 In the **Pivoting perturbation** text field, type 1.0E-8.
- 11 Click to expand the **Error** section. From the **Check error estimate** list, choose **No**.


### ICP

- 1 In the **Model Builder** window, collapse the **ICP** node.


- 2 In the **Study** toolbar, click  **Compute**.

## RESULTS


### *Inductive Power Absorbed by Electrons*

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type Inductive Power Absorbed by Electrons in the **Label** text field.

### *Surface 1*

- 1 Right-click **Inductive Power Absorbed by Electrons** 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 **Inductive Power Absorbed by Electrons** toolbar, click  **Plot**.

Add a second study step that will use the solutions of the previous study as initial conditions and will ramp up  $V_{rf}$  using the **Auxiliary sweep**.


Increase the **Number of elements** in the extra dimension to 45 to describe the periodic excitation caused by the RF bias.

## ADD STUDY



- 1 In the **Home** 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-Time Periodic**.
- 4 Click **Add Study** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Frequency-Time Periodic

- 1 In the **Settings** window for **Frequency-Time Periodic**, 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 **ICP, Frequency-Time Periodic**.
- 6 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.
- 7 Click  **Add**.
- 8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vrf (Voltage amplitude of rf bias)		V

- 9 Click  **Range**.
- 10 In the **Range** dialog box, type 0 in the **Start** text field.
- 11 In the **Step** text field, type 5.
- 12 In the **Stop** text field, type 100.
- 13 Click **Replace**.
- 14 In the **Settings** window for **Frequency-Time Periodic**, locate the **Study Extensions** section.
- 15 From the **Run continuation for** list, choose **No parameter**.
- 16 From the **Reuse solution from previous step** list, choose **Yes**.
- 17 In the **Model Builder** window, click **Study 2**.
- 18 In the **Settings** window for **Study**, type ICP/CCP in the **Label** text field.
- 19 In the **Study** toolbar, click  **Get Initial Value**.

RESULTS

Capacitive Power Deposition, Period Averaged (ptp) I, Current and Voltage, Metal Contact I (ptp) I, Electric Potential, Period Averaged (ptp) I, Electron Density, Period Averaged (ptp) I, Electron Temperature, Period Averaged (ptp) I, Magnetic Flux Density

*Norm (mf) I, Magnetic Flux Density Norm, Revolved Geometry (mf) I, Pressure (spf) I, Temperature (ht) I, Velocity (spf) I, Velocity, 3D (spf) I*

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Electron Density, Period Averaged (ptp) I, Electron Temperature, Period Averaged (ptp) I, Electric Potential, Period Averaged (ptp) I, Capacitive Power Deposition, Period Averaged (ptp) I, Current and Voltage, Metal Contact I (ptp) I, Magnetic Flux Density Norm (mf) I, Magnetic Flux Density Norm, Revolved Geometry (mf) I, Velocity (spf) I, Pressure (spf) I, Velocity, 3D (spf) I, and Temperature (ht) I**.

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

## RESULTS

### ICP/CCP

1 In the **Model Builder** window, expand the **ICP/CCP>Solver Configurations** node, then click **Results>Group 6**.

2 In the **Settings** window for **Group**, type ICP/CCP in the **Label** text field.

### ICP/CCP

#### *Solution 2 (sol2)*

1 In the **Model Builder** window, expand the **ICP/CCP>Solver Configurations>Solution 2 (sol2)>Stationary Solver I** node, then click **Fully Coupled I**.

2 In the **Settings** window for **Fully Coupled**, locate the **Results While Solving** section.

3 Select the **Plot** check box.

4 From the **Plot group** list, choose **Electron Density, Period Averaged (ptp) I**.

5 Click to expand the **Method and Termination** section. In the **Initial damping factor** text field, type 1.


## PLASMA, TIME PERIODIC (PTP)

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

2 In the **Settings** window for **Plasma, Time Periodic**, locate the **Extra Dimension Settings** section.


3 In the  $N$  text field, type 45.

### ICP/CCP


In the **Study** toolbar, click  **Compute**.

## RESULTS


### *Inductive Power Absorbed by Electrons ICP/CCP*

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type Inductive Power Absorbed by Electrons ICP/CCP in the **Label** text field.

### *Surface 1*

- 1 Right-click **Inductive Power Absorbed by Electrons ICP/CCP** 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 **Inductive Power Absorbed by Electrons ICP/CCP** toolbar, click  **Plot**.

### *Inductive Power Absorbed by Electrons ICP/CCP*

- 1 In the **Model Builder** window, under **Results>ICP/CCP** click **Inductive Power Absorbed by Electrons ICP/CCP**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **ICP/CCP/Solution 2 (3) (sol2)**.

### *Current and Voltage, Metal Contact 1 (ptp) 1*

- 1 In the **Model Builder** window, click **Current and Voltage, Metal Contact 1 (ptp) 1**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Parameter selection (Vrf)** list, choose **Last**.
- 4 In the **Current and Voltage, Metal Contact 1 (ptp) 1** toolbar, click  **Plot**.
- 5 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

