Model created in COMSOL Multiphysics 6.4

Model of a CF4/O2 Inductively Coupled Plasma Reactor

Introduction

This tutorial model studies an inductively coupled plasma (ICP) reactor in a mixture of CF_4/O_2. The plasma chemistry is based on Ref. 1 and the electron impact reactions are taken from LxCat (Ref. 2, Ref. 3, and Ref. 4). The plasma model is solved self-consistently with the **Magnetic Fields**, **Laminar Flow** and **Heat Transfer in Fluids** interfaces.

Model Definition

Electron transport is modeled by solving the continuity equation, the momentum equation under the drift-diffusion approximation, and the mean electron energy equation (for detailed information on electron transport, see *Theory for the Drift Diffusion Interface* in the *Plasma Module User's Guide*)

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

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

The source coefficients in the above equations are determined by the plasma chemistry. The electron rate expression is defined as

$$R_e = N_A \sum_j \nu_{e,j} r_j$$

where $\nu_{e,j}$ is the stoichiometric coefficient, and the reaction rate is defined as

$$r_j = k_j^f \prod_{i \in \mathrm{react}} c_i^{-\nu_{i,j}} + k_j^r \prod_{i \in \mathrm{prod}} c_k^{\nu_{i,j}}$$

where k_j^f is the forward rate constant and k_j^r is the reversed rate constant. Both the Electron Impact Reaction feature and Reaction feature can contribute to the electron rate expression. However, when using the Reaction feature it is important to note that the associated electron energy gain or loss is not included in the source term of the electron mean energy equation.

The rate constants can be computed from electron impact cross-section data

$$k^f = N_A \gamma \int_0^\infty \varepsilon \sigma(\varepsilon) f(\varepsilon) d\varepsilon$$

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

When *Townsend coefficients* are used, the reaction rate is defined as

$$r_j = \frac{\alpha_j}{N_n}|\Gamma_e| \prod_{i \neq e \in \text{react}} c_i^{-\nu_{i,j}}$$

where α_j/N_n is the reduced Townsend coefficient for reaction j (SI unit: m^2) and Γ_e is the electron flux as defined above (SI unit: $1/(m^2 \cdot s)$). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges.

The total electron energy loss or gained is calculated by summing the collisional energy changes from all reactions defined with the Electron Impact Reaction feature as

$$S_{\text{en}} = -\sum_j r_j \Delta\varepsilon_j F$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (SI unit: V) and F is the Faraday constant (SI unit: C/mol). For excitation and ionization collisions $\Delta\varepsilon_j$ corresponds to the energy of the excited state being excited/deexcited or ionized, for attachment $\Delta\varepsilon_j$ is set to zero, and for elastic collisions

$$\Delta\varepsilon = 2\frac{m_e}{m_k}\frac{3}{2}\left[T_e(eV) - \frac{k_B}{e}T_{\text{gas}}(K)\right]$$

where m_e and m_k are the electron and heavy species mass in kg, T_e is the electron temperature in eV, and T_{gas} is the gas temperature in K.

For heavy species, the following equation is solved for the mass fraction of each species (for detailed information on the transport of the nonelectron species, see *Theory for the Heavy Species Transport Interface* in the *Plasma Module User's Guide*):

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

The electrostatic field is computed using the following equation:

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

The space charge density ρ is automatically computed based on the plasma chemistry specified in the model using the formula

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

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

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

$$(j\omega\sigma - \omega^2\varepsilon_0)\mathbf{A} + \nabla\times(\mu_0^{-1}\nabla\times\mathbf{A}) = \mathbf{J}^{\mathrm{e}}$$

In the cold plasma approximation, the electromagnetic wave "sees" a plasma defined by the plasma conductivity, which is set in the **Plasma Conductivity Coupling** multiphysics node:

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

where n_e is the electron density, q is the electron charge, m_e is the electron mass, ν_e is the collision frequency, and ω is the angular frequency. The Joule heating term responsible for heating the electrons is set in the **Electron Heat Source** multiphysics node.

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 conditions for the electron and electron energy fluxes, respectively:

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

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

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.

PLASMA CHEMISTRY

The plasma chemistry is based on Ref. 1. The electron impact cross sections used in this model are retrieved from different databases from LxCat: Ref. 2, Ref. 3, and Ref. 4. The data from Ref. 2 further refers to Ref. 5 and Ref. 6. The model includes 29 species: electrons, CF_4, CF_3, CF_2, CF, CF_3^+, CF_2^+, CF^+, F_2, F_2^+, F, F^+, F^-, O_2, O_2^+, O, O^+, O^-, O_2^*, O^*, C, C^+, CO_2, CO_2^+, CO, CO^+, COF, COF_2, and FO.

Results and Discussion

The model contains two studies. In the first study, a base case is solved to provide initial conditions to a subsequent study where the oxygen mole fraction of the gas feed is parameterized. The ICP reactor is operated at 25 mTorr at the pump port with a mass flow of 50 SCCM. The input power is kept constant at 250 W.

Figure 1 shows the power density absorbed by the electrons by Joule heating caused by the coil induced currents. The power density has a typical profile found in ICP reactors with a maximum value just below the coil and being practically negligible in the reactor center because the electric fields are shielded by the dense plasma.

Figure 2, Figure 3, and Figure 4 show maximum values for the electron density, electron temperature, atomic oxygen number density, and atomic fluorine number density as a function of the molecular oxygen mole fraction in the reactor feed. These results are consistent with the experimental and model data of Ref. 1.

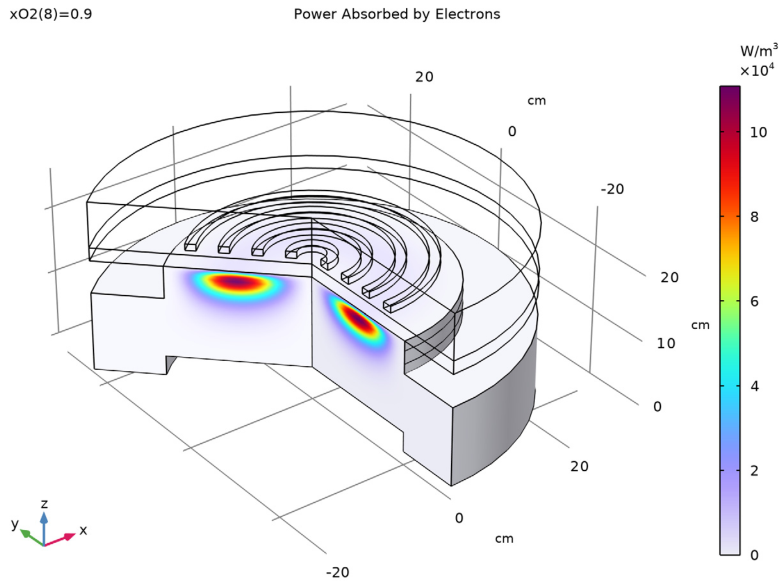

Figure 1: Power absorbed by the electrons for an oxygen mole fraction of 0.9.

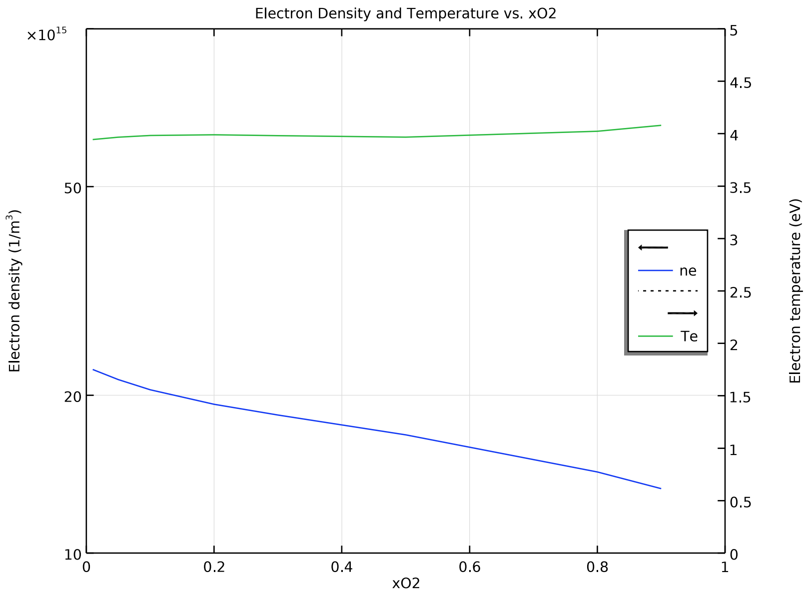

Figure 2: Maximum values of electron density and electron temperature as a function of oxygen mole fraction.

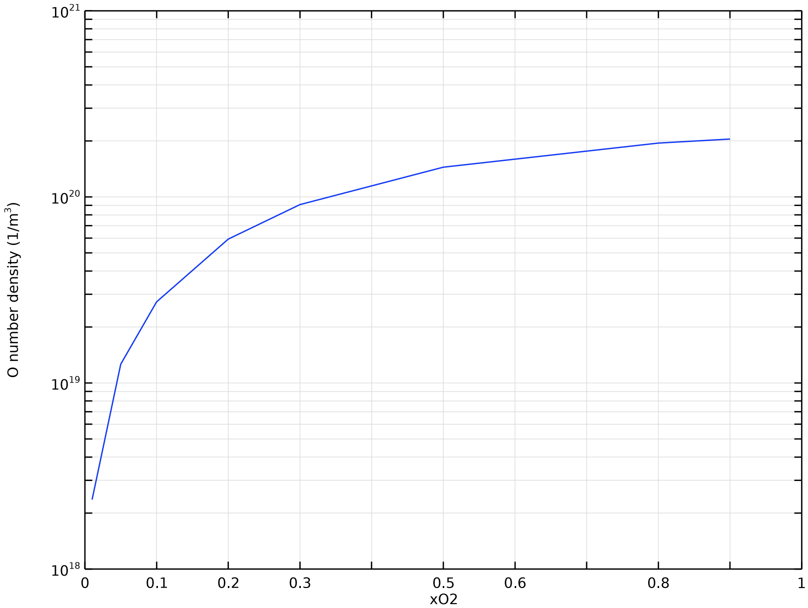

Figure 3: Maximum value of atomic oxygen number density as a function of oxygen mole fraction.

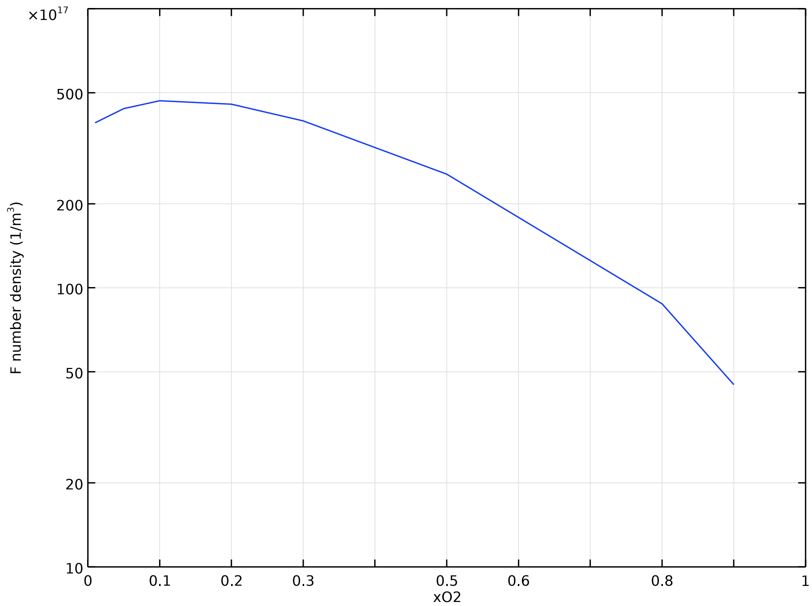

Figure 4: Maximum value of atomic fluorine number density as a function of oxygen mole fraction.

References

1. T. Kimura and M. Noto, "Experimental study and global model of inductively coupled CF4/O2 discharges," *J. Appl. Phys.*, vol. 100, no. 063303, pp. 1–9, 2006; doi.org/10.1063/1.2345461.

2. Bordage database, www.lxcat.net, retrieved on 2025.

3. Morgan database, www.lxcat.net, retrieved on 2025.

4. Phelps database, www.lxcat.net, retrieved 2025.

5. M.C. Bordage, P. Segur, and A. Chouki, "Determination of a set of electron impact cross sections in tetrafluoromethane consistent with experimental determination of swarm parameters," *J. Appl. Phys.*, vol. 80, no. 3, pp. 1325–1336, 1996; doi.org/10.1063/1.362931.

6. M.C. Bordage, P. Segur, L.G. Christophorou, and J.K. Olthoff, "Boltzmann analysis of electron swarm parameters in CF4 using independently assessed electron-collision cross

sections," *J. Appl. Phys.*, vol. 86, no. 7, pp. 3558–3566, 1999; doi.org/10.1063/1.371258.

Application Library path: `Plasma_Module/Inductively_Coupled_Plasmas/icp_cf4_o2`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Plasma** > **Nonisothermal Plasma Flow** > **Inductively Coupled Plasma**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics** > **Frequency–Stationary**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Import parameters to use in the model.

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

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `CF4_O2_icp_param.txt`.

In the following, create a geometry for an ICP reactor.

GEOMETRY 1

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 `Wc`.

4 In the **Height** text field, type `Hc`.

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 `Wc`.

4 In the **Height** text field, type `Window_thickness`.

5 Locate the **Position** section. In the **z** text field, type `Hc`.

Rectangle 3 (r3)

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 `Wc`.

4 In the **Height** text field, type `Coil_chamber_height`.

5 Locate the **Position** section. In the **z** text field, type `Hc+Window_thickness`.

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 `Coil_width`.

4 In the **Height** text field, type `Coil_height`.

5 Locate the **Position** section. In the **r** text field, type `First_coil_r`.

6 In the **z** text field, type `Hc+Window_thickness+First_coil_z`.

7 Click **Build All Objects**.

Array 1 (arr1)

1 In the **Geometry** toolbar, click **Transforms** and choose **Array**.

2 In the **Settings** window for **Array**, locate the **Size** section.

3 In the **r size** text field, type 4.

4 Locate the **Displacement** section. In the **r** text field, type Coils_spacing.

5 Select the object **r4** only.

6 Click **Build All Objects**.

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 Ww.

4 In the **Height** text field, type Wh.

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 Inw.

4 In the **Height** text field, type Inh.

5 Locate the **Position** section. In the **r** text field, type Wc-Inw.

6 In the **z** text field, type Hc-Inh.

Line Segment 1 (ls1)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 On the object **r5**, select Point 4 only.

3 In the **Settings** window for **Line Segment**, locate the **Endpoint** section.

4 From the **Specify** list, choose **Coordinates**.

5 In the **r** text field, type 15.

6 In the **z** text field, type Wh.

Line Segment 2 (ls2)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 In the **r** text field, type Wc-Inw.

5 In the **z** text field, type Hc-Inh+1.5[cm].

6 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

7 In the **r** text field, type `Wc-Inw`.

8 In the **z** text field, type `Hc-Inh+3.5[cm]`.

9 Click **Build All Objects**.

GEOMETRY 1

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

Set material properties to be used by the different physics interfaces in this model.

ADD MATERIAL

1 In the **Materials** 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 the **Add to Component** button in the window toolbar.

5 In the tree, select **Built-in** > **Glass (quartz)**.

6 Click the **Add to Component** button in the window toolbar.

7 In the tree, select **Built-in** > **Copper**.

8 Click the **Add to Component** button in the window toolbar.

9 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Copper (mat3)

1 Click the **Zoom Extents** button in the **Graphics** toolbar.

2 Select Domains 5–8 only.

Glass (quartz) (mat2)

1 In the **Model Builder** window, click **Glass (quartz) (mat2)**.

2 Select Domain 3 only.

Air (mat1)

1 In the **Model Builder** window, click **Air (mat1)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

3 Click **Clear Selection**.

4 Select Domains 2 and 4 only.

Define explicit selections to be used later for boundary conditions and meshing.

DEFINITIONS

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 5–8 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 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 4, 6, 22, 27–32, and 34 only.

Define a Maximum operator to be used during plotting.

Maximum 1 (maxop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Maximum**.

2 Select Domain 2 only.

In the Magnetic Fields interface the first thing to do is to set the domains where the physics is to be solved. After, add a Coil feature, select the coil domain, and set the coil power.

MAGNETIC FIELDS (MF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Magnetic Fields (mf)**.

2 In the **Settings** window for **Magnetic Fields**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domains 2–8 only.

Domain Coil 1

1 In the **Physics** toolbar, click **Domains** and choose **Domain Coil**.

2 In the **Settings** window for **Domain Coil**, locate the **Domain Selection** section.

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

4 Locate the **Coil** section. Select the **Coil group** checkbox.

5 From the **Coil excitation** list, choose **Power**.

6 In the P_{coil} text field, type `Pw`.

MAGNETIC FIELDS (MF)

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

Set the domains where the Heat Transfer in Fluids interface is to be solved and set a constant temperature as boundary condition.

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.

Temperature 1

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

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

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

In the Laminar Flow interface, set the domain where the physics is to be solved, and add an inlet and outlet to the system.

LAMINAR FLOW (SPF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domain 2 only.

5 Locate the **Physical Model** section. In the p_{ref} text field, type `p0`.

Inlet 1

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

2 Select Boundary 31 only.

3 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

4 From the list, choose **Mass flow**.

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

6 In the Q_{sccm} text field, type `Qf`.

Outlet 1

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

2 Select Boundary 28 only.

LAMINAR FLOW (SPF)

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

HEAT TRANSFER IN FLUIDS (HT)

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

PLASMA (PLAS)

Add isotropic diffusion for ions because the density of the negative ions can drop sharply when approaching the reactor edges and cause instability.

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

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

3 In the tree, select the checkbox for the node **Physics** > **Stabilization**.

4 Click **OK**.

5 In the **Model Builder** window, under **Component 1 (comp1)** click **Plasma (plas)**.

6 In the **Settings** window for **Plasma**, locate the **Domain Selection** section.

7 Click **Clear Selection**.

8 Select Domain 2 only.

9 Locate the **Transport Settings** section. Select the **Mixture diffusion correction** checkbox.

10 Click to expand the **Inconsistent Stabilization** section. Select the **Isotropic diffusion for ions** checkbox.

11 In the $\delta_{id,i}$ text field, type `0.1`.

Plasma Model 1

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

2 In the **Settings** window for **Plasma Model**, locate the **Electron Density and Energy** section.

3 From the **Electron transport properties** list, choose **From electron impact reactions** to estimate the electron transport parameters from the existent reactions.

Initial Values 1

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

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $n_{e,0}$ text field, type `1E15[1/m^3]`.

4 In the ε_0 text field, type `2[V]`.

THE PLASMA CHEMISTRY IMPORT FEATURE

The next steps have instructions to use the **Plasma Chemistry Import** feature to import a file that automatically creates the CF4/O2 plasma chemistry.

The following is set or created automatically:

a Species properties

b Electron impact reactions

c Heavy species reactions

d Surface reactions

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

Plasma Chemistry Import 1

1 In the **Physics** toolbar, click **Global** and choose **Plasma Chemistry Import**.

2 In the **Settings** window for **Plasma Chemistry Import**, locate the **Plasma Chemistry Import** section.

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `CF4_O2_icp_plasma_chemistry.txt`.

5 Click **Import**.

Select where the surface reactions are to be used.

Surface Reactions - Ions

1 In the **Model Builder** window, click **Surface Reactions - Ions**.

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

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

Surface Reactions - Neutrals

1 In the **Model Builder** window, click **Surface Reactions - Neutrals**.

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

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

4 Select Boundaries 4, 6, 22, 27, 29, 30, 32, and 34 only.

Add boundary conditions for the electron transport equations, Poisson's equation.

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 **Walls**.

Ground 1

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

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

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

Add an **Inlet** feature to set the mole fraction of CF4 and O2 in the feed gas. The mole fraction of all other neutral species (fragments, excited states and others) should be fixed to a small number to say that they have negligible presence in the feed gas.

Inflow 1

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 (1)
CF4	1-x02

5 Click **Add**.

6 In the table, enter the following settings:

Species names	Mole fraction (1)
02	x02

7 Click **Add**.

8 In the table, enter the following settings:

Species names	Mole fraction (1)
O	xinlet

9 Click + **Add**.

10 In the table, enter the following settings:

Species names	Mole fraction (1)
O1D	xinlet

11 Click + **Add**.

12 In the table, enter the following settings:

Species names	Mole fraction (1)
O2a1Dg	xinlet

13 Click + **Add**.

14 In the table, enter the following settings:

Species names	Mole fraction (1)
F2	xinlet

15 Click + **Add**.

16 In the table, enter the following settings:

Species names	Mole fraction (1)
F	xinlet

17 Click + **Add**.

18 In the table, enter the following settings:

Species names	Mole fraction (1)
CF3	xinlet

19 Click + **Add**.

20 In the table, enter the following settings:

Species names	Mole fraction (1)
CF2	xinlet

21 Click + **Add**.

22 In the table, enter the following settings:

Species names	Mole fraction (1)
CF	xinlet

23 Click + **Add**.

24 In the table, enter the following settings:

Species names	Mole fraction (1)
C	xinlet

25 Click + **Add**.

26 In the table, enter the following settings:

Species names	Mole fraction (1)
FO	xinlet

27 Click + **Add**.

28 In the table, enter the following settings:

Species names	Mole fraction (1)
COF	xinlet

29 Click + **Add**.

30 In the table, enter the following settings:

Species names	Mole fraction (1)
COF2	xinlet

31 Click + **Add**.

32 In the table, enter the following settings:

Species names	Mole fraction (1)
CO2	xinlet

33 Click + **Add**.

34 In the table, enter the following settings:

Species names	**Mole fraction (1)**
`CO`	`xinlet`

35 Select Boundary 31 only.

Use the **Outflow** feature to specify that the neutral species have no transport due to diffusion at the outlet.

Outflow 1

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

2 Select Boundary 28 only.

In the following, set the CF4 mass fraction to be computed from a mass constraint, set species initial conditions, and set additional entropy to some excited states.

Species: CF4

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Plasma (plas)** > **Group - Species** node, then click **Species: CF4**.

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

3 Select the **From mass constraint** checkbox.

Species: F-

1 In the **Model Builder** window, click **Species: F-**.

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: CF3+

1 In the **Model Builder** window, click **Species: CF3+**.

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

3 Select the **Initial value from electroneutrality constraint** checkbox.

Species: CF2+

1 In the **Model Builder** window, click **Species: CF2+**.

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: CF+

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

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]`.

4 Click to expand the **Species Thermodynamic Parameters** section. In the Δh text field, type `13.618`.

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 x_0 text field, type `xO2`.

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]`.

4 Locate the **Species Thermodynamic Parameters** section. In the Δh text field, type `12.06`.

Species: F2+

1 In the **Model Builder** window, click **Species: F2+**.

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

3 In the n_0 text field, type `1E10[1/m^3]`.

4 Locate the **Species Thermodynamic Parameters** section. In the Δh text field, type `15.69`.

Species: F+

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

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

3 In the Δh text field, type `17.687`.

4 Locate the **General Parameters** section. In the n_0 text field, type `1E10[1/m^3]`.

Species: CO2+

1 In the **Model Builder** window, click **Species: CO2+**.

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

3 In the n_0 text field, type `1E10[1/m^3]`.

4 Locate the **Species Thermodynamic Parameters** section. In the Δh text field, type `13.3`.

Species: CO+

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

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

3 In the Δh text field, type `14`.

4 Locate the **General Parameters** section. In the n_0 text field, type `1E10[1/m^3]`.

Species: C+

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

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

3 In the n_0 text field, type `1E10[1/m^3]`.

4 Locate the **Species Thermodynamic Parameters** section. In the Δh text field, type `11.26`.

PLASMA (PLAS)

Group - Species

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

2 In the **Model Builder** window, collapse the **Plasma (plas)** node.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 In the table, clear the **Use** checkbox for **Plasma (plas)**.

4 Locate the **Sequence Type** section. From the list, choose **User-controlled mesh**.

Size 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size 1**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Finer**.

Free Triangular 1

1 In the **Model Builder** window, click **Free Triangular 1**.
2 In the **Settings** window for **Free Triangular**, locate the **Domain Selection** section.
3 Click **Clear Selection**.
4 Select Domains 2–4 only.

Boundary Layer Properties 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Mesh 1** > **Boundary Layers 1** node, then click **Boundary Layer Properties 1**.
2 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.
3 In the **Number of layers** text field, type 4.
4 In the **Stretching factor** text field, type 1.4.
5 In the **Thickness adjustment factor** text field, type 1.

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 **Distribution** section.
3 From the **Distribution type** list, choose **Predefined**.
4 In the **Number of elements** text field, type 30.
5 In the **Element ratio** text field, type 20.
6 From the **Growth rate** list, choose **Exponential**.
7 Select the **Symmetric distribution** checkbox.
8 Locate the **Boundary Selection** section. From the **Selection** list, choose **Coil Boundaries**.

Mapped 1

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Move Up**.
2 Right-click **Mapped 1** and choose **Move Up**.
3 In the **Settings** window for **Mapped**, click **Build All**.

A first study is used to provide initial conditions to subsequent studies.

BASE CASE

1 In the **Model Builder** window, click **Study 1**.
2 In the **Settings** window for **Study**, type `Base Case` in the **Label** text field.
3 In the **Study** toolbar, click **Get Initial Value**.

RESULTS

Electric Potential (plas), Electron Density (plas), Electron Temperature (plas), Magnetic Flux Density (mf), Magnetic Flux Density, Revolved Geometry (mf), Pressure (spf), Temperature (ht), Velocity (spf), Velocity, 3D (spf)
Right-click and choose **Group**.

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

BASE CASE

Step 1: Frequency–Stationary
1 In the **Model Builder** window, expand the **Base Case** > **Solver Configurations** node, then click **Base Case** > **Step 1: Frequency–Stationary**.
2 In the **Settings** window for **Frequency–Stationary**, locate the **Study Settings** section.
3 In the **Frequency** text field, type `13.56e6`.

Solution 1 (sol1)
1 In the **Model Builder** window, expand the **Base Case** > **Solver Configurations** > **Solution 1 (sol1)** > **Stationary Solver 1** node, then click **Fully Coupled 1**.
2 In the **Settings** window for **Fully Coupled**, click to expand the **Results While Solving** section.
3 Select the **Plot** checkbox.
4 Click **Run**.

RESULTS

Electron Density (plas)
Add a second study to do a parameterization on the oxygen mole fraction. Since we already have a previous solution the initial damping factor can be set to 1.

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–Stationary**.

4 Click the **Add Study** button in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Frequency–Stationary

1 In the **Settings** window for **Frequency–Stationary**, locate the **Study Settings** section.

2 In the **Frequency** text field, type `13.56e6`.

3 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Base Case, Frequency–Stationary**.

6 In the **Model Builder** window, click **Study 2**.

7 In the **Settings** window for **Study**, type `x02 Sweep` in the **Label** text field.

8 In the **Study** toolbar, click **Get Initial Value**.

RESULTS

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

Right-click and choose **Group**.

xO2 Sweep

In the **Settings** window for **Group**, type `x02 Sweep` in the **Label** text field.

XO2 SWEEP

Solver Configurations

In the **Model Builder** window, expand the **xO2 Sweep > Solver Configurations** node.

Solution 2 (sol2)

1 In the **Model Builder** window, expand the **xO2 Sweep > Solver Configurations > Solution 2 (sol2) > Stationary Solver 1** node, then click **Fully Coupled 1**.

2 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.

3 In the **Initial damping factor** text field, type `1`.

4 Locate the **Results While Solving** section. Select the **Plot** checkbox.

5 In the table, enter the following settings:

Plot group	Plot window
Electron Density (plas) 1	Graphics

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xO2 (Oxygen mole fraction)	`0.01 0.05 0.1 0.2 0.3 0.5 0.8 0.9`	

5 Click to expand the **Advanced Settings** section. Select the **Reuse solution from previous step** checkbox.

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

Prepare plots to show the electron density, electron temperature, F number density, and O number density as functions of the O2 mole fraction.

RESULTS

Electron Density and Temperature vs. xO2

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Electron Density and Temperature vs. xO2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **xO2 Sweep/Solution 2 (sol2)**.

Global 1

1 Right-click **Electron Density and Temperature vs. xO2** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	**Unit**	**Description**
`maxop1(plas.ne)`	`1/m^3`	`Maximum 1`

4 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

Legends
`ne`

Global 2

1 Right-click **Global 1** and choose **Duplicate**.

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

3 In the table, enter the following settings:

Expression	**Unit**	**Description**
`maxop1(plas.Te)`	`V`	`Maximum 1`

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Te`

Electron Density and Temperature vs. xO2

1 In the **Model Builder** window, click **Electron Density and Temperature vs. xO2**.

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

3 From the **Title type** list, choose **Label**.

4 Locate the **Plot Settings** section. Select the **Two y-axes** checkbox.

5 In the table, select the **Plot on secondary y-axis** checkbox for **Global 2**.

6 Select the **y-axis label** checkbox. In the associated text field, type Electron density (1/m³).

7 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Electron temperature (eV)`.

8 Locate the **Axis** section. Select the **y-axis log scale** checkbox.

9 Select the **Manual axis limits** checkbox.

10 In the **x minimum** text field, type `0`.

11 In the **x maximum** text field, type `1`.

12 In the **y minimum** text field, type `1e16`.

13 In the **y maximum** text field, type `1e17`.

14 In the **Secondary y minimum** text field, type `0`.

15 In the **Secondary y maximum** text field, type `5`.

16 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

17 In the **Electron Density and Temperature vs. xO2** toolbar, click **Plot**.

O Density vs. xO2

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `O Density vs. xO2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **xO2 Sweep/Solution 2 (sol2)**.

Global 1

1 Right-click **O Density vs. xO2** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
`maxop1(plas.n_wO)`	`1/m^3`	`Maximum 1`

O Density vs. xO2

1 In the **Model Builder** window, click **O Density vs. xO2**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** checkbox. In the associated text field, type `O number density (1/m<sup>3</sup>)`.

6 Locate the **Axis** section. Select the **y-axis log scale** checkbox.

7 Select the **Manual axis limits** checkbox.

8 In the **x minimum** text field, type `0`.

9 In the **x maximum** text field, type `1`.

10 In the **y minimum** text field, type `1e18`.

11 In the **y maximum** text field, type `1e21`.

12 Locate the **Legend** section. Clear the **Show legends** checkbox.

13 In the **O Density vs. xO2** toolbar, click **Plot**.

F Density vs. xO2

1 Right-click **O Density vs. xO2** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `F Density vs. xO2` in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type `F number density (1/m<sup>3</sup>)`.

4 Locate the **Axis** section. In the **y maximum** text field, type `1e20`.

Global 1

1 In the **Model Builder** window, expand the **F Density vs. xO2** node, then click **Global 1**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
maxop1(plas.n_wF)	1/m^3	Maximum 1

4 In the **F Density vs. xO2** toolbar, click **Plot**.

Prepare a plot to show the power absorbed by electrons. First, create a dataset with a selection of the plasma domain only.

Revolution 2D 4

1 In the **Model Builder** window, expand the **Results > Datasets** node.

2 Right-click **Results > Datasets > Revolution 2D 3** and choose **Duplicate**.

Selection

1 In the **Results** toolbar, click **Attributes** and choose **Selection**.

2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 2 only.

Power Absorbed by Electrons

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Power Absorbed by Electrons` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Revolution 2D 1**.

Volume 1

1 Right-click **Power Absorbed by Electrons** and choose **Volume**.

2 In the **Settings** window for **Volume**, locate the **Data** section.

3 From the **Dataset** list, choose **Revolution 2D 4**.

4 Locate the **Expression** section. In the **Expression** text field, type `mf.Qrh`.

Power Absorbed by Electrons

1 In the **Model Builder** window, click **Power Absorbed by Electrons**.

2 In the **Settings** window for **3D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **Label**.

4 Locate the **Color Legend** section. Select the **Show units** checkbox.

5 In the **Power Absorbed by Electrons** toolbar, click **Plot**.