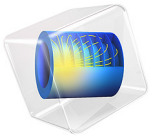

Model created in COMSOL Multiphysics 6.4

Hydrogen Global Model Coupled with the Two-Term Boltzmann Equation

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Introduction

This tutorial studies the chemistry of a hydrogen plasma in moderate pressures. The main goals are to show how to prepare a global model to study a chemistry and study the influence of the electron energy distribution function (EEDF). This are important steps that need to be done before moving to a space dependent model.

In this model, it is shown how to solve a plasma global model fully self-consistently with the Boltzmann equation in the two-term approximation.

The chemistry and model here presented are based on the work from Ref. 1 and Ref. 2. The results are in general good agreement with the ones from Ref. 1. However, a detailed comparison is not attempted since the models and chemistry have important differences. The reference used for the plasma chemistry and the chemistry here is closer to the simplified chemistry presented in Ref. 2 which does not include negative ions. Regarding the model, the main differences are that the model used here: (i) does not compute the vibrational temperature or solve for the vibrational states, and (ii) solves for the electron mean energy equation which uses power as an input.

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

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

where ρ is the mass density (SI unit: kg/m^3), w_k is the mass fraction, $w_{f,k}$ is the mass fraction in the feed, m_f and m_o are the mass-flow rates of the total feed and outlet, and R_k is the rate expression (SI unit: kg/(m^3·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's total mass or pressure into account, the mass-continuity equation can also be solved:

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

The electron number density is obtained from electroneutrality:

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

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

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

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

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

solver; (ii) if the LFA is used, the reduced electric field must be given as input to the Boltzmann solver and the electron mean energy comes from averaging over the computed EEDF.

This work uses the LEA. The first part uses a Maxwellian EEDF and the subsequent part solves the Boltzmann equation in the two-term approximation (B2T).

Coupling the B2T with a space-dependent model is computationally very expensive. Therefore, it is recommended to first explore the influence of the EEDF using a global (volume-averaged) model, since it can run simulations in a fraction of the time of a space-dependent model while retaining the tendencies of volume-averaged physical quantities.

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 (SI unit: W/m^3) is given as:

$$Q = -V \sum_j H_j r_j + V \sum_j \Delta\varepsilon_j F r_j$$

where $\Delta\varepsilon_j$ is the electron energy loss from reaction j (SI unit: V) and F is the Faraday constant (SI unit: C/mol). The last term in the equation above is only added for electron impact reactions to account for the energy loss or gain by the electron. Note that the electron enthalpy is set to zero and does not contribute to H_j. For electron impact reactions resulting in excitation and ionization $\Delta\varepsilon_j$ corresponds to the energy of the excited state being excited/deexcited or ionized, for attachment $\Delta\varepsilon_j$ is set to zero, and for elastic collisions

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

where m_e and m_k are the electron and heavy species mass in kg, T_e is the electron temperature in eV, and T_{gas} is the gas temperature in K. 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 the simplified chemistry presented in table 4 of Ref. 2 and is presented in Table 1. The electron impact cross sections are from Ref. 4 and were retrieved from Ref. 5, and the rates are from Ref. 6 and Ref. 7. The model includes eight species: electrons, H_2, H, H_2^+, H^+, H_3^+, and two excited states of hydrogen corresponding to the levels $n = 2$ and $n = 3$ that are represented by Hn2 and Hn3.

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

Reaction	Formula	Type	$\Delta\varepsilon$(eV)
1	e+H2=>e+H2	Elastic	-
2	e+H2=>e+H2	Vibrational excitation	0.516-1.5
3	e+H2=>e+2H	Dissociation	7.93-11.72 and17.22-17.53
4	e+H2=>e+H2	Excitation	12.4-14.6
5	e+H2=>e+H+Hn2	Dissociative excitation	14.68
6	e+H2=>e+H+Hn3	Dissociative excitation	16.57
7	e+H2=>2e+H2+	Ionization	15.4
8	e+H2=>2e+H+H+	Ionization	19
9	e+H=>e+H	Elastic	-
10	e+H=>e+Hn2	Excitation	10.2043
11	e+H=>e+Hn3	Charge transfer	12.1
12	e+H=>e+H	Excitation	12.755 and 13.0615
13	e+H=>2e+H+	Ionization	13.6057
14	e+H3+=>3H	Recombination	0
15	e+H2+=>H+Hn2	Recombination	0.01
16	e+H2+=>H+Hn3	Recombination	0.01
17	e+H+=>Hn2	Recombination	0
18	e+H+=>Hn3	Recombination	0
19	Hn2+H2=>H3++e	Ionization	-
20	Hn3+H2=>H3++e	Ionization	-
21	H2+H2+=>H3++H	Ionization	-
22	H2+H2=>2H+H2	Dissociation	-
23	2H+H2=>H2+H2	Association	-

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

Reaction	Formula	Type	$\Delta\varepsilon$(eV)
24	H2+H=>3H	Dissociation	-
26	3H=>H2+H	Association	-

In addition to the volume reactions, the surface reaction listed in Table 2 are also implemented.

TABLE 2: SURFACE REACTIONS.

Reaction	Formula	Sticking coefficient
1	H=>0.5H2	0.02
2	Hn2=>H	1
3	Hn3=>H	1
4	H+=>H	1
5	H2+=>H2	1
6	H3+=>H2+H	1

Results and Discussion

In Ref. 1, a key parameter in the experiments is the power density that is estimated from the volume of the plasma and the input power. In the global model presented here, the volume needs to be fixed and the parameterization is made over power, which is an input to the electron mean energy equation. The dimensions of the domain were found to match the values of the power density given in table 1 of Ref. 1. These dimensions are used to estimate losses by transport and the plasma volume. However, if the dimensions that are used to estimate the diffusion length are used also to estimate the heat losses by transport the temperature obtained is too low. This makes sense since the region that the plasma occupies is smaller than the reactor chamber Ref. 2. When using dimensions closer to a typical reactor chamber (from Ref. 2) to estimate the heat losses by transport, the gas temperature is in good agreement with Ref. 1.

When making the parameterization in power note that the pressure varies according to table 1 of Ref. 1.

Figure 1 shows the computed EEDFS for the different power densities under study. The EEDFS are similar to the ones obtained in Ref. 1 and present the same behavior that the high-energy tail decreases with increasing power density. Present in Figure 1 is also a

Maxwellian EEDF corresponding to the last power density. As can be seen, the computed EEDF deviates strongly from a Maxwellian. However, quantities such as the gas temperature, electron temperature, electron density, H mole fraction, and neutral number densities do not change significantly, as shown in figures Figure 2 through Figure 5.

Figure 2 shows the gas temperature and the H mole fraction as a function of the power density. These results are in good agreement with the results presented in figure 18 of Ref. 1.

The ion number densities presented in Figure 3 also agree well with results in figure 11 of Ref. 1, the dominant ion being H_3^+ with densities between 10^{11} and 10^{12} cm^{-3} and H_2^+ being the ion with lowest density.

Figure 6 shows the relative rates of the main ionization mechanisms. The dominating ionization mechanism is the collision quenching of H-excited states that creates H_3^+. Electron impact ionization of H_2 has some importance at low powers but its relative contribution decreases fast with power. Ionization from H atoms plays a minor role. The results are in agreement with those in figure 12(a) of Ref. 1.

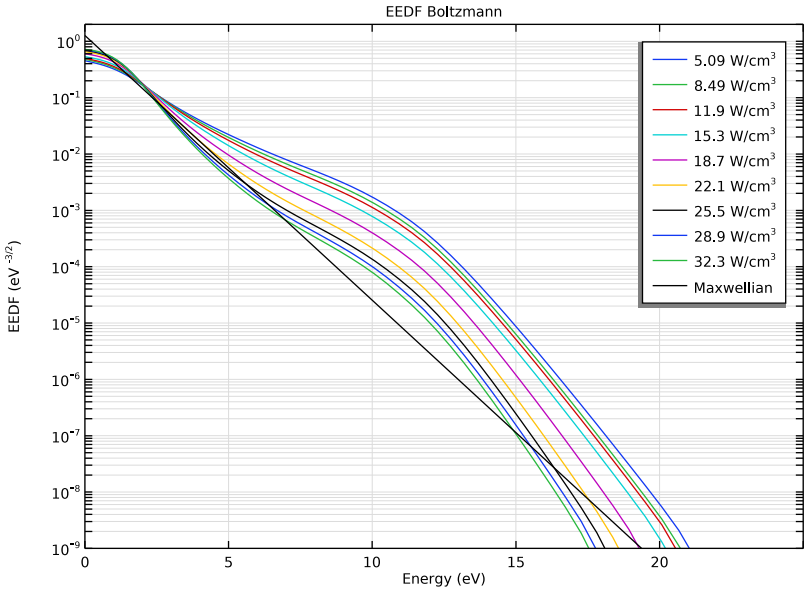

Figure 1: Computed EEDF for different power densities and a Maxwellian EEDF corresponding to the highest power density.

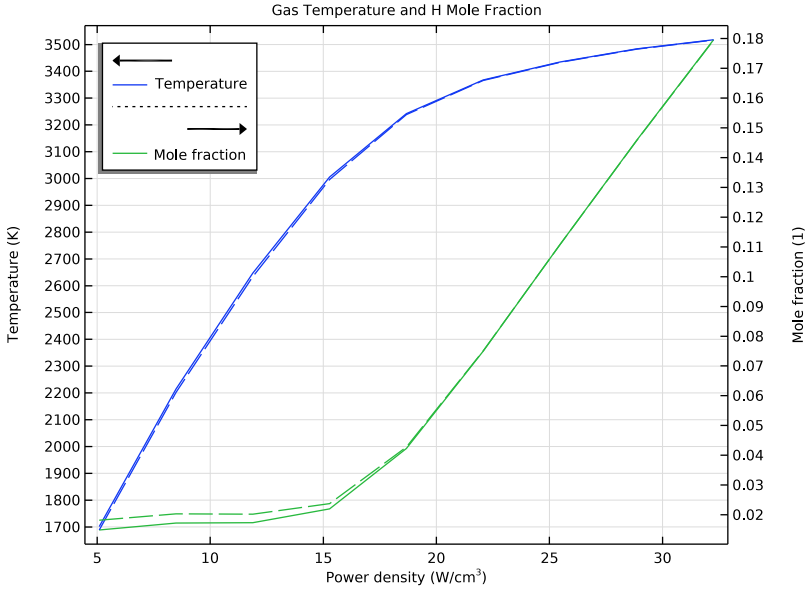

Figure 2: Gas temperature and H atom mole fraction as a function of the power density using a Maxwellian EEDF (solid) and solving for the B2T(dashed).

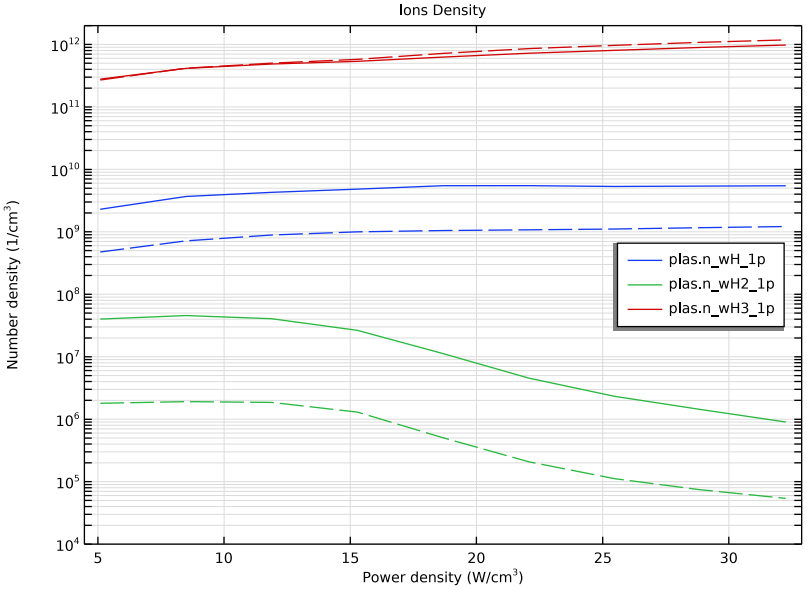

Figure 3: Ion number densities as a function of the power density using a Maxwellian EEDF (solid) and solving for the B2T (dashed).

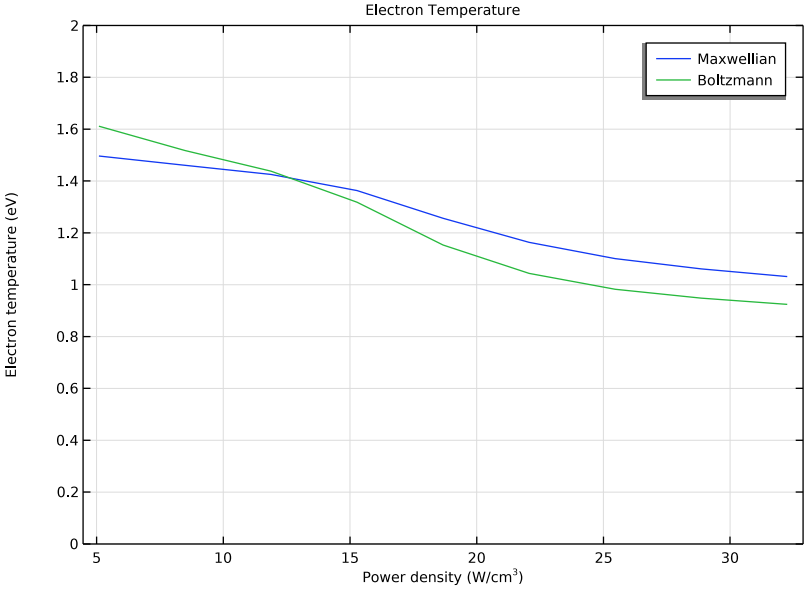

Figure 4: Electron temperature as a function of the power density using a Maxwellian EEDF (solid) and solving for the B2T(dashed).

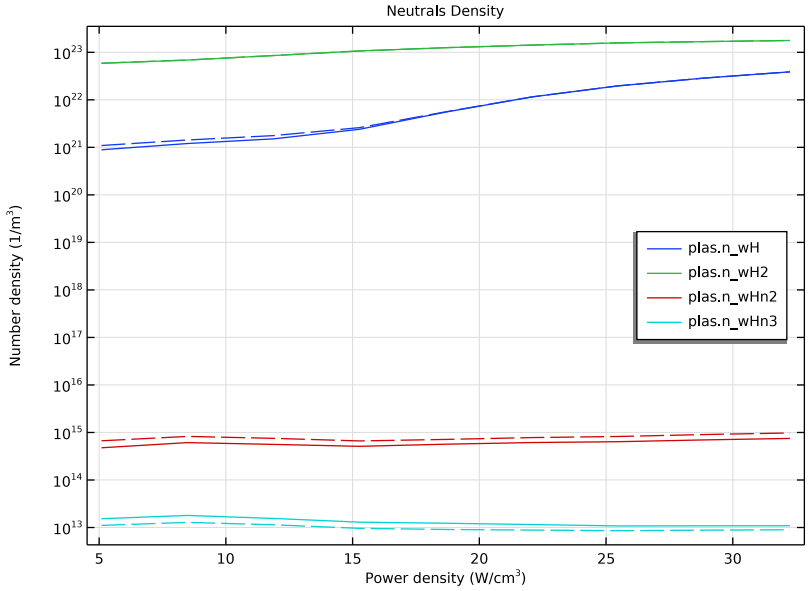

Figure 5: Neutrals number density as a function of the power density using a Maxwellian EEDF (solid) and solving for the B2T(dashed).

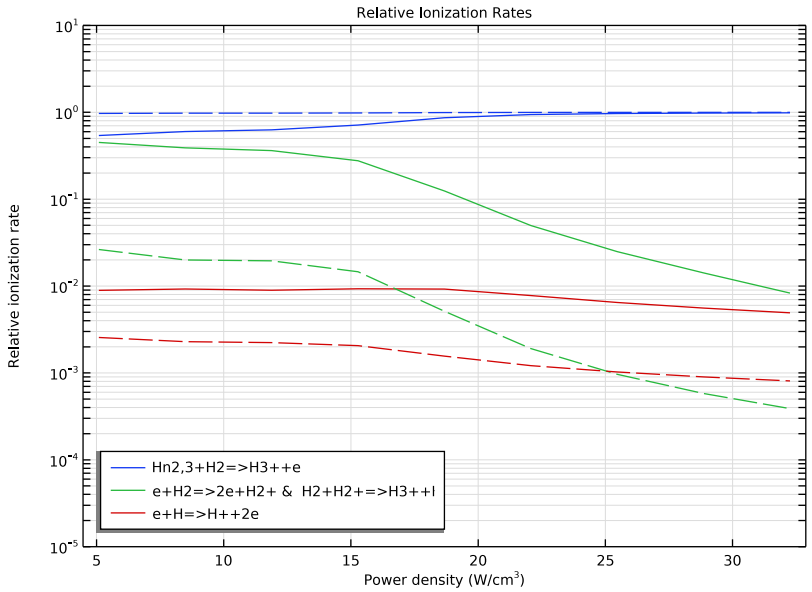

Figure 6: Relative ionization rates as a function of the power density using a Maxwellian EEDF (solid) and solving for the B2T(dashed).

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6. M. Capitelli, C.M. Ferreira, B.F. Gordiets and A.I. Osipov, *Plasma Kinetics in Atmospheric Gases*, Springer, 2000.

7. R.K. Janev, W.D. Langer, K. Evans, Jr. and D.E. Post, Jr. *Elementary Processes in Hydrogen-Helium Plasmas*, Springer-Verlag, 1987.

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

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**.

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
W	2.5[cm]	0.025 m	Plasma width
H	3[cm]	0.03 m	Plasma height
Wg	5[cm]	0.05 m	Width for heat
Hg	6[cm]	0.06 m	Height for heat
p0	5[kPa]	5000 Pa	Pressure
pw	300[W]	300 W	Power
Qs	500	500	Mass flow
pd	pw/Vol	5.093E6 W/m³	Power density
Vol	(pi*W^2*H)	5.8905E-5 m³	Plasma volume
f0	2.45e9[Hz]	2.45E9 Hz	Excitation frequency
w0	f0*2*pi	1.5394E10 Hz	Angular frequency
hl_ions	0.05	0.05	Correction factor for ions

DEFINITIONS

Variables 1

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

Define variables for diffusion lengths.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
Lamb_diff	((pi/H)^2+(2.405/W)^2)^-0.5	m	Diffusion length for species
Lamb_diff_heat	((pi/Hg)^2+(2.405/Wg)^2)^-0.5	m	Diffusion length for heat

Interpolation 1 (int1)

1 In the **Definitions** toolbar, click **Interpolation**.

Define an interpolation function that gives the pressure as a function of power. This function is used to set the pressure of the reactor.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the **Function name** text field, type pfnc.

4 In the table, enter the following settings:

t	f(t)
300	1400
600	2500
1000	5200
1500	8400
2000	11000

5 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

6 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
pfnc	Pa

7 In the **Argument** table, enter the following settings:

Argument	Unit
t	W

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

GEOMETRY 1

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 W.

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

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

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

Plasma Model 1

Set the pressure (using the interpolation function previously defined), mass flow, power absorbed by the electrons, an estimation of the plasma sheath voltage drop (for the mean kinetic energy lost per ion lost), 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 p_A text field, type `pfnc(pw)`.

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

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

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

7 Locate the **Heat Transfer to Surfaces** section. In the Λ_S text field, type `Lamb_diff_heat`.

THE PLASMA CHEMISTRY IMPORT FEATURE

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

The following is set or created automatically:

a Species properties

b Reaction group features for hydrogen

c Surface reactions

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

Plasma Chemistry Import 1

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

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

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `H2_plasma_chemistry.txt`.

5 Click **Import**.

Set some properties of the species and the surface reactions.

Set H2 to be the species that the mass fraction is found from mass constraint.

Species: H2

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Plasma (plas)** > **Group - Species** node, then click **Species: H2**.

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`.

Group - Species

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

Set different aspects of surface reactions: diffusion length, recombination of H 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: H=>0.5H2

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Plasma (plas)** > **Group - Surface Reactions** node, then click **1: H=>0.5H2**.

2 Select Boundary 2 only.

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

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 `Lamb_diff`.

2: Hn2=>H

1 In the **Model Builder** window, click **2: Hn2=>H**.

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 **Sticking coefficient and diffusion**.

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

3: Hn3=>H

1 In the **Model Builder** window, click **3: Hn3=>H**.

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 **Sticking coefficient and diffusion**.

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

4: H+=>H

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

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_l text field, type `hl_ions`.

5: H2+=>H2

1 In the **Model Builder** window, click **5: H2+=>H2**.

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_l text field, type `hl_ions`.

6: H3+=>H2+H

1 In the **Model Builder** window, click **6: H3+=>H2+H**.

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_l text field, type `hl_ions`.

Group - Surface Reactions

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

MESH 1

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

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

3 From the **Element size** list, choose **Extremely coarse**.

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

STUDY 1

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

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

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

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** checkbox.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
pw (Power)	`range(300,200,2000)`	`W`

6 From the **Run continuation for** list, choose **No parameter**.

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

8 In the **Study** toolbar, click = **Compute**.

In the following create plots for the gas temperature, H mole fraction, electron temperature, ion densities, neutral densities, and relative ionization rates.

RESULTS

Gas Temperature and H Mole Fraction

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

2 In the **Settings** window for **1D Plot Group**, type `Gas Temperature and H Mole Fraction` in the **Label** text field.

Global 1

1 Right-click **Gas Temperature and H Mole Fraction** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.T	K	Temperature

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

5 In the **Expression** text field, type `pw/plas.Vol_gm`.

6 In the **Unit** field, type `W/cm^3`.

Global 2

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

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.x_wH	1	Mole fraction

Gas Temperature and H Mole Fraction

1 In the **Model Builder** window, click **Gas Temperature and H Mole Fraction**.

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Power density (W/cm<sup>3</sup>)`.

6 Select the **Two y-axes** checkbox.

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

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

Ions Density

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

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

Global 1

1 Right-click **Ions Density** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wH_1p	1/cm^3	Number density
plas.n_wH2_1p	1/cm^3	Number density
plas.n_wH3_1p	1/cm^3	Number density

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

5 In the **Expression** text field, type pw/plas.Vol_gm.

6 In the **Unit** field, type W/cm^3.

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

8 Select the **Expression** checkbox.

9 In the **Ions Density** toolbar, click **Plot**.

Ions Density

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

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type Power density (W/cm³).

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

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

8 In the **y minimum** text field, type 1e4.

9 In the **y maximum** text field, type 2e12.

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

Electron Temperature

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

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

Global 1

1 Right-click **Electron Temperature** 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	Maxwellian

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

5 In the **Expression** text field, type `pw/plas.Vol_gm`.

6 In the **Unit** field, type `W/cm^3`.

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

Electron Temperature

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

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Power density (W/cm<sup>3</sup>)`.

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

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

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

9 In the **y maximum** text field, type `2`.

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

Neutrals Density

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

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

Global 1

1 Right-click **Neutrals Density** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
plas.n_wH	1/m^3	Number density
plas.n_wH2	1/m^3	Number density

Expression	Unit	Description
plas.n_wHn2	1/m^3	Number density
plas.n_wHn3	1/m^3	Number density

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

5 In the **Expression** text field, type `pw/plas.Vol_gm`.

6 In the **Unit** field, type `W/cm^3`.

7 Locate the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

8 Select the **Expression** checkbox.

9 In the **Neutrals Density** toolbar, click **Plot**.

Neutrals Density

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

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Power density (W/cm<sup>3</sup>)`.

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

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

Relative Ionization Rates

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

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

Global 1

1 Right-click **Relative Ionization Rates** 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.r_rg3_1+plas.r_rg3_2)/ (plas.r_rg3_1+plas.r_rg3_2+ plas.r_rg3_3+plas.r_rg2_21+ plas.r_rg1_7)`	1	`Hn2,3+H2=>H3++e`
`(plas.r_rg3_3+ plas.r_rg2_21)/ (plas.r_rg3_1+plas.r_rg3_2+ plas.r_rg3_3+plas.r_rg2_21+ plas.r_rg1_7)`	1	`e+H2=>2e+H2+ &  H2+H2+=>H3++H`
`plas.r_rg1_7/(plas.r_rg3_1+ plas.r_rg3_2+plas.r_rg3_3+ plas.r_rg2_21+plas.r_rg1_7)`	1	`e+H=>H++2e`

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

5 In the **Expression** text field, type `pw/plas.Vol_gm`.

6 In the **Unit** field, type `W/cm^3`.

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

8 In the **Relative Ionization Rates** toolbar, click **Plot**.

Relative Ionization Rates

1 In the **Model Builder** window, click **Relative Ionization Rates**.

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Power density (W/cm<sup>3</sup>)`.

6 Select the **y-axis label** checkbox. In the associated text field, type `Relative ionization rate`.

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

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

9 In the **y minimum** text field, type `1e-5`.

10 In the **y maximum** text field, type `10`.

11 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

In the next part of this example the global model is solved self-consistently with the Boltzmann equation in the two-term approximation.

Choose to solve the Boltzmann equation in the two-term approximation in the HF limit and set the reduced angular frequency. Reduce the maximum energy of the EEDF domain (this value is found from trial-and-error and verifying that the high energy region of the EEDF is weekly populated for values larger than 50 eV).

Before solving the global model and the Boltzmann equation it is necessary to obtain initial conditions for the EEDF. This is done with the **EEDF Initialization** study that only solves for the EEDF. This solution is used as initial condition to a subsequent study.

PLASMA (PLAS)

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

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

3 In the **Settings** window for **Plasma**, locate the **Electron Energy Distribution Function Settings** section.

4 From the **Electron energy distribution function** list, choose **Boltzmann equation, two-term approximation (linear)**.

5 Select the **Oscillating field** checkbox.

6 In the ω/N text field, type `w0/plas.Nn`.

7 In the ε_{max} text field, type `50[V]`.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **EEDF Initialization**.

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

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

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

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

STUDY 2

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

RESULTS

EEDF Initialization

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

The next study solves the global and the Boltzmann equation in the two-term approximation fully coupled. The power is parameterized from 300 to 2000 W. The EEDF previously computed is used as initial conditions.

STUDY 3

Step 1: Stationary

1. In the **Model Builder** window, under **Study 3** 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 2, EEDF Initialization**.
6. Locate 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
pw (Power)	`range(300,200,2000)`	`W`

9. From the **Run continuation for** list, choose **No parameter**.
10. From the **Reuse solution from previous step** list, choose **Yes**.
11. In the **Model Builder** window, click **Study 3**.
12. In the **Settings** window for **Study**, locate the **Study Settings** section.
13. Clear the **Generate default plots** checkbox.
14. In the **Study** toolbar, click **Compute**.
15. In the **Label** text field, type `Boltzmann EEDF`.
16. In the **Model Builder** window, collapse the **Boltzmann EEDF** node.

INITIALIZATION EEDF

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

2 In the **Settings** window for **Study**, type `Initialization EEDF` in the **Label** text field.

MAXWELLIAN EEDF

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

2 In the **Settings** window for **Study**, type `Maxwellian EEDF` in the **Label** text field.

3 In the **Model Builder** window, collapse the **Maxwellian EEDF** node.

INITIALIZATION EEDF

In the **Model Builder** window, collapse the **Initialization EEDF** node.

In the same plots prepared before add the results when solving for the EEDF.

RESULTS

Global 3

1 In the **Model Builder** window, under **Results** > **Gas Temperature and H Mole Fraction** right-click **Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (sol3)**.

4 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Cycle (reset)**.

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

Global 4

1 In the **Model Builder** window, under **Results** > **Gas Temperature and H Mole Fraction** right-click **Global 2** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (sol3)**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

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

Global 2

1 In the **Model Builder** window, under **Results** > **Ions Density** right-click **Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (sol3)**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Cycle (reset)**.

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

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

Global 2

1 In the **Model Builder** window, under **Results** > **Electron Temperature** right-click **Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (sol3)**.

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

Expression	Unit	Description
`plas.Te`	`V`	`Boltzmann`

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

Global 2

1 In the **Model Builder** window, under **Results** > **Neutrals Density** right-click **Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (sol3)**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Cycle (reset)**.

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

Global 2

1 In the **Model Builder** window, under **Results** > **Relative Ionization Rates** right-click **Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (sol3)**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Cycle (reset)**.

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

Prepare a plot to show the computed EEDF for the different applied powers.

Boltzmann EEDF/Solution 3 (5) (sol3)

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

2 Right-click **Results** > **Datasets** > **Boltzmann EEDF/Solution 3 (sol3)** and choose **Duplicate**.

3 In the **Settings** window for **Solution**, locate the **Solution** section.

4 From the **Component** list, choose **Extra Dimension from Plasma (plas_eedf_xdim)**.

EEDF Boltzmann

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

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (5) (sol3)**.

4 In the **Label** text field, type `EEDF Boltzmann`.

Line Graph 1

1 Right-click **EEDF Boltzmann** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.fcap`.

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

6 In the **Expression** text field, type `plas.xeedf`.

7 Click to expand the **Legends** section. Select the **Show legends** checkbox.

8 From the **Legends** list, choose **Evaluated**.

9 In the **Legend** text field, type `eval(plas.Pgm/plas.Vol_gm, W/cm^3) W/cm<sup> 3</sup>`.

10 In the **EEDF Boltzmann** toolbar, click **Plot**.

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Boltzmann EEDF/Solution 3 (5) (sol3)**.

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

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `plas.fmax`.

6 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Black**.

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

8 In the table, enter the following settings:

Legends
Maxwellian

EEDF Boltzmann

1 In the **Model Builder** window, click **EEDF Boltzmann**.

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Energy (eV)`.

6 Select the **y-axis label** checkbox. In the associated text field, type `EEDF (eV <sup>-3/2</sup>)`.

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

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

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

10 In the **x maximum** text field, type `25`.

11 In the **y minimum** text field, type `1e-9`.

12 In the **y maximum** text field, type `2`.

13 In the **EEDF Boltzmann** toolbar, click  **Plot**.