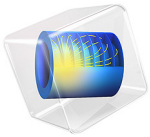

Global Model of an SF6/Argon Plasma

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Introduction

This tutorial studies the chemistry of a SF_6/argon plasma in moderate pressures using a global model. The main goal is to show how to prepare a model with a mixture of different elements (in this case Ar and SF_6) in which one of the species can dissociate by electron impact into many fragments (SF_6 dissociates into SF_x, F, and S) and where multiple negative ions exist.

A simplified plasma chemistry is used to discuss the main aspects of such discharges. It is important to keep in mind that a benchmark is not attempted and the idea is to provide a template that can be used to develop more complex and precise chemistries. In fact, quite probably it will be necessary to modify the data used and add more reactions to achieve experimental verification. The chemistry is based on Ref. 1, Ref. 2, Ref. 3, and Ref. 4.

Model Definition

The model used in this work considers that the spatial distribution of the different quantities in the plasma reactor can be treated as uniform. Without the 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 or the influence of the EEDF is to be studied.

When using a plasma global 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·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·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·s)). The sum in the last two terms is over all surfaces where there are surface reactions.

To take possible variations of the system 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

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

and if 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 be either analytic or can be 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 work uses the LEA and a Maxwellian EEDF.

The present study also solves the gas heat equation

$$V\rho C_p \frac{dT}{dt} = m_f \sum_k w_{f,k}(h_{f,k} + h_k) + Q + Q_S$$

where C_p is the specific heat at constant pressure of the mixture, T is the gas temperature, $h_{f,k}$ is the enthalpy of species k in the feed, h_k is the enthalpy of species k. The heat source from collisions is given by

$$Q = -V\sum_j H_j r_j + V \sum_{j,\,\text{elastic}} 2\frac{m_e}{m_k}\frac{3}{2}\left[T_e(eV) - \frac{k_B}{e}T_{\text{gas}}(K)\right]Fr_j$$

where the first term on the left side is the energy release from reactions, H_j is the reaction enthalpy, and r_j is the reaction rate. The last term is the energy gain from elastic collisions between electrons and heavy species. Heat losses by transport are including in a simplified form:

$$Q_S = k\frac{T_S - T}{\Lambda_S^2}V$$

where k is the thermal conductivity of the mixture, T_S is the surface temperature, and Λ_S is the diffusion length.

PLASMA CHEMISTRY

The plasma chemistry is based on Ref. 1, Ref. 2 and Ref. 3. The electron impact cross sections for SF_6 are from Ref. 4 and Ref. 6, and for F and F_2 are from Ref. 5 and Ref. 7. Argon cross sections are from Ref. 8. All cross-section data were directly retrieved from Ref. 9. For the rate constants of heavy species reactions were given generic order of magnitude values characteristic of the reaction type. The model includes 28 species: electrons, SF_x, SF_x^+, SF_x^-, F_x, F_x^+, F_x^-, Ar, Ars, and Ar^+.

This plasma chemistry is completely prepared in text data files and then imported using the Plasma Chemistry Add-in. Five reaction groups are created as listed in Table 1.

TABLE 1: REACTION GROUP FEATURES INCLUDED IN THIS MODEL.

Reaction group for	Type	No. of reactions included
SF_x	Electron Impact Reactions	32
F_x	Electron Impact Reactions	14
Ar	Electron Impact Reactions	5
Ion–ion	Heavy Species Reactions	56
Neutral–neutral	Heavy Species Reactions	9

In addition to the volume reactions, 11 surface reactions are also implemented.

Results and Discussion

On this work, 3 studies are made. In the first study, a base case is solved using a stationary solver for an input power of 2000 W and an argon mole fraction of 0.1. In the second study, a power sweep is solved for the input power ranging from 2000 W down to 300 W. In the third study, the argon mole fraction is swept from 0.1 to 0.9. For all cases the pressure is kept constant at 20 mTorr, a Maxwellian electron energy distribution function is used, and the heavy species heat equation is solved for.

Figure 1 shows the number densities of negatively charged species as a function of input power. The values are in agreement with Ref. 1. The density of F^- shows significant increase with power because of higher dissociation degree.

Figure 2 shows the electron temperature as a function of input power. The electron temperature decreases with power increase in agreement with Ref. 1 suggesting that the plasma is better confined at higher powers.

Figure 3 shows the gas temperature as a function of input power. The gas temperature increases significantly with power as expected. The values are in a reasonable range for the present operation conditions.

Figure 4 shows the number densities of positively charged species as a function of the argon mole fraction. As expected, the Ar^+ density increases with the argon mole fraction as more argon is available to ionize.

Figure 5 shows the electronegativity as a function of argon mole fraction. As expected, the electronegativity drops as the mixture becomes lean in SF_6 but the dominant charged species are still ions even at 90% argon.

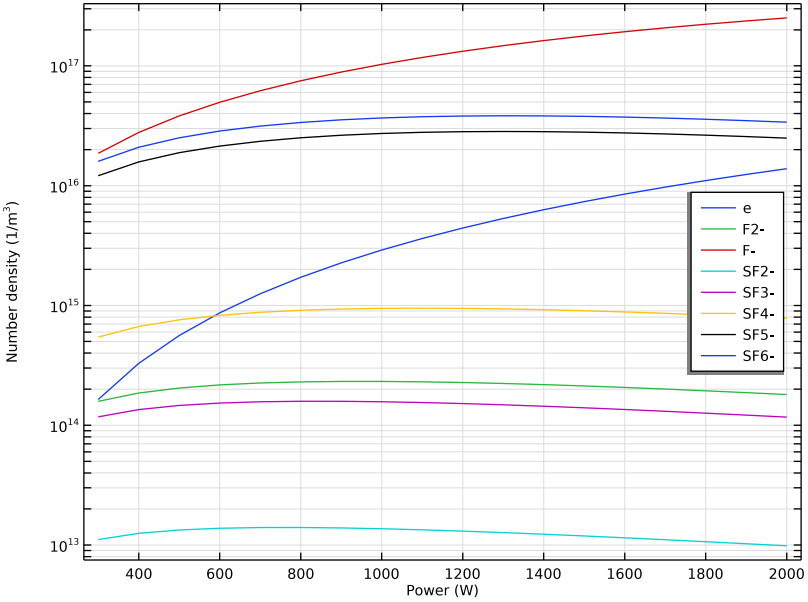

Figure 1: Number densities of negatively charged species as a function of input power.

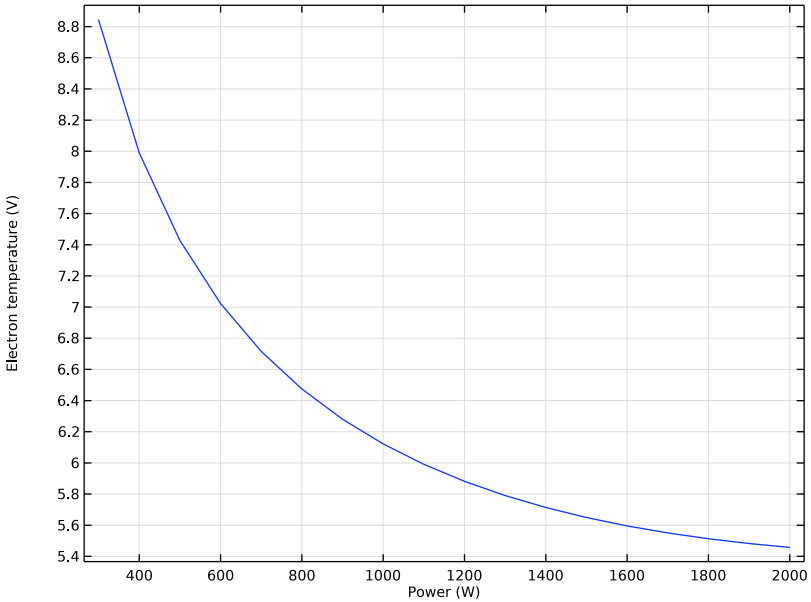

Figure 2: Electron temperature as a function of input power.

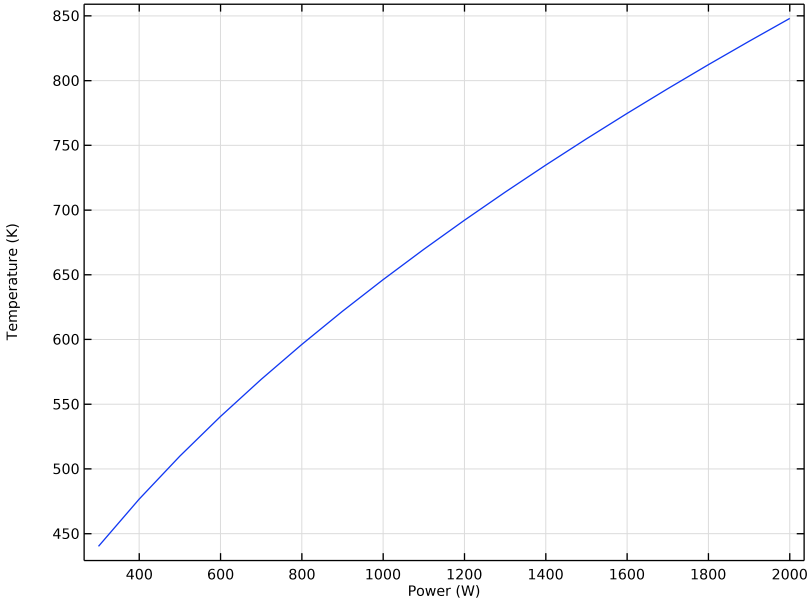

Figure 3: Gas temperature as a function of input power.

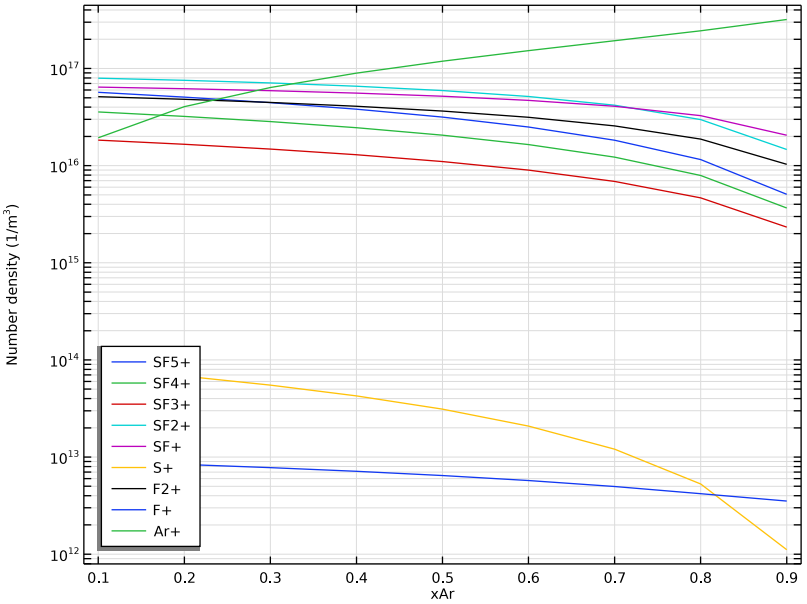

Figure 4: Number densities of positively charged species as a function of argon mole fraction.

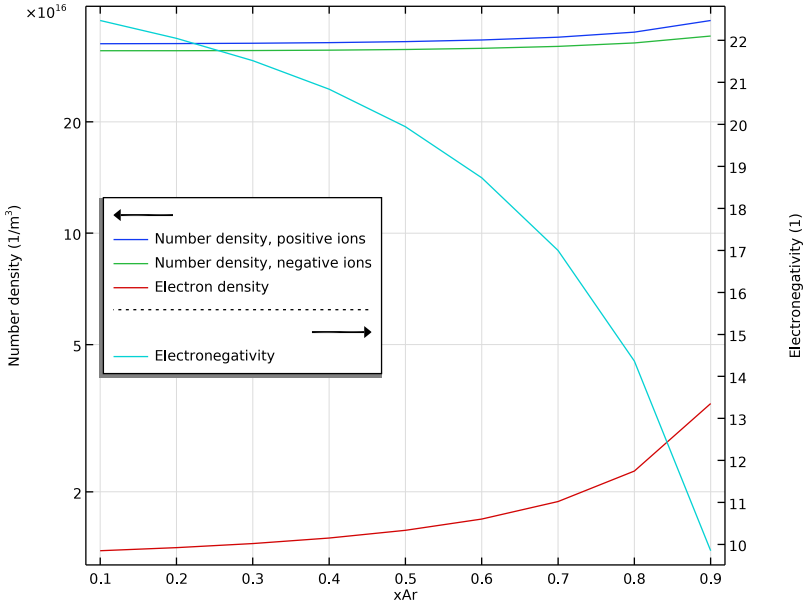

Figure 5: Electronegativity as a function of argon mole fraction.

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1. M. Mao, Y.N. Wang, and A. Bogaerts, "Numerical study of the plasma chemistry in inductively coupled SF6 and SF6/Ar plasmas used for deep silicon etching applications," *J. Phys. D: Appl. Phys.*, vol. 44, no. 43, p. 435202, 2011.

2. G. Kokkoris and others, "A global model for SF6 plasmas coupling reaction kinetics in the gas phase and on the surface of the reactor walls," *J. Phys. D: Appl. Phys*, vol. 42, no. 5, p. 055209, 2009.

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4. L.G. Christophorou and J.K. Olthoff, "Electron interactions with SF6," *J. Phys. Chem. Ref. Data*, vol. 29, no. 3, pp. 267–330, 2000 (www.lxcat.net/Christophorou , retrieved May 2024).

5. V. Gedeon and others, "B-spline R-matrix-with-pseudostates calculations for electron-impact excitation and ionization of fluorine," *Phys. Rev. A*, vol. 89, no. 5, p. 052713, 2014.

6. Biagi database, www.lxcat.net/Biagi, retrieved on 2024.

7. Morgan database, www.lxcat.net/Morgan, retrieved on 2024.

8. Phelps database, www.lxcat.net, retrieved 2017.

9. www.lxcat.net/IST-Lisbon, retrieved May 2024.

Application Library path: `Plasma_Module/Global_Modeling/sf6_argon_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** > **Stationary**.

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 In the table, enter the following settings:

Name	Expression	Value	Description
Qfeed	100	100	Feed mass flow in SCCM
Temp	315[K]	315 K	Gas temperature
pA	20[mTorr]	2.6664 Pa	Gas pressure
Pinp	2000[W]	2000 W	Power input from source
abs_to_inp	0.5	0.5	Power absorption ratio
Pabs	Pinp*abs_to_inp	1000 W	Power absorbed by plasma
xAr	0.1	0.1	Argon mole fraction
width	19[cm]	0.19 m	Chamber radius
height	17[cm]	0.17 m	Chamber height
lambda_diff	((pi/height)^2+(2.405/width)^2)^-0.5	0.044644 m	Diffusion length for heat

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**.

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

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 `width`.

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

5 Click **Build All Objects**.

PLASMA (PLAS)

Choose to solve for a global model of a constant pressure reactor and include the heavy species energy equation.

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

5 Locate the **Transport Settings** section. Select the **Calculate thermodynamic properties** checkbox.

6 Click to expand the **Heavy Species Energy Balance** section. Select the **Include heavy species energy conservation equation** checkbox.

Plasma Model 1

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

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_0 text field, type `Temp`.

4 In the p_A text field, type `pA`.

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

6 In the T_f text field, type `Temp`.

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

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

9 In the ε_i text field, type `10[V]`.

10 Locate the **Heat Transfer to Surfaces** section. In the T_S text field, type `Temp`.

11 In the Λ_S text field, type `lambda_diff`.

THE PLASMA CHEMISTRY ADD-IN

The next steps have instructions to first import the **Plasma Chemistry** add-in and then to use this add-in to import a file that automatically creates the SF6/Ar plasma chemistry.

The following is set or created automatically:

a Species properties

b Reaction group features for SF6, F2 and Ar

c Surface reactions

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

In the **Developer** toolbar, click **Add-in Libraries**.

ADD-IN LIBRARIES

1. In the **Add-in Libraries** window, select **Plasma Module** > **plasma_chemistry** in the tree.
2. In the tree, select the checkbox for the node **Plasma Module** > **plasma_chemistry** (if it is not already selected).
3. Click **Done** to load the add-in and close the **Add-in Libraries** window.
4. In the **Developer** toolbar, click **Add-ins** and choose **Plasma Chemistry** > **Plasma Chemistry**.

GLOBAL DEFINITIONS

Plasma Chemistry 1

1. In the **Model Builder** window, under **Global Definitions** click **Plasma Chemistry 1**.
2. In the **Settings** window for **Plasma Chemistry**, locate the **Plasma Chemistry Import** section.
3. Click **Browse**.
4. Browse to the model's Application Libraries folder and double-click the file `SF6_Ar_plasma_chemistry.txt`.
5. Click **Import**.

Set properties for some species and group all the species nodes.

Set SF6 to be the species that the mass fraction is found from mass constraint.

PLASMA (PLAS)

Species: SF6

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Plasma (plas)** click **Species: SF6**.
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-xAr`.

Species: Ar

1. In the **Model Builder** window, click **Species: Ar**.
2. In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the x_{feed} text field, type `xAr`.

Species: F2+

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

2 In the **Settings** window for **Species**, click to expand the **Species Thermodynamic Parameters** section.

3 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`.

Species: Ars

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

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

3 In the Δh text field, type `11.50`.

Species: Ar+

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

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

3 In the Δh text field, type `15.80`.

Species: Ar, Species: Ar+, Species: Ars, Species: F, Species: F+, Species: F-, Species: F2, Species: F2+, Species: F2-, Species: S, Species: S+, Species: SF, Species: SF+, Species: SF2, Species: SF2+, Species: SF2-, Species: SF3, Species: SF3+, Species: SF3-, Species: SF4, Species: SF4+, Species: SF4-, Species: SF5, Species: SF5+, Species: SF5-, Species: SF6, Species: SF6-, Species: e

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Plasma (plas)**, Ctrl-click to select **Species: e**, **Species: SF6**, **Species: SF5+**, **Species: F**, **Species: SF4+**, **Species: SF3+**, **Species: SF2+**, **Species: F2**, **Species: SF+**, **Species: S+**, **Species: F2-**, **Species: SF4**, **Species: F-**, **Species: SF5**, **Species: SF2-**, **Species: SF3-**, **Species: SF4-**, **Species: SF5-**, **Species: SF6-**, **Species: SF**, **Species: SF2**, **Species: SF3**, **Species: S**, **Species: F2+**, **Species: F+**, **Species: Ar**, **Species: Ars**, and **Species: Ar+**.

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

Group - Species

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

2 In the **Model Builder** window, collapse the **Group - Species** node.

Set different aspects of surface reactions: recombination of F at the surface (set in the **Forward sticking coefficient** field), and add a correction factor for ions (this is an estimate of the drop of the ion density near the surface to better estimate the losses by transport).

1: F=>0.5F2

1 In the **Model Builder** window, click **1: F=>0.5F2**.

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

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

2: SF5+=>SF5

1 In the **Model Builder** window, click **2: SF5+=>SF5**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

3: SF4+=>SF4

1 In the **Model Builder** window, click **3: SF4+=>SF4**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

4: SF3+=>SF3

1 In the **Model Builder** window, click **4: SF3+=>SF3**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

5: SF2+=>SF2

1 In the **Model Builder** window, click **5: SF2+=>SF2**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

6: SF+=>SF

1 In the **Model Builder** window, click **6: SF+=>SF**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

7: S+=>S

1 In the **Model Builder** window, click **7: S+=>S**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

8: F2+=>F2

1 In the **Model Builder** window, click **8: F2+=>F2**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

9: F+=>F

1 In the **Model Builder** window, click **9: F+=>F**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

10: Ar+=>Ar

1 In the **Model Builder** window, click **10: Ar+=>Ar**.

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

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

4 Locate the **Reaction Formula** section. From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `0.25`.

11: Ars=>Ar

1 In the **Model Builder** window, click **11: Ars=>Ar**.

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

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

10: Ar+=>Ar, 11: Ars=>Ar, 1: F=>0.5F2, 2: SF5+=>SF5, 3: SF4+=>SF4, 4: SF3+=>SF3, 5: SF2+=>SF2, 6: SF+=>SF, 7: S+=>S, 8: F2+=>F2, 9: F+=>F

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Plasma (plas)**, Ctrl-click to select **1: F=>0.5F2**, **2: SF5+=>SF5**, **3: SF4+=>SF4**, **4: SF3+=>SF3**, **5: SF2+=>SF2**, **6: SF+=>SF**, **7: S+=>S**, **8: F2+=>F2**, **9: F+=>F**, **10: Ar+=>Ar**, and **11: Ars=>Ar**.

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

Group - Surface Reactions

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

2 In the **Model Builder** window, collapse the **Group - Surface Reactions** node.

In the following prepare a base study with an input power of 2000 W, the results of this base study can be used as the initial values for the following parametric studies.

STUDY 1 - BASE CASE

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

2 In the **Settings** window for **Study**, type `Study 1 - Base Case` in the **Label** text field.

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

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

In the following measure number densities of all the species, which can be used to benchmark with reference results.

RESULTS

Global Evaluation 1

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

2 Right-click **Results** > **Derived Values** and choose **Global Evaluation**.

3 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

4 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wSF6	1/m^3	SF6
plas.n_wSF5	1/m^3	SF5
plas.n_wSF4	1/m^3	SF4
plas.n_wSF3	1/m^3	SF3
plas.n_wSF2	1/m^3	SF2
plas.n_wSF	1/m^3	SF
plas.n_wS	1/m^3	S
plas.n_wF	1/m^3	F
plas.n_wF2	1/m^3	F2
plas.n_wSF5_1p	1/m^3	SF5+
plas.n_wSF4_1p	1/m^3	SF4+
plas.n_wSF3_1p	1/m^3	SF3+
plas.n_wSF2_1p	1/m^3	SF2+
plas.n_wSF_1p	1/m^3	SF+
plas.n_wS_1p	1/m^3	S+
plas.n_wF_1p	1/m^3	F+
plas.n_wF2_1p	1/m^3	F2+
plas.n_wSF6_1m	1/m^3	SF6-
plas.n_wSF5_1m	1/m^3	SF5-
plas.n_wSF4_1m	1/m^3	SF4-
plas.n_wSF3_1m	1/m^3	SF3-
plas.n_wSF2_1m	1/m^3	SF2-
plas.n_wF_1m	1/m^3	F-
plas.n_wF2_1m	1/m^3	F2-
plas.ne	1/m^3	e

5 Click **Evaluate**.

In the following prepare a parameterization of the input power from 2000 to 300 W with a step of 100 W.

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 - POWER SWEEP

1 In the **Settings** window for **Study**, type `Study 2 - Power Sweep` in the **Label** text field.

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

Step 1: Stationary

1 In the **Model Builder** window, under **Study 2 - Power Sweep** click **Step 1: Stationary**.

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

3 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 **Study 1 - Base Case, Stationary**.

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

7 Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Pinp (Power input from source)		W

9 In the table, click to select the cell at row number 1 and column number 2.

10 Click **Range**.

11 In the **Range** dialog, type 2000 in the **Start** text field.

12 In the **Step** text field, type -100.

13 In the **Stop** text field, type 300.

14 Click **Add**.

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

In the following create plots for the number densities of neutral, positive, and negative species respectively as a function of input power. The electron temperature, electronegativity and gas temperature are also plotted with respect to input power.

RESULTS

Species densities vs. Power - Neutral

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

2 In the **Settings** window for **1D Plot Group**, type `Species densities vs. Power - Neutral` in the **Label** text field.

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

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

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `Power (W)`.

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

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

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

Global 1

1 Right-click **Species densities vs. Power - Neutral** 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_wSF6	1/m^3	SF6
plas.n_wSF5	1/m^3	SF5
plas.n_wSF4	1/m^3	SF4
plas.n_wSF3	1/m^3	SF3
plas.n_wSF2	1/m^3	SF2
plas.n_wSF	1/m^3	SF
plas.n_wS	1/m^3	S
plas.n_wF2	1/m^3	F2
plas.n_wF	1/m^3	F

Expression	Unit	Description
plas.n_wAr	1/m^3	Ar
plas.n_wArs	1/m^3	Ars

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

5 In the **Species densities vs. Power - Neutral** toolbar, click **Plot**.

Species densities vs. Power - Positive

1 In the **Model Builder** window, right-click **Species densities vs. Power - Neutral** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Species densities vs. Power - Positive` in the **Label** text field.

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

Global 1

1 In the **Model Builder** window, expand the **Species densities vs. Power - Positive** 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_wSF5_1p	1/m^3	SF5+
plas.n_wSF4_1p	1/m^3	SF4+
plas.n_wSF3_1p	1/m^3	SF3+
plas.n_wSF2_1p	1/m^3	SF2+
plas.n_wSF_1p	1/m^3	SF+
plas.n_wS_1p	1/m^3	S+
plas.n_wF2_1p	1/m^3	F2+
plas.n_wF_1p	1/m^3	F+
plas.n_wAr_1p	1/m^3	Ar+

5 In the **Species densities vs. Power - Positive** toolbar, click **Plot**.

Species densities vs. Power - Negative

1 In the **Model Builder** window, right-click **Species densities vs. Power - Positive** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Species densities vs. Power - Negative` in the **Label** text field.

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

Global 1

1 In the **Model Builder** window, expand the **Species densities vs. Power - Negative** 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.ne`	`1/m^3`	`e`
`plas.n_wF2_1m`	`1/m^3`	`F2-`
`plas.n_wF_1m`	`1/m^3`	`F-`
`plas.n_wSF2_1m`	`1/m^3`	`SF2-`
`plas.n_wSF3_1m`	`1/m^3`	`SF3-`
`plas.n_wSF4_1m`	`1/m^3`	`SF4-`
`plas.n_wSF5_1m`	`1/m^3`	`SF5-`
`plas.n_wSF6_1m`	`1/m^3`	`SF6-`

5 In the **Species densities vs. Power - Negative** toolbar, click **Plot**.

Electron Temperature vs. Power

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

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

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

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

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `Power (W)`.

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

Global 1

1 Right-click **Electron Temperature vs. Power** 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.Te	V	Electron temperature

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

Electronegativity vs. Power

1 In the **Model Builder** window, right-click **Electron Temperature vs. Power** and choose **Duplicate**.

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

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

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

5 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Electronegativity (1)`.

6 Locate the **Legend** section. Select the **Show legends** checkbox.

7 From the **Position** list, choose **Middle right**.

Global 2

1 Right-click **Electronegativity vs. Power** and choose **Global**.

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

3 Select the **Plot on secondary y-axis** checkbox.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
plas.nm/plas.ne	1	Electronegativity

Global 1

1 In the **Model Builder** window, 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.np	1/m^3	Number density, positive ions

Expression	Unit	Description
plas.nm	1/m^3	Number density, negative ions
plas.ne	1/m^3	Electron density

5 In the **Electronegativity vs. Power** toolbar, click **Plot**.

6 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

Gas Temperature vs. Power

1 In the **Model Builder** window, right-click **Electron Temperature vs. Power** and choose **Duplicate**.

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

Global 1

1 In the **Model Builder** window, expand the **Gas Temperature vs. Power** 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.T	K	Temperature

5 In the **Gas Temperature vs. Power** toolbar, click **Plot**.

Electron Temperature vs. Power, Electronegativity vs. Power, Gas Temperature vs. Power, Species densities vs. Power - Negative, Species densities vs. Power - Neutral, Species densities vs. Power - Positive

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Species densities vs. Power - Neutral**, **Species densities vs. Power - Positive**, **Species densities vs. Power - Negative**, **Electron Temperature vs. Power**, **Electronegativity vs. Power**, and **Gas Temperature vs. Power**.

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

Power Sweep

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

2 In the **Model Builder** window, collapse the **Power Sweep** node.

In the following prepare a parameterization of the argon feed mole fraction xAr from 0.1 to 0.9 with a step of 0.1.

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 **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 3 - XAR SWEEP

1 In the **Settings** window for **Study**, type `Study 3 - xAr Sweep` in the **Label** text field.

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

Step 1: Stationary

1 In the **Model Builder** window, under **Study 3 - xAr Sweep** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Values of Dependent Variables** section.

3 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 **Study 2 - Power Sweep, Stationary**.

6 From the **Parameter value (Pinp (W))** list, choose **2000 W**.

7 Locate the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

8 Click **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xAr (Argon mole fraction)		

10 In the table, click to select the cell at row number 1 and column number 2.

11 Click **Range**.

12 In the **Range** dialog, type `0.1` in the **Start** text field.

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

14 In the **Stop** text field, type `0.9`.

15 Click **Add**.

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

In the following duplicate the same set of plots created for the Power sweep, make sure the correct dataset is selected, and change the x axis to argon feed mole fraction xAr.

RESULTS

xAr Sweep

1. In the **Model Builder** window, right-click **Power Sweep** and choose **Duplicate**.
2. In the **Settings** window for **Group**, type `xAr Sweep` in the **Label** text field.

Species densities vs. xAr - Neutral

1. In the **Model Builder** window, expand the **xAr Sweep** node, then click **Species densities vs. Power - Neutral 1**.
2. In the **Settings** window for **1D Plot Group**, type `Species densities vs. xAr - Neutral` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 3 - xAr Sweep/ Solution 3 (sol3)**.
4. Locate the **Plot Settings** section. In the **x-axis label** text field, type `xAr`.
5. In the **Species densities vs. xAr - Neutral** toolbar, click **Plot**.
6. Locate the **Legend** section. From the **Position** list, choose **Lower left**.

Species densities vs. xAr - Positive

1. In the **Model Builder** window, under **Results** > **xAr Sweep** click **Species densities vs. Power - Positive 1**.
2. In the **Settings** window for **1D Plot Group**, type `Species densities vs. xAr - Positive` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 3 - xAr Sweep/ Solution 3 (sol3)**.
4. Locate the **Plot Settings** section. In the **x-axis label** text field, type `xAr`.
5. In the **Species densities vs. xAr - Positive** toolbar, click **Plot**.
6. Locate the **Legend** section. From the **Position** list, choose **Lower left**.

Species densities vs. xAr - Negative

1. In the **Model Builder** window, under **Results** > **xAr Sweep** click **Species densities vs. Power - Negative 1**.
2. In the **Settings** window for **1D Plot Group**, type `Species densities vs. xAr - Negative` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 3 - xAr Sweep/ Solution 3 (sol3)**.
4. Locate the **Plot Settings** section. In the **x-axis label** text field, type `xAr`.
5. In the **Species densities vs. xAr - Negative** toolbar, click **Plot**.

Electron Temperature vs. xAr

1 In the **Model Builder** window, under **Results** > **xAr Sweep** click **Electron Temperature vs. Power 1**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3 - xAr Sweep/ Solution 3 (sol3)**.

4 Locate the **Plot Settings** section. In the **x-axis label** text field, type `xAr`.

5 In the **Electron Temperature vs. xAr** toolbar, click **Plot**.

Electronegativity vs. xAr

1 In the **Model Builder** window, under **Results** > **xAr Sweep** click **Electronegativity vs. Power 1**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3 - xAr Sweep/ Solution 3 (sol3)**.

4 Locate the **Plot Settings** section. In the **x-axis label** text field, type `xAr`.

5 In the **Electronegativity vs. xAr** toolbar, click **Plot**.

6 Locate the **Legend** section. From the **Position** list, choose **Middle left**.

Gas Temperature vs. xAr

1 In the **Model Builder** window, under **Results** > **xAr Sweep** click **Gas Temperature vs. Power 1**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3 - xAr Sweep/ Solution 3 (sol3)**.

4 Locate the **Plot Settings** section. In the **x-axis label** text field, type `xAr`.

5 In the **Gas Temperature vs. xAr** toolbar, click **Plot**.

xAr Sweep

In the **Model Builder** window, collapse the **Results** > **xAr Sweep** node.