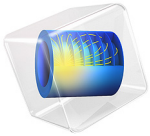

Chlorine Discharge Global Model

Introduction

Plasma discharges containing Chlorine are commonly used to etch semiconductors and metals in microelectronics fabrication. Cl_2 has low dissociation energy and very low threshold energy for dissociative attachment, and atomic chlorine has large electron affinity. As a consequence, a Cl_2 plasma has substantial levels of electronegativity and dissociation. Quantification of the negative ion and atomic chlorine density is important to understand the reactor operation. In particular chlorine atoms are accepted to be a main reactant for plasma etching.

In this study, model results of chlorine and electron density for absorbed powers between 25 and 600 W and for working pressures between 1 and 100 mTorr are presented. To explore such a large parametric region, a global (volume-averaged) model is used because it can run simulations in a fraction of the time of a space-dependent model while retaining the tendencies of volume-averaged physical quantities.

Model results of several relevant quantities such as atomic chlorine density, electron density, and electron temperature are in good agreement with measurements performed in inductively coupled plasma reactors found in the literature.

You can find more information about global models and Chlorine plasmas in Ref. 1, Ref. 2, and Ref. 3 and in the references therein.

Model Definition

The model used in this work considers that the spatial information of the different quantities in the plasma reactor can be treated as uniform or can be introduced using analytic models. Without the spatial derivatives the numerical solution of the equation set becomes considerably simpler and the computational time is reduced. In the following it is taken advantage of the fast computational time to investigate a broad region of parameters with a complex plasma chemistry.

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 study uses the LEA and a Maxwellian EEDF to computed the electron impact rate coefficients.

In this work are simulated cylindrical reactors with several dimensions corresponding to inductively coupled plasma reactors used by different experimental groups. The simulations are performed for a reactor operating at constant pressure. Moreover, the mass-flow rate of the outlet is found by assuming that the feed and the surface reactions cannot change the total mass of the system

$$m_o = m_f + \sum_l h_l A_l M_{f,l} .$$

Note that the surface reactions used in these simulations do not change the mass of the system.

However the mass-continuity equation is not solved, the mass density can still change as a result of a change in the mean molar mass, thus accounting for changes in the number density (due to dissociation and association) to maintaining a constant pressure.

The expressions used for the mean kinetic energy lost per electron lost and the mean kinetic energy lost per ion lost are deduced from theory and numerical solution and are explained in Ref. 1and references therein. The gas temperature is a function of pressure and absorbed power and is based on experimental data Ref. 1.

PLASMA CHEMISTRY

It is used the plasma chemistry suggested in Ref. 2 and presented in Table 1that consists of 10 species and 44 reactions.

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon$(eV)
1	e+Cl2=>e+Cl2	Momentum	0
2	e+Cl=>e+Cl	Momentum	0

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon(\mathrm{eV})$
3	e+Cl2=>Cl+Cl+e	Dissociation	4
4	e+Cl2=>2e+Cl2+	Ionization	11.5
5	e+Cl2=>2e+Cl+Cl+	Ionization	14.25
6	e+Cl2=>3e+2Cl+	Ionization	28.5
7	e+Cl2=>Cl+Cl-	Attachment	0
8	e+Cl2v1=>Cl+Cl-	Attachment	0
9	e+Cl2v2=>Cl+Cl-	Attachment	0
10	e+Cl2v3=>Cl+Cl-	Attachment	0
11	e+Cl2=>Cl++Cl-+e	Ionization/Attachment	14.25
12	e+Cl2=>e+Cl2v1*	Excitation	0.07
13	e+Cl2=>e+Cl2v2*	Excitation	0.14
14	e+Cl2=>e+Cl2v3*	Excitation	0.21
15	e+Cl2v1=>e+Cl2v2*	Excitation	0.07
16	e+Cl2v2=>e+Cl2v3*	Excitation	0.07
17	e+Cl2v1=>e+Cl2v3*	Excitation	0.14
18	e+Cl2+=>2Cl	Excitation	0
19	e+Cl=>e+Cl12*	Excitation	1.35
20	e+Cl=>e+Cl52*	Excitation	10.17
21	e+Cl=>Cl++2e	Ionization	14.25
22	e+Cl12=>Cl++2e	Ionization	10.18
23	e+Cl52=>Cl++2e	Ionization	4.08
24	e+Cl-=>Cl+2e	Ionization	2.36
25	e+Cl-=>Cl++3e	Ionization	16.61
26	Cl52=>Cl	Radiation decay	0
27	Cl2++Cl-=>3Cl	Ion-ion recombination	0
28	Cl2++Cl-=>Cl+Cl2	Ion-ion recombination	0
29	Cl++Cl-=>2Cl	Ion-ion recombination	0
30	Cl2+Cl+=>Cl+Cl2+	Charge exchange	0
31	Cl2v1+Cl+=>Cl+Cl2+	Charge exchange	0
32	Cl2v2+Cl+=>Cl+Cl2+	Charge exchange	0
33	Cl2v3+Cl+=>Cl+Cl2+	Charge exchange	0

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	FORMULA	TYPE	$\Delta\varepsilon(\mathrm{eV})$
34	2Cl+Cl2=>2Cl2	Association	0
35	2Cl+Cl=>Cl2+Cl	Association	0
36	Cl+Cl2v3=>Cl+Cl2v2	Deexcitation	0
37	Cl+Cl2v2=>Cl+Cl2v1	Deexcitation	0
38	Cl+Cl2v1=>Cl+Cl2v0	Deexcitation	0

*The reaction set includes the inverse reaction with the rate coefficient obtained by detailed balance.

The model also include the surface reactions presented in Table 2.

TABLE 2: TABLE OF SURFACE REACTIONS.

REACTION	FORMULA	STICKING COEFFICIENT
1	Cl2+=>Cl2	1
2	Cl+=>Cl	1
3	Cl2v1=>Cl2	1
4	Cl2v2=>Cl2	1
5	Cl2v3=>Cl2	1
6	Cl12=>Cl	1
7	Cl52=>Cl	1
8	Cl=>0.5Cl2	Ref. 1

The rate at which positive ions are lost to the wall is computed from the Bohm velocity and the density that an ion have near the surface. The ion density at the surface is estimated from theory Ref. 1 and Ref. 3 and is introduced in the model using the correction factor h_l. Negative ions are assumed to be confined in the plasma bulk.

The rate at which neutral species are lost to the wall involves the information of diffusional losses, of the particle mean velocity, and of the sticking coefficient Ref. 1 and Ref. 3. The wall recombination of neutral chlorine atoms is an important aspect of chlorine containing discharges since it influences the degree of dissociation of the discharge. The sticking coefficient for the recombination of Cl at the surface is obtained by fitting experimental data Ref. 1. All other neutral excited species revert to ground state with sticking coefficient equal to one.

Results and Discussion

In this section are presented simulations results that can be compared with measurements and simulations reported in Ref. 1. The measurements are for inductively coupled plasma

reactors with radius R and length L, operate at a given volumetric flow (Q_f), and sweep either the input power or the pressure. The power absorbed by the plasma that is used in the simulations is estimated in Ref. 1. The parameters used in the simulations are summarized in Table 3, and are labeled with the name of the authors that perform the measurements. Overall the numeric results are consistent with those of Ref. 1 and agree well for most experimental conditions.

TABLE 3: REACTOR PARAMETERS USED IN THE SIMULATIONS.

AUTHOR	R(cm)	L(cm)	Q_f(sccm)	P_{abs}(W)	P(mTorr)
Corr and others	10	8.5	10	25-300 300	10 1-100
Malyshev and Donnelly	18.5	20	100	50-650	10
Efremov and others	15	14	20	300	1-100

Figure 1 and Figure 2 present electron and Cl number density as a function of the absorbed power for the experimental conditions of Corr and others and Malyshev and Donnelly. The atomic Chlorine density for the conditions of Corr and others and the electron density for the conditions of Malyshev and Donnelly (Figure 2) agree well with measurements. The electron density for the conditions of Corr and others (Figure 1) is highly overestimated when compared with measurements but is consistent with the simulation results of Ref. 1. The electronegativity, also presented in Figure 1, only agrees well with measurements at higher absorbed powers.

Figure 3 presents electron and Cl number density as a function of the reactor pressure for the experimental conditions of Corr and others. There is a fair agreement for all conditions with the model capturing the tendencies but slightly underestimating the Cl density and overestimating the electron density.

Figure 4 presents the electron temperature as a function of the reactor pressure for the experimental conditions of Efremov and others. The model agrees well with measurements capturing the decrease of the electron temperature with pressure. However, the measured temperature decreases at a faster rate with pressure at higher pressures.

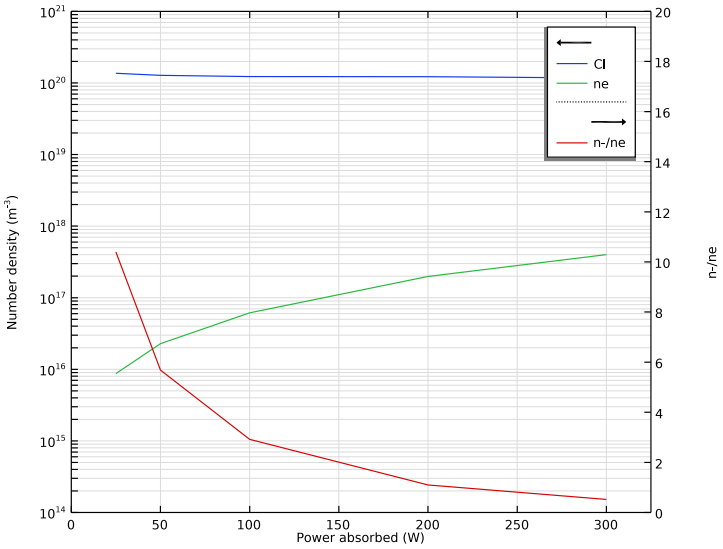

Figure 1: Model results for the electron and Cl densities, and for the electronegativity as a function of the absorbed power for the conditions of Corr and others: P=10 mTorr, Q_f=10 sccm, R=10 cm, and L=8.5 cm.

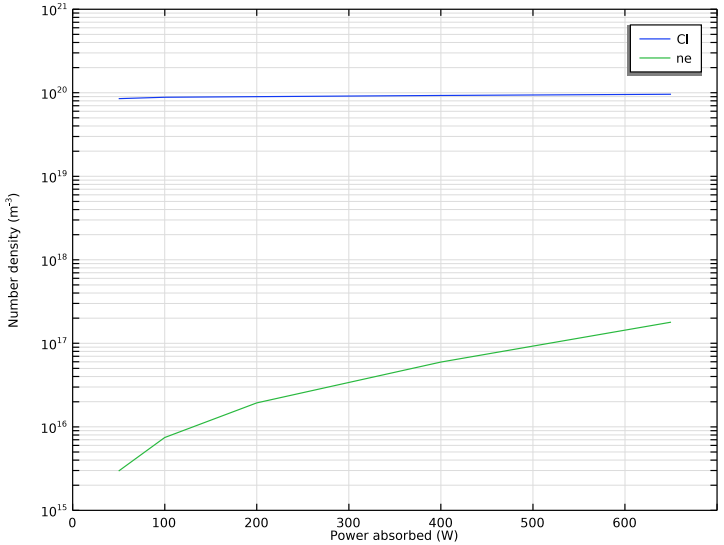

Figure 2: Model results for the electron and Cl densities as a function of the absorbed power for the conditions of Malyshev and Donnelly: P=10 mTorr, Q_f=100 sccm, R=8.5 cm, and L=20 cm.

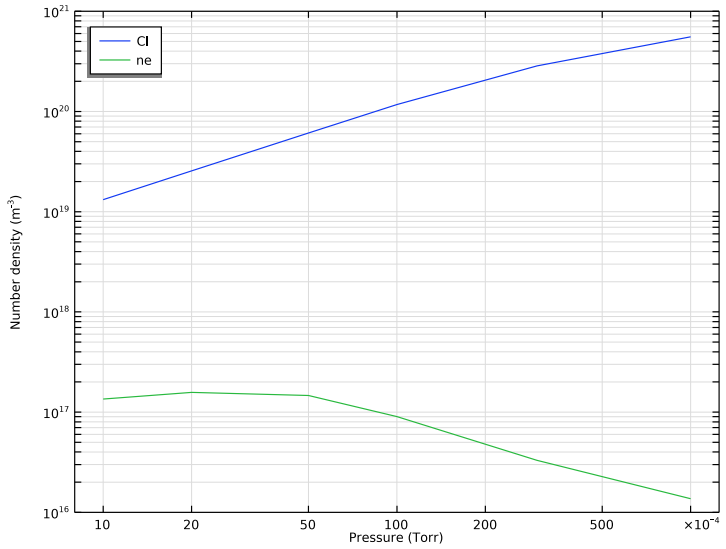

Figure 3: Model results for the electron and Cl densities as a function of pressure. The Cl density is for the conditions of Corr and others: P_{abs}=300 W, Q_f=10 sccm, R=10 cm, and L=8.5 cm. The electron density is for the conditions of Efremov and others: P_{abs}=300 W, Q_f=20 sccm, R=25 cm, and L=14 cm.

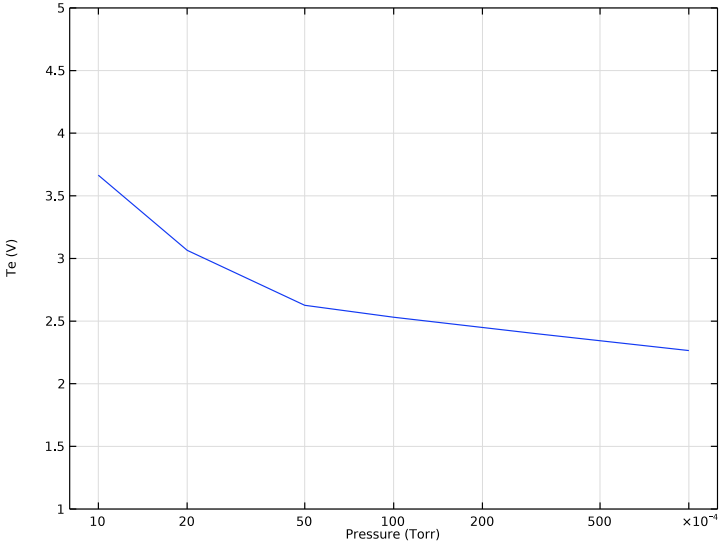

Figure 4: Model results for the electron temperature as a function of pressure for the conditions of Efremov and others: P_{abs}=300 W and Q_f=20 sccm, R=15 cm, and L=14 cm.

References

1. E.G. Thorsteinsson, and J.T. Gudmundsson, "A global (volume averaged) model of a chlorine discharge," *Plasma Sources Sci. Technol.*, vol. 19, p. 015001 (15pp), 2010.

2. E. Kemaneci, E. Carbone, J-P. Booth, W. Graef, J. van Dijk, and G. Kroesen, "Global (volume-averaged) model of inductively coupled chlorine plasma: influence of Cl wall recombination and external heating on continuous and pulse-modulated plasmas," *Plasma Sources Sci. Technol.*, vol. 23, p. 045002 (14pp), 2014.

3. M.A. Lieberman and A.J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, John Wiley & Sons, 2005.

Application Library path: `Plasma_Module/Global_Modeling/chlorine_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**.

ROOT

Construct a cylindrical reactor with radius *Rad* and length *L*. The values of *Rad* and *L* are set in the **Parameters** node.

GEOMETRY 1

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 `Rad`.

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

GLOBAL DEFINITIONS

Add parameters to be used in the simulations. The pressure and absorbed power need to be set here to be available to do a parameter sweep.

The different studies performed use different parameters so that before each new study (after the first study) it is necessary to change some of the parameters values.

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	10[cm]	0.1 m	
L	8.5[cm]	0.085 m	
Pabs	25[W]	25 W	
Qfeed	10	10	
p0	0.01[Torr]	1.3332 Pa	

DEFINITIONS

Import the file containing the energy levels to be used when defining the reactions.

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `chlorine_global_model_variables_1.txt`.

Import the file containing the variables used to define the gas temperature, the plasma and sheath potential, and the h_l correction factors.

Variables 2

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `chlorine_global_model_variables_2.txt`.

Choose to use a global model for the following simulations and set the model to work at constant pressure.

PLASMA (PLAS)

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**.

Set the background gas temperature, the working pressure, the total mass flow, the power absorbed, the mean kinetic energy lost per ion and electron lost.

The mole fraction of each species in the mass flow is set later in the species node.

Plasma Model 1

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

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

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

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 `Pabs`.

7 In the ε_e text field, type `Epsilon_e`.

8 In the ε_i text field, type `Epsilon_p+Epsilon_s`.

Add reactions relevant for the Chlorine plasma chemistry. There are about 40 volume reactions that need to be added.

For electron impact reactions it is needed to set the collision type, the rate constant and the energy loss in the collision.

For reactions between heavy species it is only necessary to set the rate constant.

Electron Impact Reaction 1

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>Cl+Cl+e`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the $\Delta\varepsilon$ text field, type `ediss`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `1.04e-13*plas.Te^(-0.29)*exp(-8.84/plas.Te)*N_A_const`.

Electron Impact Reaction 2

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>2e+Cl2+`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the $\Delta\varepsilon$ text field, type `eionCl2`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `5.12e-14*plas.Te^(0.48)*exp(-12.34/plas.Te)*N_A_const`.

Electron Impact Reaction 3

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>2e+Cl+Cl+`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the $\Delta\varepsilon$ text field, type `eionCl`.

6 Locate the **Reaction Parameters** section. In the k^{f} text field, type `2.14e-13*plas.Te^(-0.07)*exp(-25.26/plas.Te)*N_A_const`.

Electron Impact Reaction 4

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>3e+2Cl+`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the Δε text field, type `2*eionCl`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `2.27e-16*plas.Te^(1.92)*exp(-21.26/plas.Te)*N_A_const`.

Electron Impact Reaction 5

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>Cl+Cl-`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Attachment**.

5 Locate the **Reaction Parameters** section. In the k^f text field, type `(3.43e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 3.05e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 6

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v1=>Cl+Cl-`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Attachment**.

5 Locate the **Reaction Parameters** section. In the k^f text field, type `(14.06e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 12.51e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 7

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v2=>Cl+Cl-`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Attachment**.

5 Locate the **Reaction Parameters** section. In the k^f text field, type `(30.18e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 26.84e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 8

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v3=>Cl+Cl-`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Attachment**.

5 Locate the **Reaction Parameters** section. In the k^f text field, type `(46.31e-15*plas.Te^(-1.18)*exp(-3.98/plas.Te) + 41.18e-16*plas.Te^(-1.33)*exp(-0.11/(plas.Te+0.014)))*N_A_const`.

Electron Impact Reaction 9

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>Cl++Cl-+e`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `eionCl`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `2.94e-16*plas.Te^(0.19)*exp(-18.79/plas.Te)*N_A_const`.

Electron Impact Reaction 10

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>e+Cl2v1`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.99e-12*plas.Te^(-1.5)*exp(-7.51/plas.Te-0.0001/plas.Te^2)*N_A_const`.

Electron Impact Reaction 11

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>e+Cl2v2`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `ev2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3.28e-17*plas.Te^(-1.12)*exp(-0.37/plas.Te) + 2.86e-17*exp(-(log(plas.Te)+0.99)^2/(2*1.06^2)))*N_A_const`.

Electron Impact Reaction 12

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>e+Cl2v3`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `ev3`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.3e-17*plas.Te^(-1.24)*exp(-0.41/plas.Te) + 6.08e-18*exp(-(log(plas.Te)+0.94)^2/(2*1.02^2)))*N_A_const`.

Electron Impact Reaction 13

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v1=>e+Cl2v2`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `ev2-ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const`.

Electron Impact Reaction 14

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v2=>e+Cl2v3`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `ev3-ev2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const`.

Electron Impact Reaction 15

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v1=>e+Cl2v3`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `ev3-ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.25e-16*plas.Te^(-1.13)*exp(-0.36/plas.Te) + 1.06e-16*exp(-(log(plas.Te)+1.01)^2/(2*1.06^2)))*N_A_const`.

Electron Impact Reaction 16

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2+=>2Cl`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-eionCl2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `9e-14*plas.Te^(-0.5)*N_A_const`.

Electron Impact Reaction 17

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl=>e+Cl12`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `eCl12`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `4.55e-14*plas.Te^(-0.46)*exp(-2.01/plas.Te-0.001/plas.Te^2)*N_A_const`.

Electron Impact Reaction 18

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl=>e+Cl52`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `eCl52`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(7.03e-17*plas.Te^(0.55)*exp(-2.15/plas.Te-1.5/plas.Te^2-2.05/plas.Te^3))*N_A_const`.

Electron Impact Reaction 19

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl=>Cl++2e`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the Δε text field, type `eionCl`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.17e-14* plas.Te^(0.53)*exp(-13.29/plas.Te)*N_A_const`.

Electron Impact Reaction 20

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl12=>Cl++2e`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the Δε text field, type `eionCl-eCl12`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.17e-14* plas.Te^(0.53)*exp(-13.29/plas.Te)*N_A_const`.

Electron Impact Reaction 21

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl52=>Cl++2e`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the Δε text field, type `eionCl-eCl52`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(4.33e-14* plas.Te^(0.55)*exp(-0.15/plas.Te-0.85/plas.Te^2))*N_A_const`.

Electron Impact Reaction 22

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl-=>Cl+2e`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the Δε text field, type `eatt`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `9.02e-15* plas.Te^(0.92)*exp(-4.88/plas.Te)*N_A_const`.

Electron Impact Reaction 23

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl-=>Cl++3e`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Ionization**.

5 In the Δε text field, type `eatt+eionCl`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.62e-15*plas.Te^(0.72)*exp(-25.38/plas.Te)*N_A_const`.

Electron Impact Reaction 24

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v1=>e+Cl2`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-ev1`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `3.99e-12*plas.Te^(-1.5)*exp(-7.51/plas.Te-0.0001/plas.Te^2)*N_A_const*exp(ev1/plas.Te)`.

Electron Impact Reaction 25

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v2=>e+Cl2`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-ev2`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3.28e-17*plas.Te^(-1.12)*exp(-0.37/plas.Te) + 2.86e-17*exp(-(log(plas.Te)+0.99)^2/(2*1.06^2)))*N_A_const*exp(ev2/plas.Te)`.

Electron Impact Reaction 26

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v3=>e+Cl2`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-ev3`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.3e-17*plas.Te^(-1.24)*exp(-0.41/plas.Te) + 6.08e-18*exp(-(log(plas.Te)+0.94)^2/(2*1.02^2)))*N_A_const*exp(ev3/plas.Te)`.

Electron Impact Reaction 27

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v2=>e+Cl2v1`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-(ev2-ev1)`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const*exp((ev2-ev1)/plas.Te)`.

Electron Impact Reaction 28

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v3=>e+Cl2v2`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-(ev3-ev2)`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(3e-16*plas.Te^(-1.0)*exp(-0.37/plas.Te) + 4.61e-16*exp(-(log(plas.Te)+1.04)^2/(2*1.10^2)))*N_A_const*exp((ev3-ev2)/plas.Te)`.

Electron Impact Reaction 29

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2v3=>e+Cl2v1`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-(ev3-ev1)`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(1.25e-16*plas.Te^(-1.13)*exp(-0.36/plas.Te) + 1.06e-16*exp(-(log(plas.Te)+1.01)^2/(2*1.06^2)))*N_A_const*exp((ev3-ev1)/plas.Te)`.

Electron Impact Reaction 30

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl12=>e+Cl`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-eCl12`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `4.55e-14*plas.Te^(-0.46)*exp(-2.01/plas.Te-0.001/plas.Te^2)*N_A_const*exp((eCl12)/plas.Te)`.

Electron Impact Reaction 31

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl52=>e+Cl`.

4 Locate the **Collision Type** section. From the **Collision type** list, choose **Excitation**.

5 In the Δε text field, type `-eCl52`.

6 Locate the **Reaction Parameters** section. In the k^f text field, type `(7.03e-17*plas.Te^(0.55)*exp(-2.15/plas.Te-1.5/plas.Te^2-2.05/plas.Te^3))*N_A_const*exp((eCl52)/plas.Te)`.

Reaction 1

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

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

3 In the **Formula** text field, type `Cl52=>Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1e5`.

Reaction 2

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

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

3 In the **Formula** text field, type `Cl2++Cl-=>3Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5e-14*(300/Th)^0.5*N_A_const`.

Reaction 3

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

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

3 In the **Formula** text field, type `Cl2++Cl-=>Cl+Cl2`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5e-14[m^3/s]*N_A_const`.

Reaction 4

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

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

3 In the **Formula** text field, type `Cl++Cl-=>2Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5e-14*(300/Th)^0.5*N_A_const`.

Reaction 5

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

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

3 In the **Formula** text field, type `Cl2+Cl+=>Cl+Cl2+`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 6

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

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

3 In the **Formula** text field, type `Cl2v1+Cl+=>Cl+Cl2+`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 7

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

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

3 In the **Formula** text field, type `Cl2v2+Cl+=>Cl+Cl2+`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 8

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

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

3 In the **Formula** text field, type `Cl2v3+Cl+=>Cl+Cl2+`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `5.4e-16[m^3/s]*N_A_const`.

Reaction 9

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

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

3 In the **Formula** text field, type `2Cl+Cl2=>2Cl2`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `3.5e-45*exp(810/Th)*N_A_const`.

Reaction 10

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

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

3 In the **Formula** text field, type `2Cl+Cl=>Cl2+Cl`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `8.75e-46*exp(810/Th)*N_A_const`.

Reaction 11

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

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

3 In the **Formula** text field, type `Cl+Cl2v3=>Cl+Cl2v2`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1.3e-17*(Th/300)^0.5*N_A_const`.

Reaction 12

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

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

3 In the **Formula** text field, type `Cl+Cl2v2=>Cl+Cl2v1`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1.3e-17*(Th/300)^0.5*N_A_const`.

Reaction 13

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

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

3 In the **Formula** text field, type `Cl+Cl2v1=>Cl+Cl2`.

4 Locate the **Reaction Parameters** section. In the k^f text field, type `1.3e-17*(Th/300)^0.5*N_A_const`.

This model has two electron impact reactions of the elastic type: one with molecular Chlorine and another with atomic Chlorine.

These two reactions are defined using collision cross section data that needs to be imported from files.

Electron Impact Reaction 32

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl2=>e+Cl2`.

4 Locate the **Collision Type** section. In the m_r text field, type `7.720e-6`.

5 Locate the **Collision** section. From the **Specify reaction using** list, choose **Cross-section data**.

6 Locate the **Reaction Parameters** section. From the **Electron energy distribution function** list, choose **Maxwellian**.

7 Find the **Collision cross section data** subsection. Click **Load from File**.

8 Browse to the model's Application Libraries folder and double-click the file `Cl2_mom_xsec.txt`.

Electron Impact Reaction 33

1 In the **Physics** toolbar, click **Domains** and choose **Electron Impact Reaction**.

2 In the **Settings** window for **Electron Impact Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `e+Cl=>e+Cl`.

4 Locate the **Collision Type** section. In the m_r text field, type `1.510e-5`.

5 Locate the **Collision** section. From the **Specify reaction using** list, choose **Cross-section data**.

6 Locate the **Reaction Parameters** section. From the **Electron energy distribution function** list, choose **Maxwellian**.

7 Find the **Collision cross section data** subsection. Click **Load from File**.

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

In the species nodes (for heavy species) set the species data by choosing the atomic and molecular chlorine presets accordingly.

This information is used to compute the diffusion coefficients and the Bohm velocity that is used to estimate the surface losses of neutral species and positive ions, respectively.

Also for each species set the initial mole fraction (for neutrals) and the initial number density (for ions) in the reactor.

If the species is a neutral it is also possible to set the mole fraction of the total mass flow.

In this model the feed only contains molecular Chlorine so that the **Feed mole fraction** of Cl2 is set to 1.

Species: Cl2

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

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

3 Select the **From mass constraint** check box.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **Cl2**.

5 In the x_{feed} text field, type `1`.

Species: Cl

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

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

3 From the **Preset species data** list, choose **Cl**.

Species: Cl2+

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

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

3 From the **Preset species data** list, choose **Cl2**.

4 In the n_0 text field, type `1E16[1/m^3]`.

Species: Cl+

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

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

3 In the n_0 text field, type `1E14[1/m^3]`.

4 From the **Preset species data** list, choose **Cl**.

Species: Cl-

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

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

3 From the **Preset species data** list, choose **Cl**.

4 In the n_0 text field, type `1E14[1/m^3]`.

Species: Cl2v1

1 In the **Model Builder** window, click **Species: Cl2v1**.

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

3 From the **Preset species data** list, choose **Cl2**.

Species: Cl2v2

1 In the **Model Builder** window, click **Species: Cl2v2**.

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

3 From the **Preset species data** list, choose **Cl2**.

Species: Cl2v3

1 In the **Model Builder** window, click **Species: Cl2v3**.

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

3 From the **Preset species data** list, choose **Cl2**.

Species: Cl12

1 In the **Model Builder** window, click **Species: Cl12**.

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

3 From the **Preset species data** list, choose **Cl**.

Species: Cl52

1 In the **Model Builder** window, click **Species: Cl52**.

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

3 From the **Preset species data** list, choose **Cl**.

Add surface reactions to estimate the losses at the walls.

Neutral species are estimated to be lost with the same frequency at all boundaries. In Contrast, the surface losses of positive ions in this model are different at radial and longitudinal boundaries.

For each ion two surface reactions are created: one selects longitudinal boundaries and sets the longitudinal correction factor, the other select the radial boundary and sets the radial correction factor.

Surface Reaction 1

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

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

3 In the **Formula** text field, type `Cl2+=>Cl2`.

4 From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_1 text field, type `hRCl2`.

6 Select Boundary 4 only.

Surface Reaction 2

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

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

3 In the **Formula** text field, type `Cl=>0.5Cl2`.

4 From the **Specify reaction using** list, choose **Sticking coefficient and diffusion**.

5 Locate the **Reaction Parameters** section. In the γ_f text field, type `gammaCl_steel`.

6 In the Λ_{eff} text field, type `Lambda_diff`.

7 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

Surface Reaction 3

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

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

3 In the **Formula** text field, type `Cl+=>Cl`.

4 From the **Specify reaction using** list, choose **Bohm velocity**.

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

6 Select Boundary 4 only.

Surface Reaction 4

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

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

3 In the **Formula** text field, type `Cl2v1=>Cl2`.

4 From the **Specify reaction using** list, choose **Sticking coefficient and diffusion**.

5 Locate the **Reaction Parameters** section. In the Λ_{eff} text field, type `Lambda_diff`.

6 Locate the **Boundary Selection** section. From the **Selection** list, choose **All boundaries**.

5: Cl2v1=>Cl2

1 Right-click **4: Cl2v1=>Cl2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl2v2=>Cl2`.

6: Cl2v2=>Cl2

1 Right-click **5: Cl2v2=>Cl2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl2v3=>Cl2`.

7: Cl2v3=>Cl2

1 Right-click **6: Cl2v3=>Cl2** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl12=>Cl`.

8: Cl12=>Cl

1 Right-click **7: Cl12=>Cl** and choose **Duplicate**.

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

3 In the **Formula** text field, type `Cl52=>Cl`.

Surface Reaction 9

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

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

3 In the **Formula** text field, type `Cl2+=>Cl2`.

4 From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_l text field, type `hLCl2`.

6 Select Boundaries 2 and 3 only.

Surface Reaction 10

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

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

3 In the **Formula** text field, type `Cl+=>Cl`.

4 From the **Specify reaction using** list, choose **Bohm velocity**.

5 Locate the **Reaction Parameters** section. In the h_l text field, type `hLCl`.

6 Select Boundaries 2 and 3 only.

PLASMA (PLAS)

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

In the following create and run four separate studies that will do parametric sweeps.

The studies are labeled with the names of the authors that made the measurements.

Since each study needs a different set of parameters after the first study it is necessary to change some parameters such as the reactor radius and length, the absorbed power, and the total mass flow.

CORR POWER SWEEP

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

2 In the **Settings** window for **Study**, type `Corr power sweep` in the **Label** text field.

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

4 Clear the **Generate convergence plots** check box.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

Set the **Jacobian update** to **Minimal** to decrease the computational time.

3 In the **Model Builder** window, expand the **Corr power sweep>Solver Configurations> Solution 1 (sol1)>Time-Dependent 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 From the **Jacobian update** list, choose **Minimal**.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Corr power sweep** 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 `0 10^{range(-12,0.1,2)}`.

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
Pabs	25 50 100 200 300	W

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

CORR POWER SWEEP

In the **Model Builder** window, collapse the **Corr power sweep** node.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	18.5[cm]	0.185 m	
L	20[cm]	0.2 m	
Qfeed	100	100	

ADD STUDY

1 In the **Study** 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> Time Dependent**.

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

STUDY 2

Step 1: Time Dependent

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

2 In the **Output times** text field, type `0 10^{range(-12,0.1,2)}`.

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

4 In the **Settings** window for **Study**, type `Malyshev and Donnelly power sweep` in the **Label** text field.

5 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

6 Clear the **Generate convergence plots** check box.

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
Pabs	50 100 200 400 650	W

Solution 8 (sol8)

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

2 In the **Model Builder** window, expand the **Solution 8 (sol8)** node.

3 In the **Model Builder** window, expand the **Malyshev and Donnelly power sweep> Solver Configurations>Solution 8 (sol8)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, locate the **Method and Termination** section.

5 From the **Jacobian update** list, choose **Minimal**.

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

MALYSHEV AND DONNELLY POWER SWEEP

In the **Model Builder** window, collapse the **Malyshev and Donnelly power sweep** node.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	10[cm]	0.1 m	
L	8.5[cm]	0.085 m	
Pabs	300[W]	300 W	
Qfeed	10	10	

ADD STUDY

1 Go to the **Add Study** window.

2 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

3 Click **Add Study** in the window toolbar.

STUDY 3

Step 1: Time Dependent

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

2 In the **Output times** text field, type `0 10^{range(-12,0.1,2)}`.

3 In the **Model Builder** window, click **Study 3**.

4 In the **Settings** window for **Study**, type `Corr pressure sweep` in the **Label** text field.

5 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

6 Clear the **Generate convergence plots** check box.

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
p0	1e-3 2e-3 5e-3 10e-3 30e-3 100e-3	Torr

Solution 15 (sol15)

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

2 In the **Model Builder** window, expand the **Solution 15 (sol15)** node.

3 In the **Model Builder** window, expand the **Corr pressure sweep>Solver Configurations> Solution 15 (sol15)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, locate the **Method and Termination** section.

5 From the **Jacobian update** list, choose **Minimal**.

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

CORR PRESSURE SWEEP

In the **Model Builder** window, collapse the **Corr pressure sweep** node.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
Rad	15[cm]	0.15 m	
L	14[cm]	0.14 m	
Qfeed	20	20	

ADD STUDY

1 Go to the **Add Study** window.

2 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

3 Click **Add Study** in the window toolbar.

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

STUDY 4

Step 1: Time Dependent

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

2 In the **Output times** text field, type `0 10^{range(-12,0.1,2)}`.

3 In the **Model Builder** window, click **Study 4**.

4 In the **Settings** window for **Study**, type `Efremov pressure sweep` in the **Label** text field.

5 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

6 Clear the **Generate convergence plots** check box.

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
p0	`1e-3 2e-3 5e-3 10e-3 30e-3 100e-3`	`Torr`

Solution 23 (sol23)

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

2 In the **Model Builder** window, expand the **Solution 23 (sol23)** node.

3 In the **Model Builder** window, expand the **Efremov pressure sweep>Solver Configurations> Solution 23 (sol23)>Time-Dependent Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, locate the **Method and Termination** section.

5 From the **Jacobian update** list, choose **Minimal**.

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

EFREMOV PRESSURE SWEEP

1 In the **Model Builder** window, collapse the **Efremov pressure sweep** node.

Create 4 plots that show the results from the previous simulations. Each plot is labeled with the name of the authors that performed the measurements.

First create a plot with the data from the Corr study that shows the electron density, the atomic chlorine density, and the electronegativity as a function of the absorbed power.

RESULTS

Corr power sweep

1 In the **Home** toolbar, click  **Add Plot Group** and choose **1D Plot Group**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Corr power sweep/ Parametric Solutions 1 (sol2)**.

4 From the **Time selection** list, choose **Last**.

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

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** check box. In the associated text field, type `Power absorbed (W)`.

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

9 Select the **Two y-axes** check box.

10 Select the **Secondary y-axis label** check box. In the associated text field, type `n-/ne`.

11 Locate the **Axis** section. Select the **Manual axis limits** check box.

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

13 In the **x maximum** text field, type `325`.

14 In the **y minimum** text field, type `1e14`.

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

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

17 In the **Secondary y maximum** text field, type `20`.

18 Select the **y-axis log scale** check box.

Global 1

1 Right-click **Corr power sweep** 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_wCl	1/m^3	Number density
plas.ne	1/m^3	Electron density

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Pabs**.

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

6 In the table, enter the following settings:

Legends
Cl
ne

Global 2

1 In the **Model Builder** window, right-click **Corr power sweep** and choose **Global**.

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

3 Select the **Plot on secondary y-axis** check box.

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

Expression	Unit	Description
alpha	1	

5 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Pabs**.

6 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
n-/ne

8 In the **Corr power sweep** toolbar, click **Plot**.

Create a second plot with the data from the Malyshev and Donnelly study that shows the electron density, and the atomic chlorine density as a function of the absorbed power.

Malyshev and Donnelly power sweep

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type Malyshev and Donnelly power sweep in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Malyshev and Donnelly power sweep/Parametric Solutions 2 (sol9)**.

4 From the **Time selection** list, choose **Last**.

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

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** check box. In the associated text field, type `Power absorbed (W)`.

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

9 Locate the **Axis** section. Select the **Manual axis limits** check box.

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

11 In the **x maximum** text field, type `700`.

12 In the **y minimum** text field, type `1e15`.

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

14 Select the **y-axis log scale** check box.

Global 1

1 Right-click **Malyshev and Donnelly power sweep** 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_wCl`	`1/m^3`	`Number density`
`plas.ne`	`1/m^3`	`Electron density`

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Pabs**.

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Cl`
`ne`

7 In the **Malyshev and Donnelly power sweep** toolbar, click  **Plot**.

Corr and Efremov pressure sweep

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

Create a third plot with the data from the Corr and Efremov studies that shows the electron density, and the atomic chlorine density as a function of the pressure.

2 In the **Settings** window for **1D Plot Group**, type `Corr and Efremov pressure sweep` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

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

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `Pressure (Torr)`.

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

8 Locate the **Axis** section. Select the **Manual axis limits** check box.

9 In the **x minimum** text field, type `8e-4`.

10 In the **x maximum** text field, type `125e-3`.

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

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

13 Select the **x-axis log scale** check box.

14 Select the **y-axis log scale** check box.

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

Global 1

1 Right-click **Corr and Efremov pressure sweep** and choose **Global**.

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

3 From the **Dataset** list, choose **Corr pressure sweep/Parametric Solutions 3 (sol16)**.

4 From the **Time selection** list, choose **Last**.

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

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

6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **p0**.

7 From the **Parameter** list, choose **Expression**.

8 In the **Expression** text field, type `p0`.

9 From the **Unit** list, choose **Torr**.

10 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
Cl

Global 2

1 In the **Model Builder** window, right-click **Corr and Efremov pressure sweep** and choose **Global**.

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

3 From the **Dataset** list, choose **Efremov pressure sweep/Parametric Solutions 4 (sol24)**.

4 From the **Time selection** list, choose **Last**.

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

Expression	Unit	Description
plas.ne	1/m^3	Electron density

6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **p0**.

7 From the **Parameter** list, choose **Expression**.

8 In the **Expression** text field, type p0.

9 From the **Unit** list, choose **Torr**.

10 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
ne

12 In the **Corr and Efremov pressure sweep** toolbar, click **Plot**.

Efremov pressure sweep

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

Create the fourth and last plot with the data from the Efremov study that shows the electron temperature as a function of the pressure.

2 In the **Settings** window for **1D Plot Group**, type Efremov pressure sweep in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Efremov pressure sweep/ Parametric Solutions 4 (sol24)**.

4 From the **Time selection** list, choose **Last**.

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

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** check box. In the associated text field, type `Pressure (Torr)`.

8 Select the **y-axis label** check box. In the associated text field, type `Te (V)`.

9 Locate the **Axis** section. Select the **Manual axis limits** check box.

10 In the **x minimum** text field, type `8e-4`.

11 In the **x maximum** text field, type `125e-3`.

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

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

14 Select the **x-axis log scale** check box.

15 Locate the **Legend** section. Clear the **Show legends** check box.

Global 1

1 Right-click **Efremov pressure sweep** 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 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **p0**.

5 From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `p0`.

7 From the **Unit** list, choose **Torr**.

8 In the **Efremov pressure sweep** toolbar, click  **Plot**.