Model created in COMSOL Multiphysics 6.4

Global Model of a CF4/O2 Plasma Reactor for Silicon Etching

This model is licensed under the COMSOL Software License Agreement 6.4.
All trademarks are the property of their respective owners. See www.comsol.com/trademarks.

Introduction

This tutorial studies the etching of silicon using a CF_4/O_2 plasma using a global model. The plasma and surface chemistries are based on Ref. 1 and Ref. 2, and the electron impact reactions are taken from LxCat (Ref. 3, Ref. 4, and Ref. 5).

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

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

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 $R_{\mathrm{surf},k,l}$ 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 and Ref. 2. The electron impact cross sections used in this model are retrieved from different databases from LxCat: Ref. 3, Ref. 4, and Ref. 5. The data from Ref. 3 further refers to Ref. 6 and Ref. 7. The model solves for 29 volume 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, O_2^*, O^*, C, C^+, CO_2, CO_2^+, CO, CO^+, COF, COF_2, and FO.

The enchant products in the gaseous phase Si, SiF, SiF_2, SiF_3, and SiF_4 are assumed not to influence the plasma discharge. Reactions with these species are not included and these species are not solved for.

The following surface species are also included: Si(s), SiF(s), SiF_2(s), and SiF_3(s). The model solves for the site fraction of each species and Si(s) is set to be the empty site species. The empty site species is not solved for and its site fraction is obtained from the total site constraint.

When modeling surface species with a stationary solver, one of the surface species needs to be specified as an empty site species to be computed from a surface site constraint.

In this model, the etching process begins with fluorine atom adsorption at surface sites (Table 1) followed by chemical etching, which is negligible under the current conditions (Table 2), and ion-enhanced etching and sputtering (Table 3).

TABLE 1: F ADSORPTION REACTIONS AT SURFACE SITES.

Formula
F+Si(s)=>SiF(s)
F+SiF(s)=>SiF2(s)
F+SiF2(s)=>SiF3(s)

TABLE 2: CHEMICAL ETCHING.

Formula
F+SiF3(s)=>SiF4

TABLE 3: ION-ENHANCED ETCHING AND SPUTTERING REACTIONS.

Formula
I^++Si(s)=>I+Si
I^++SiF(s)=>I+SiF
I^++SiF2(s)=>I+SiF2
I^++SiF3(s)=>I+SiF3

In Table 3, I^+ denotes an ion that becomes neutralized upon reaching the surface and removes surface species into the gas phase, with a specified yield that depends on the ion energy. In the present model, the ion energy is treated as a parameter.

When explicitly solving for surface sites, rather than using a generic reaction to represent wall interactions, it is necessary to specify all possible reactions involving the available surface sites. For example, a generic wall recombination might be written as F=>0.5F2, but in a surface-site-based formulation, this process is represented as shown in Table 4.

TABLE 4: F RECOMBINATION AT THE SURFACE.

FORMULA
F+SiF(s)=>Si(s)+F2
F+SiF2(s)=>SiF(s)+F2
F+SiF3(s)=>SiF2(s)+F2

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 200 W, pressure of 350 mTorr, and an oxygen mole fraction (x_{O2}) of 0.01. In the second study, the oxygen mole fraction is varied between 0.01 and 0.8 for 15, 25, and 50 V of ion energy. The ion energy is assumed to be the same for all ion and is only used to compute the yield of ion enhanced etching reactions.

The etching rate of Si (E_{Si}) is define by the flux of Si containing species from the surface, $\Gamma_{ESi} = \Gamma_{Si} + \Gamma_{SiF} + \Gamma_{SiF2} + \Gamma_{SiF3} + \Gamma_{SiF4}$, divided by the density of Si, $n_{Si} = 5.0 \times 10^{28}\ \mathrm{m}^{-3}$:

$$E_{Si} = \frac{\Gamma_{ESi}}{n_{Si}}.$$

In the plasma interface, fluxes at surfaces are defined by `Rsurf` variables. For an individual *Surface Reaction* feature defined as F+Si(s)=>Si+F the flux of Si at the surface is defined by the variable `plas.Rsurf_#_Si_surf`, where # is the reaction number. In a *Surface Reaction Group* the flux of a given species at the surface is defined by the variable `plas.Rsurf_srg#_SpeciesName_surf`, where # is the *Surface Reaction Group* number. This variable sums over all reactions involving that species. In the present model all surface reactions that cause removal of Si from the surface (except chemical etching that is negligible for the present conditions) are grouped in a *Surface Reaction Group* labeled as “Waffer - Ion Enhance Etching and Sputtering”. This way, the flux of Si containing species used to compute etching can be computed by the sum of the variables `plas.Rsurf_srg5_Si_surf`, `plas.Rsurf_srg5_SiF_surf`, `plas.Rsurf_srg5_SiF2_surf`, and `plas.Rsurf_srg5_SiF3_surf`.

Figure 1 shows the etching rate as a function of the F number density (n_F) for several ion energies. Three regimes are observed in agreement with Ref. 8 (page 584) where a detailed explanation is provided. Here, only the key points are summarized. In the first regime (up to about 15% of x_{O2}) both E_{Si} and n_F increase with x_{O2}. This is explained by the "burning" of CF_x species creating F atoms. In the second regime (from 15% to 40% of x_{O2}) E_{Si} starts to decrease with x_{O2} even if n_F continues to increase. Ref. 8 explains this trend as the result of competition of O atoms in surface sites $SiF_x(s)$. However, in the present model, such surface mechanisms are not included and that might explain why the etching rate variation is smaller in this regime. We could say that in the present model the second regime described in Ref. 8 is absent and what is observed is a direct transition to the third regime where both E_{Si} and n_F decrease with x_{O2}, which is believed to be due to oxygen dilution.

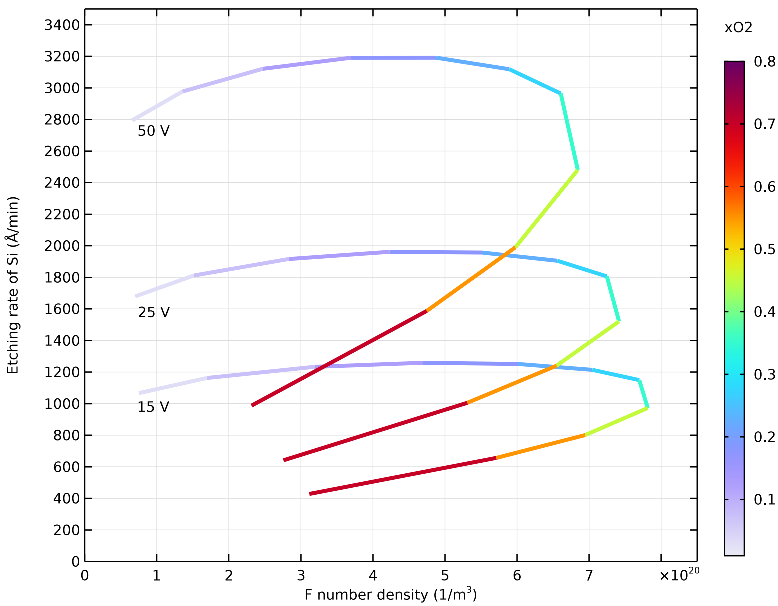

Figure 1: Silicon etching rate as a function of atomic fluorine number density at ion energies of 10, 25, and 50 V. The color scale represents the mole fraction of oxygen.

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. P. Ho, J.E. Johannes, R.J. Buss, and E. Meeks, "Chemical Reaction Mechanisms for Modeling the Fluorocarbon Plasma Etch of Silicon Oxide and Related Materials," Sandia Report SAND2001-1292, 2001; doi.org/10.2172/782704

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

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

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

6. 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.

7. 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.

8. M.A. Lieberman and A.J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, John Wiley & Sons, 2025.

Application Library path: `Plasma_Module/Surface_Processing/cf4_o2_si_etching_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_si_etching_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_Si_etching_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 the 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-x02`.

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 `x02`.

This model assumes that etchant products do not influence the discharge. To *not* solve for the etchant products in the gaseous phase, use a Species Constraint Group species to constrain their densities to their initial values.

Species Constraint Group 1

1. In the **Physics** toolbar, click **Domains** and choose **Species Constraint Group**.
2. Select Domain 1 only.
3. In the **Settings** window for **Species Constraint Group**, locate the **Species Group** section.
4. Click **Add**.
5. In the table, enter the following settings:

Species names
Si

6. Click **Add**.
7. In the table, enter the following settings:

Species names
Si
SiF

8. Click **Add**.

9 In the table, enter the following settings:

Species names
Si
SiF
SiF2

10 Click **Add**.

11 In the table, enter the following settings:

Species names
Si
SiF
SiF2
SiF3

12 Click **Add**.

13 In the table, enter the following settings:

Species names
Si
SiF
SiF2
SiF3
SiF4

In the following, select the boundaries for each of the Surface Reaction Group features.

Group - Species

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

Surface Reactions - Side Walls

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

2 Select Boundaries 3 and 4 only.

Surface Reactions - Wafer - Adsorption, Chemical Etching, and Recombination

1 In the **Model Builder** window, click **Surface Reactions - Wafer - Adsorption, Chemical Etching, and Recombination**.

2 Select Boundary 2 only.

Surface Reactions - Wafer - Lumped

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

2 Select Boundary 2 only.

Surface Reactions - Wafer Radical Abstraction

1 In the **Model Builder** window, click **Surface Reactions - Wafer Radical Abstraction**.

2 Select Boundary 2 only.

Surface Reactions - Wafer - Ion Enhanced Etching and Sputtering

1 In the **Model Builder** window, click **Surface Reactions - Wafer - Ion Enhanced Etching and Sputtering**.

2 Select Boundary 2 only.

Select Si(s) to be identified as an empty site species. This way, the site fraction for Si(s) is not solved for. Instead, it is obtained from total site conservation.

Species: Si(s)

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

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

3 Select the **Empty site species** checkbox.

Use a time-dependent solver to provide good initial conditions for a subsequent stationary solver where parameterizations are made.

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

Step 1: Time Dependent

1 In the **Model Builder** window, under **Base Case** click **Step 1: Time Dependent**.

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

3 In the **Output times** text field, type `10^{range(log10(1.0e-7),1/2,log10(50))}`.

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

Add a stationary study to parameterize the O2 mole fraction and ion energy.

Since the solution from a previous study is used to provide initial conditions and solutions from previous steps are reused, it is possible to increase the initial damping factor to 1. This will reduce the computation time.

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

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

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

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.

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
Eion (Ion energy)	15 25 50	V

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xO2 (O2 mole fraction)	0.01 0.05 0.1 0.15 0.2 0.25 0.3 0.4 0.5 0.6 0.8	

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

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

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

RESULTS

Create plots to show the electron density, electron temperature, electronegativity, species number density, site fraction, and etching rate.

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 **Study 2/Solution 2 (sol2)**.

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

5 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

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

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

Electron Temperature

1 In the **Model Builder** window, 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

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 **Legend** section.

3 From the **Position** list, choose **Upper right**.

Electronegativity

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

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

Global 1

1 In the **Model Builder** window, expand the **Electronegativity** 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.alphaN	1	Electronegativity

4 In the **Electronegativity** toolbar, click **Plot**.

Neutral Species Number Density

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

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

3 Locate the **Title** section. 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 Number density (1/m³).

6 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Neutral Species Number 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.n_wCF4	1/m^3	CF4
plas.n_wF2	1/m^3	F2
plas.n_wF	1/m^3	F
plas.n_wO2	1/m^3	O2
plas.n_wO	1/m^3	O
plas.n_wCOF2	1/m^3	COF2
plas.n_wCO2	1/m^3	CO2
plas.n_wCO	1/m^3	CO

Neutral Species Number Density

1 In the **Model Builder** window, click **Neutral Species Number Density**.

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

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

4 From the **Parameter selection (Eion)** list, choose **Last**.

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

Global 1

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

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

3 Find the **Include** subsection. Clear the **Solution** checkbox.

4 In the **Neutral Species Number Density** toolbar, click **Plot**.

Charged Species Number Density

1 In the **Model Builder** window, right-click **Neutral Species Number Density** and choose **Duplicate**.

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

Global 1

1 In the **Model Builder** window, expand the **Charged Species Number Density** node, then click **Global 1**.

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

3 Click **Clear Table**.

4 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wCF3_1p	1/m^3	CF3+
plas.n_wF2_1p	1/m^3	F2+
plas.n_wF_1p	1/m^3	F+
plas.n_wF_1m	1/m^3	F-
plas.n_wO_1p	1/m^3	O+
plas.n_wO_1m	1/m^3	O-
plas.n_wCO2_1p	1/m^3	CO2+
plas.n_wCO_1p	1/m^3	CO+

5 In the **Charged Species Number Density** toolbar, click **Plot**.

Site Fraction

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

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

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

4 From the **Parameter selection (Eion)** list, choose **Last**.

5 Locate the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Plot Settings** section.

7 Select the **y-axis label** checkbox. In the associated text field, type `Site fraction (1)`.

Global 1

1 Right-click **Site Fraction** 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
Zk_Si_surf	1	Si(s)
Zk_SiF_surf	1	SiF(s)
Zk_SiF2_surf	1	SiF2(s)
Zk_SiF3_surf	1	SiF3(s)

4 Locate the **Legends** section. Find the **Include** subsection. Clear the **Solution** checkbox.

5 In the **Site Fraction** toolbar, click **Plot**.

Etching Rate vs. F Number Density

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

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

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

4 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

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

6 In the **Parameter values (Eion (V))** list box, select **15**.

Global 1

1 Right-click **Etching Rate vs. F Number 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.Rsurf_srg5_Si_surf+ plas.Rsurf_srg5_SiF_surf+ plas.Rsurf_srg5_SiF2_surf+ plas.Rsurf_srg5_SiF3_surf)*N_A_const/ (5E28[m^-3])	Å/min	

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `plas.n_wF`.

6 Click to expand the **Coloring and Style** section. From the **Width** list, choose **3**.

7 Locate the **Legends** section. Clear the **Show legends** checkbox.

Color Expression 1

1 Right-click **Global 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `xO2`.

4 In the **Etching Rate vs. F Number Density** toolbar, click **Plot**.

Global 2

1 In the **Model Builder** window, under **Results** > **Etching Rate vs. F Number Density** right-click **Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

4 From the **Parameter selection (Eion)** list, choose **From list**.

5 In the **Parameter values (Eion (V))** list box, select **25**.

6 In the **Etching Rate vs. F Number Density** toolbar, click **Plot**.

Color Expression 1

1 In the **Model Builder** window, expand the **Global 2** node, then click **Color Expression 1**.

2 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

3 Clear the **Color legend** checkbox.

Global 3

1 In the **Model Builder** window, under **Results** > **Etching Rate vs. F Number Density** right-click **Global 2** and choose **Duplicate**.

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

3 In the **Parameter values (Eion (V))** list box, select **50**.

4 In the **Etching Rate vs. F Number Density** toolbar, click **Plot**.

Etching Rate vs. F Number Density

1 In the **Model Builder** window, click **Etching Rate vs. F Number Density**.

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

3 Select the **Show titles** checkbox.

4 Locate the **Axis** section. Select the **Manual axis limits** checkbox.

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

6 In the **x maximum** text field, type `8.5e20`.

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

8 In the **y maximum** text field, type `3500`.

9 In the **Etching Rate vs. F Number Density** toolbar, click **Plot**.

Annotation 1

1 Right-click **Etching Rate vs. F Number Density** and choose **Annotation**.

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

3 In the **Text** text field, type `50 V`.

4 Locate the **Position** section. In the **R** text field, type `0.6e20`.

5 In the **Z** text field, type `2800`.

6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

Annotation 2

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

2 In the **Settings** window for **Annotation**, locate the **Position** section.

3 In the **Z** text field, type `1650`.

4 Locate the **Annotation** section. In the **Text** text field, type `25 V`.

Annotation 3

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

2 In the **Settings** window for **Annotation**, locate the **Position** section.

3 In the **Z** text field, type `1050`.

4 Locate the **Annotation** section. In the **Text** text field, type `15 V`.

Color Expression 1

1 In the **Model Builder** window, under **Results** > **Etching Rate vs. F Number Density** > **Global 1** click **Color Expression 1**.

2 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

3 In the **Color legend title** text field, type `x02`.

Etching Rate vs. F Number Density

1 In the **Model Builder** window, under **Results** click **Etching Rate vs. F Number Density**.

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

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

4 Select the **y-axis label** checkbox. In the associated text field, type `Etching rate of Si (Å/min)`.

5 In the **Etching Rate vs. F Number Density** toolbar, click **Plot**.