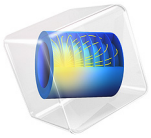

Model created in COMSOL Multiphysics 6.4

Global Model of a CF4/O2 Plasma Reactor

Introduction

This tutorial studies the plasma chemistry of a CF_4/O_2 plasma at low pressure using a global model. The plasma chemistry is based on Ref. 1 and the electron impact reactions are taken from LxCat (Ref. 2, Ref. 3, and Ref. 4).

Model Definition

The model used in this work assumes that the spatial distribution of the different quantities in the plasma reactor can be treated as uniform. Without spatial derivatives, the numerical solution of the equation set becomes considerably simpler and the computation time is reduced. These advantages make a global model a good first approach to study a plasma reactor, especially when complex chemistries are involved.

When using a global plasma model the species densities and the electron temperature are treated as volume-averaged quantities. Detailed information on the global model can be found in the section *Theory for Global Models* in the *Plasma Module User's Guide*. For heavy species the following equation is solved for the mass fraction

$$V\rho\frac{d}{dt}(w_k) = m_f w_{f,k} - m_o w_k + VR_k + \sum_l h_l A_l R_{\text{surf},k,l} M_k - w_k \sum_l h_l A_l M_{f,l}$$

where ρ is the mass density (SI unit: kg/m^3), w_k is the mass fraction, $w_{f,k}$ is the mass fraction in the feed, m_f and m_o are the mass-flow rates of the total feed and outlet, and R_k is the rate expression (SI unit: $kg/(m^3 \cdot s)$). The fourth term on the right-hand side accounts for surface losses and creation, where A_l is the surface area, h_l is a dimensionless correction term, V is the reactor volume, M_k is the species molar mass (SI unit: kg/mol) and $R_{\text{surf},k,l}$ is the surface rate expression (SI unit: $mol/(m^2 \cdot s)$) at a surface l. The last term is introduced because the species mass balance equations are written in the nonconservative form and it used the mass-continuity equation to replace for the mass density time derivative. In the last term $M_{f,l}$ is the inward mass flux of surface l (SI unit: $kg/(m^2 \cdot s)$). The sum in the last two terms is over all surfaces where there are surface reactions.

To take possible variations of the system's total mass or pressure into account, the mass-continuity equation can also be solved:

$$V\frac{d\rho}{dt} = m_f - m_o + \sum_l h_l A_l M_{f,l}\,.$$

The electron number density is obtained from electroneutrality:

$$n_e = \sum_{k=1}^{N} Z_k n_k$$

Using the local energy approximation (LEA), the electron energy density n_ε (SI unit: V/ m^3) is computed from

$$V\frac{dn_\varepsilon}{dt} = VR_\varepsilon + \frac{P_{\text{abs}}}{e} + \sum_l \sum_{\text{ions}} h_l A_l R_{\text{surf},k,l} N_a(\varepsilon_e + \varepsilon_i)$$

where R_ε is the electron energy loss due to inelastic and elastic collisions, P_{abs} is the power absorbed by the electrons (SI unit: W), and e is the elementary charge. The last term on the right side accounts for the kinetic energy transported to the surface by electrons and ions. The summation is over all positive ions, ε_e is the mean kinetic energy lost per electron lost, ε_i is the mean kinetic energy lost per ion lost, and N_a is Avogadro's number. If using the local field approximation (LFA) the electron mean energy equation is not solved and the electron mean energy can be: (i) provided as a function of the electric field; or (ii) obtained by solving the Boltzmann equation in the two-term approximation.

The rate coefficients for electron impact reactions can be computed by appropriate averaging of cross sections over an EEDF. The EEDF can either be analytic or obtained by solving the steady-state Boltzmann equation in the two-term approximation coupled with the equation system (*The Boltzmann Equation, Two-Term Approximation Interface* in the *Plasma Module User's Guide*). When solving for the EEDF, the coupling between the equations is as follows: (i) if the LEA is used, the electron mean energy obtained from the electron mean energy equation is given as input to the Boltzmann solver; (ii) if the LFA is used, the reduced electric field must be given as input to the Boltzmann solver and the electron mean energy comes from averaging over the computed EEDF.

This model uses the LEA and a Maxwellian EEDF, as in Ref. 1.

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 using a time-dependent solver for an input power of 120 W and an oxygen mole fraction of 0.01. In the second study, the power is kept at 120 W and the oxygen mole fraction is varied between 0 and 1 for pressures of 8, 15, and 25 mTorr.

Figure 1, Figure 2, Figure 3, and Figure 4 show the electron density, electron temperature, F number density, and O number density, respectively. In general, there is good agreement with the results from Ref. 1.

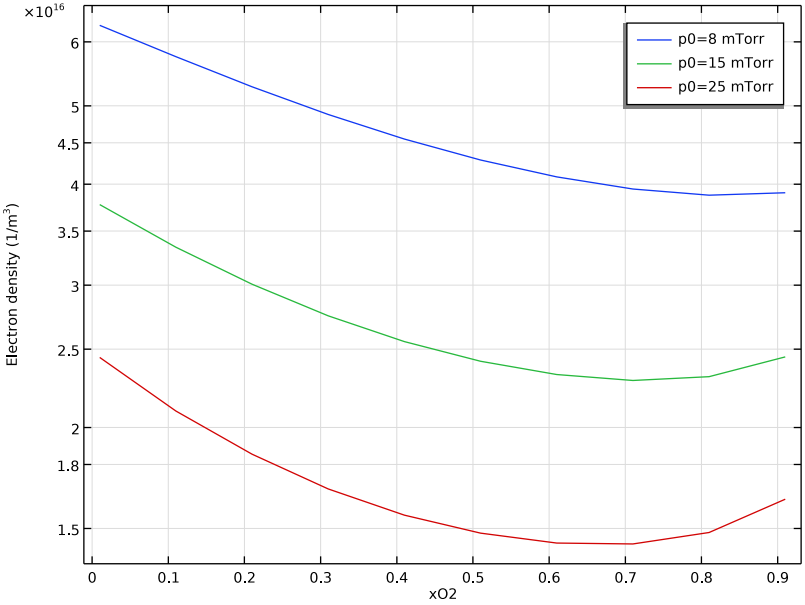

Figure 1: Electron number density as a function of oxygen mole fraction for several pressures.

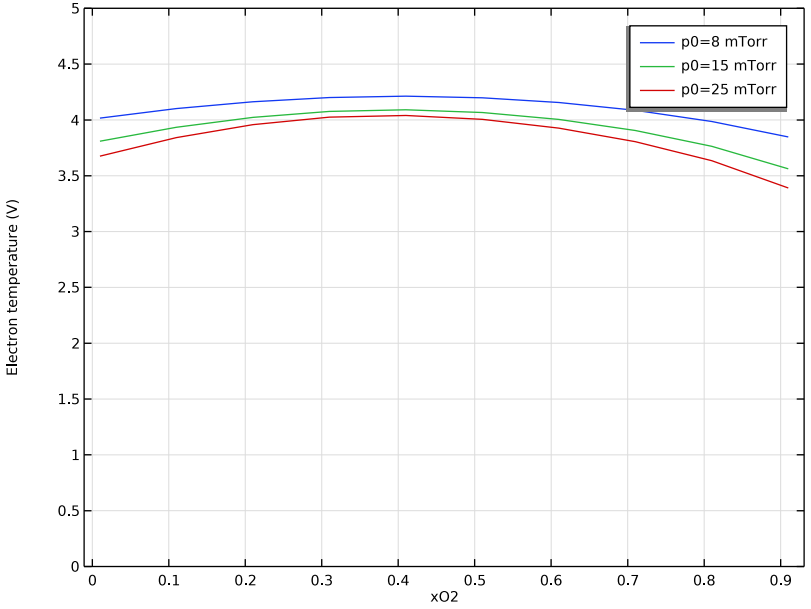

Figure 2: Electron temperature as a function of oxygen mole fraction for several pressures.

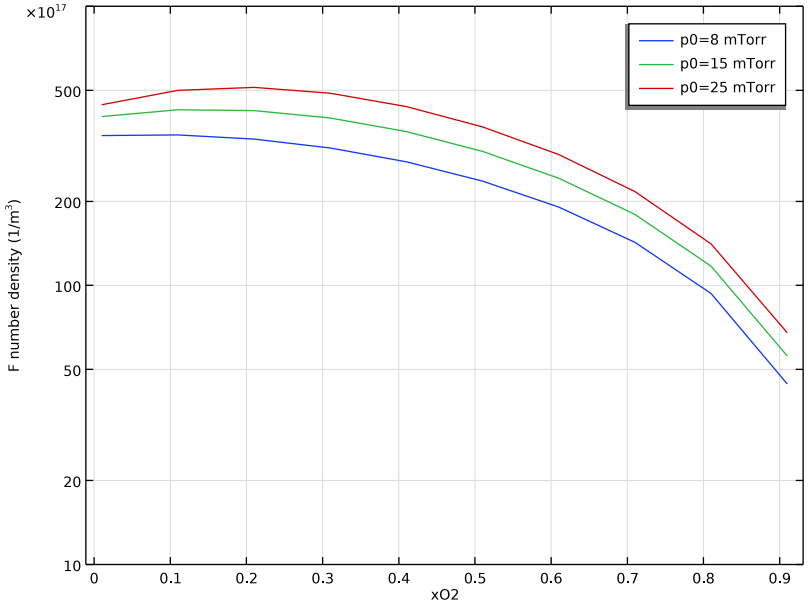

Figure 3: F number density as a function of oxygen mole fraction for several pressures.

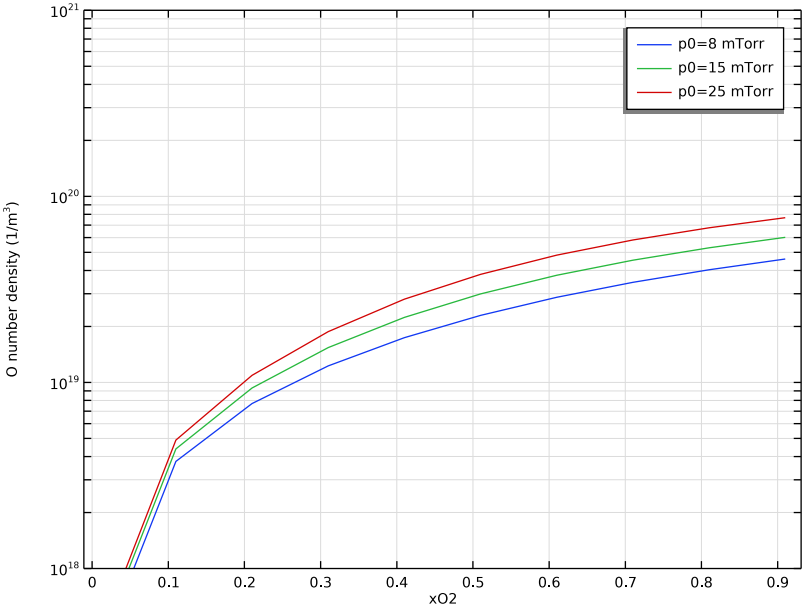

Figure 4: O number density as a function of oxygen mole fraction for several pressures.

References

1. T. Kimura and M. Noto, "Experimental study and global model of inductively coupled CF_4/O_2 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, p. 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/Global_Modeling/cf4_o2_global_model`

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** > **Plasma (plas)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies** > **Time Dependent**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Add some parameters to be used 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_global_model_parameters.txt`.

Set the domain dimensions. The volume and surface areas used in the global model of the reactor are obtained automatically from this geometry.

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 `R0`.

4 In the **Height** text field, type `L0`.

PLASMA (PLAS)

Choose to solve for a global model of a constant pressure reactor.

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

2 In the **Settings** window for **Plasma**, locate the **Diffusion Model** section.

3 From the **Diffusion model** list, choose **Global**.

4 Locate the **Plasma Properties** section. Select the **Use reduced electron transport properties** checkbox.

5 Locate the **Reactor** section. From the **Reactor type** list, choose **Constant pressure**.

Plasma Model 1

Set the pressure, mass flow, power absorbed by the electrons, and an estimation of the plasma sheath voltage drop (for the mean kinetic energy lost per ion lost).

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 **Model Inputs** section.

3 In the T text field, type `Tgas`.

4 In the p_{A} text field, type `p0`.

5 Locate the **Total Mass Flow** section. In the Q_{sccm} text field, type `Qfeed`.

6 Locate the **Mean Electron Energy Specification** section. In the P_{abs} text field, type `pw`.

7 In the ε_e text field, type `2*plas.Te`.

8 In the ε_i text field, type `Vp`.

THE PLASMA CHEMISTRY IMPORT FEATURE

The next steps show how 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** Reaction group features for CF4/O2
- **c** 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_plasma_chemistry.txt`.
5. Click **Import**.

Set some properties of the species and the surface reactions.

Set CF4 to be the species for which the mass fraction is found from a mass constraint.

Set the feed mole fraction for CF4 and O2.

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.
4. Locate the **General Parameters** section. In the x_{feed} text field, type `1-xO2`.

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_{feed} text field, type `xO2`.

PLASMA (PLAS)

Group - Species

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

Surface Reactions - All Surfaces

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

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

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

Next, use a time-dependent study to find a solution for the base case. The solution from this study will provide initial conditions for a second study that sweeps for pressure and oxygen mole fraction.

BASE CASE

1 In the **Model Builder** window, click **Study 1**.

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

3 Clear the **Generate default plots** checkbox.

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

5 In the **Label** text field, type `Base Case`.

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 **General Studies** > **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: Stationary

1 In the **Settings** window for **Stationary**, click to expand the **Values of Dependent Variables** section.

2 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

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

4 From the **Study** list, choose **Base Case, Time Dependent**.

5 From the **Time (s)** list, choose **Last**.

6 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

7 From the **Sweep type** list, choose **All combinations**.

8 Click **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
p0 (Gas pressure)	8 15 25	mTorr

10 Click **Add**.

11 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xO2 (O2 mole fraction)		

12 In the table, click to select the cell at row number 2 and column number 2.

13 Click **Range**.

14 In the **Range** dialog, type `0.01` in the **Start** text field.

15 In the **Step** text field, type `0.1`.

16 In the **Stop** text field, type `0.95`.

17 Click **Replace**.

18 In the **Settings** window for **Stationary**, locate the **Study Extensions** section.

19 From the **Reuse solution from previous step** list, choose **Yes**.

Since you already have a solution from a previous study and are reusing the solution from the previous step, you can set the initial damping factor to 1.

Solution 2 (sol2)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node.

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

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

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

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

7 In the **Settings** window for **Study**, type `xO2 and Pressure Sweep` in the **Label** text field.

8 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

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

RESULTS

Create plots to show the electron density, electron temperature, F number density, and O number density.

Electron Density

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

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

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

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

Global 1

1 Right-click **Electron Density** 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
`plas.ne`	`1/m^3`	`Electron density`

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

5 From the **Parameter selection (p0)** list, choose **From list**.

6 In the **Parameter values (p0 (mTorr))** list box, select **8**.

7 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

8 In the **Electron Density** toolbar, click **Plot**.

Global 2

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

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

3 In the **Parameter values (p0 (mTorr))** list box, select **15**.

4 In the **Electron Density** toolbar, click **Plot**.

Global 3

1 Right-click **Global 2** and choose **Duplicate**.

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

3 In the **Parameter values (p0 (mTorr))** list box, select **25**.

4 In the **Electron Density** toolbar, click **Plot**.

Electron Density

1 In the **Model Builder** window, click **Electron Density**.

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

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

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

5 In the **y maximum** text field, type `3e17`.

6 In the **Electron Density** toolbar, click **Plot**.

7 Select the **y-axis log scale** checkbox.

Electron Temperature

1 Right-click **Electron Density** and choose **Duplicate**.

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

Global 1

1 In the **Model Builder** window, expand the **Electron Temperature** 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
`plas.Te`	`V`	`Electron temperature`

Global 2

1 In the **Model Builder** window, click **Global 2**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
`plas.Te`	`V`	`Electron temperature`

Global 3

1 In the **Model Builder** window, click **Global 3**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.Te	V	Electron temperature

4 In the **Electron Temperature** toolbar, click **Plot**.

Electron Temperature

1 In the **Model Builder** window, click **Electron Temperature**.

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

3 Clear the **y-axis log scale** checkbox.

4 In the **y minimum** text field, type 0.

5 In the **y maximum** text field, type 5.

6 In the **Electron Temperature** toolbar, click **Plot**.

F Density

1 Right-click **Electron Temperature** and choose **Duplicate**.

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

Global 1

1 In the **Model Builder** window, expand the **F Density** 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
plas.n_wF	1/m^3	Number density

Global 2

1 In the **Model Builder** window, click **Global 2**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wF	1/m^3	Number density

Global 3

1 In the **Model Builder** window, click **Global 3**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wF	1/m^3	Number density

F Density

1 In the **Model Builder** window, click **F Density**.

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

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

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

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

6 In the **y maximum** text field, type `1e20`.

7 In the **F Density** toolbar, click **Plot**.

O Density

1 Right-click **F Density** and choose **Duplicate**.

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

Global 1

1 In the **Model Builder** window, expand the **O Density** 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
plas.n_wO	1/m^3	Number density

Global 2

1 In the **Model Builder** window, click **Global 2**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wO	1/m^3	Number density

Global 3

1 In the **Model Builder** window, click **Global 3**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wO	1/m^3	Number density

O Density

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

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

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

4 Locate the **Axis** section. In the **y maximum** text field, type `1e21`.

5 In the **O Density** toolbar, click **Plot**.