Argon Boltzmann Analysis

Introduction

The electron energy distribution function (EEDF) plays an important role in the overall behavior of discharges. Analytic forms of the EEDF exist such as Maxwellian or Druyvesteyn, but in some cases they fail to fit the discharge physics. Factors such as ionization degree (n_e/N), mole fraction of excited species, and reduced angular frequency of the electromagnetic field can all influence the shape of the EEDF. This can lead to differences in the magnitude of electron impact rate coefficients which are in turn used in a fluid model for the electron density and mean electron energy. This tutorial example shows how these factors influence the EEDF and the rate coefficients for argon.

Model Definition

This model is based on the results obtained in Ref 1. In this model, the x-coordinate represents electron energy, ε (eV), rather than physical space. First a set of electron impact collision cross sections are read from a file. The first time the model is solved, the EEDF is assumed to be Maxwellian:

$$f(\varepsilon) = \varphi^{-3/2}\beta_1 \exp(-(\varepsilon\beta_2/\varphi)) \tag{1}$$

where

$$\beta_1 = \Gamma(5/2)^{3/2}\Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2)\Gamma(3/2)^{-1} \tag{2}$$

Subsequently, the Two-term Boltzmann equation is solved which computes the EEDF rather than assuming a specific form. The Two-term Boltzmann equation is:

$$\frac{\partial}{\partial\varepsilon}\left(Wf - D\frac{\partial f}{\partial\varepsilon}\right) = S \tag{3}$$

where f is the EEDF ($\mathrm{eV}^{-3/2}$) and

$$W = -\gamma\varepsilon^2\sigma_\varepsilon - 3a\left(\frac{n_e}{N_n}\right)A_1 \tag{4}$$

and

$$D = \frac{\gamma}{3}\left(\frac{E}{N_n}\right)^2\left(\frac{\varepsilon}{\sigma_m}\right) + \frac{\gamma k_b T}{q}\varepsilon^2\sigma_\varepsilon + 2a\left(\frac{n_e}{N_n}\right)(A_2 + \varepsilon^{3/2}A_3) \quad (5)$$

For definitions of the quantities in the equations Equation 4 and Equation 5, see the chapter The Boltzmann Equation, Two-Term Approximation Interface in the *Plasma Module User's Guide*.

At zero energy, the condition that energy flux is zero must hold:

$$\mathbf{n} \cdot \left(Wf - D\frac{\partial f}{\partial \varepsilon}\right) = 0 \quad (6)$$

and as $\varepsilon \to \infty, f \to 0$. In practice, this boundary condition is applied by setting f to zero for a suitably large ε. The default maximum ε is 100 eV by default.

Results and Discussion

Solving the Boltzmann equation allows various conditions for ionization degree, mole fraction of excited species and reduced angular frequencies to be tested.

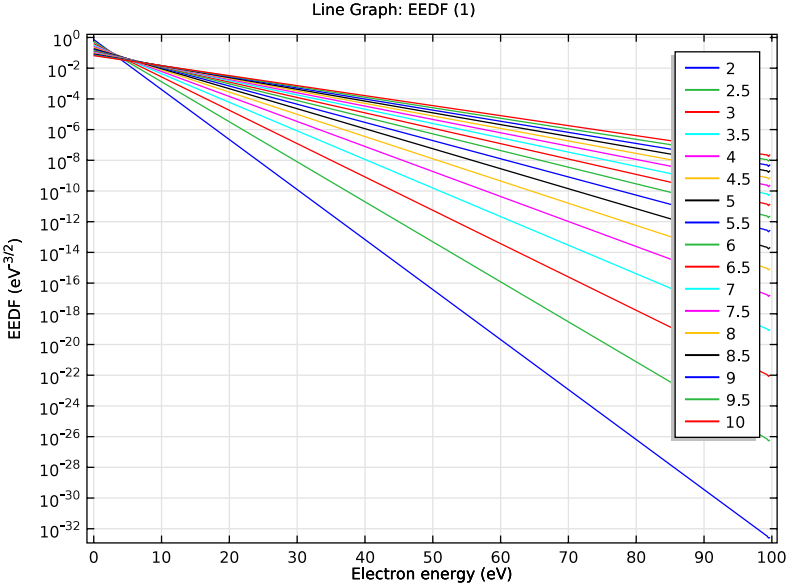

Figure 1: Maxwellian EEDF for a range of different mean electron energies.

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Figure 1 shows the distribution function assuming Maxwellian. Electron-electron collisions tend to make the shape of the EEDF closer to a Maxwellian distribution. The influence of different degrees of ionization is shown in Figure 2.

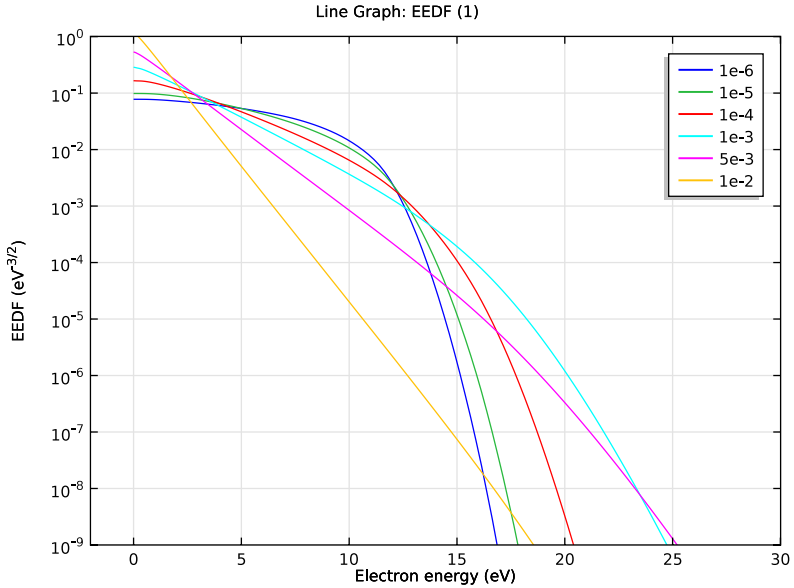

Figure 2: EEDF in argon for an applied reduced electric field of 10 Td for different degrees of ionization.

As the ionization degree increases, the EEDF tends to become more Maxwellian (which would be represented by a linear line on a log scale). The electron-electron collisions tend to push the electrons at the tail to higher energies, which will have an effect on the rate coefficients for electron impact reactions with a high activation energy.

The effect on the rate coefficients can be seen in Figure 3. The ionization rate coefficient is substantially higher at a given mean electron energy when the ionization degree is higher.

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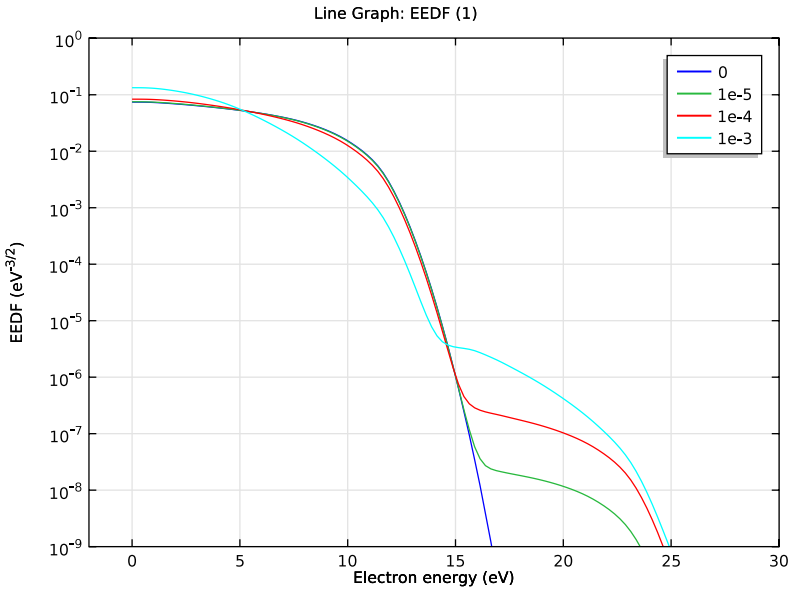

Figure 3: Plot of ionization rate coefficient versus mean electron energy for different ionization degrees.

If the mole fraction of electronically excited species is non zero then superelastic collisions can influence the shape of the EEDF. Figure 4 plots the EEDF for different mole fractions of electronically excited argon. The superelastic collisions leads to a high energy tail in the distribution function. This results in an increase in the magnitude of the ionization rate coefficients.

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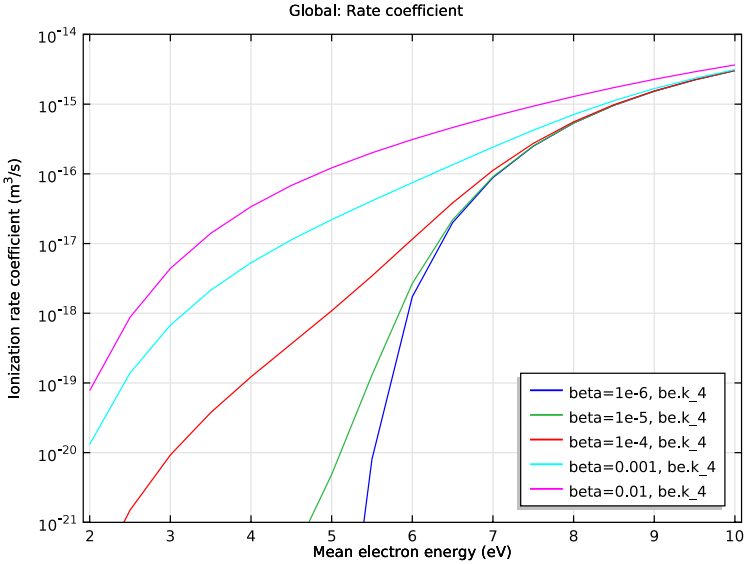

Figure 4: EEDF for argon at a reduced electric field of 10 Td for different mole fractions of electronically excited argon.

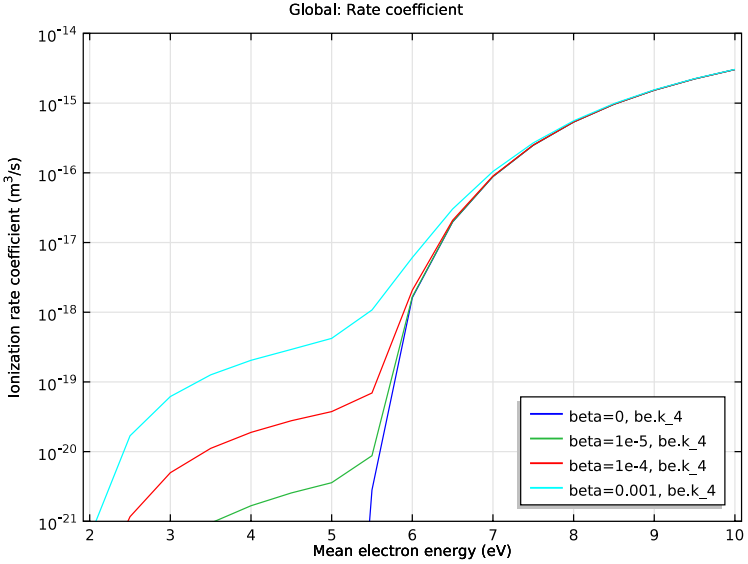

Figure 5: Ionization rate coefficient for different mole fractions of electronically excited argon.

Finally, the influence of a high frequency oscillating field on the EEDF is studied by applying different reduced angular frequencies. The EEDF is plotted in Figure 6.

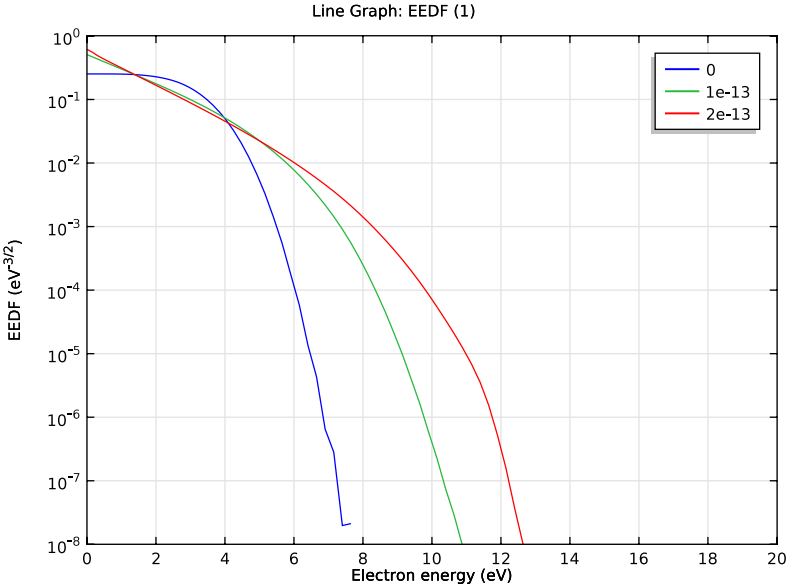

Figure 6: Plot of EEDF for different reduced angular frequencies for the same mean electron energy.

Reference

1. G.J.M. Hagelaar and L.C. Pitchford, "Solving the Boltzmann Equation to Obtain Electron Transport Coefficients and Rate Coefficients for Fluid Models," *Plasma Sources Science and Technology*, vol. 14, pp. 722–733, 2005.

Model Library path: `Plasma_Module/Two-term_Boltzmann_Equation/boltzmann_argon`

Modeling Instructions

MODEL WIZARD

1 Go to the **Model Wizard** window.

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2 Click the **ID** button.

3 Click **Next**.

4 In the **Add physics** tree, select **Plasma>Boltzmann Equation, Two-Term Approximation (be)**.

5 Click **Add Selected**.

6 Click **Next**.

7 Find the **Studies** subsection. In the tree, select **Preset Studies>Mean Energies**.

8 Click **Finish**.

GLOBAL DEFINITIONS

Begin by defining beta, the ionization degree, as a global parameter. This makes it available for selection as a parameter in a parametric sweep.

Parameters

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

2 In the **Parameters** settings window, locate the **Parameters** section.

3 In the table, enter the following settings:

NAME	EXPRESSION	DESCRIPTION
beta	1e-6	Ionization degree

GEOMETRY 1

Notice that the geometry and mesh are automatically generated for this physics interface and they very rarely need to be changed.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION

1 In the **Model Builder** window, under **Model 1** click **Boltzmann Equation, Two-Term Approximation**.

2 In the **Boltzmann Equation, Two-Term Approximation** settings window, locate the **Cross Section Import** section.

3 In the edit field, type `Ar_xsecs.txt`.

Zero Probability 1

1 Right-click **Model 1>Boltzmann Equation, Two-Term Approximation** and choose **Zero Probability**.

2 Select Boundary 2 only.

Zero Energy Flux 1

1 In the **Model Builder** window, right-click **Boltzmann Equation, Two-Term Approximation** and choose **Zero Energy Flux**.

2 Select Boundary 1 only.

STUDY 1

Step 1: Mean Energies

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Mean Energies**.

2 In the **Mean Energies** settings window, locate the **Study Settings** section.

3 In the **Mean energies** edit field, type `range(2,0.5,10)`.

4 In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

RESULTS

EEDF (be)

1 In the **Model Builder** window, under **Results** click **EEDF (be)**.

2 In the **1D Plot Group** settings window, click to expand the **Axis** section.

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

4 Click the **Zoom Extents** button on the Graphics toolbar.

5 Click the **Plot** button.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION

1 In the **Model Builder** window, under **Model 1** click **Boltzmann Equation, Two-Term Approximation**.

2 In the **Boltzmann Equation, Two-Term Approximation** settings window, click to expand the **Electron Energy Distribution Function Settings** section.

3 From the **Electron energy distribution function** list, choose **Boltzmann**.

4 Locate the **Boltzmann Properties** section. From the **Electron-electron collisions** list, choose **On**.

Now parameterize the ionization degree of the argon.

Boltzmann Model 1

1 In the **Model Builder** window, under **Model 1>Boltzmann Equation, Two-Term Approximation** click **Boltzmann Model 1**.

2 In the **Boltzmann Model** settings window, locate the **Mole Fraction Settings** section.

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3 In the x_{Ar} edit field, type `1`.

4 In the x_{Ars} edit field, type `0`.

5 Locate the **Boltzmann Settings** section. In the β edit field, type `beta`.

6 In the n_e edit field, type `1E18`.

Initial Values 1

1 In the **Model Builder** window, under **Model 1>Boltzmann Equation, Two-Term Approximation** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the $T_{d,0}$ edit field, type `10`.

ROOT

In the **Model Builder** window, right-click the root node and choose **Add Study**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Find the **Studies** subsection. In the tree, select **Preset Studies>Reduced Electric Fields**.

3 Click **Finish**.

STUDY 2

Step 1: Reduced Electric Fields

1 In the **Model Builder** window, under **Study 2** click **Step 1: Reduced Electric Fields**.

2 In the **Reduced Electric Fields** settings window, locate the **Study Settings** section.

3 In the **Reduced electric fields** edit field, type `10`.

4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click **Add**.

6 In the table, enter the following settings:

PARAMETER VALUE LIST
`1e-6 1e-5 1e-4 1e-3 5e-3 1e-2`

7 In the **Model Builder** window, right-click **Study 2** and choose **Compute**.

RESULTS

EEDF (be) 1

1 In the **1D Plot Group** settings window, locate the **Axis** section.

2 Select the **Manual axis limits** check box.

3 In the **x minimum** edit field, type `-2`.

4 In the **x maximum** edit field, type `30`.

5 In the **y minimum** edit field, type `10^(-9)`.

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

7 In the **Model Builder** window, under **Results>EEDF (be) 1** click **Line Graph 1**.

8 In the **Line Graph** settings window, click to expand the **Legends** section.

9 From the **Legends** list, choose **Manual**.

10 In the table, enter the following settings:

LEGENDS
1e-6
1e-5
1e-4
1e-3
5e-3
1e-2

11 Click the **Plot** button.

Now parameterize the mole fraction of excited argon atoms.

ROOT

In the **Model Builder** window, right-click the root node and choose **Add Study**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Find the **Studies** subsection. In the tree, select **Preset Studies>Reduced Electric Fields**.

3 Click **Finish**.

STUDY 3

Step 1: Reduced Electric Fields

1 In the **Model Builder** window, under **Study 3** click **Step 1: Reduced Electric Fields**.

2 In the **Reduced Electric Fields** settings window, locate the **Study Settings** section.

3 In the **Reduced electric fields** edit field, type `10`.

4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

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5 Click **Add**.

6 In the table, enter the following settings:

PARAMETER VALUE LIST
0 1e-5 1e-4 1e-3

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION

Boltzmann Model 1

1 In the **Model Builder** window, under **Model 1>Boltzmann Equation, Two-Term Approximation** click **Boltzmann Model 1**.

2 In the **Boltzmann Model** settings window, locate the **Boltzmann Settings** section.

3 In the β edit field, type `0`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} edit field, type `1-beta`.

5 In the x_{Ars} edit field, type `beta`.

STUDY 3

In the **Model Builder** window, right-click **Study 3** and choose **Compute**.

RESULTS

EEDF (be) 2

1 In the **Model Builder** window, under **Results** click **EEDF (be) 2**.

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

3 Select the **Manual axis limits** check box.

4 In the **x minimum** edit field, type `-2`.

5 In the **x maximum** edit field, type `30`.

6 In the **y minimum** edit field, type `10^(-9)`.

7 In the **y maximum** edit field, type `1`.

8 In the **Model Builder** window, under **Results>EEDF (be) 2** click **Line Graph 1**.

9 In the **Line Graph** settings window, click to expand the **Legends** section.

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

11 In the table, enter the following settings:

LEGENDS
0
1e-5
1e-4
1e-3

12 Click the **Plot** button.

Now use the parametric sweep feature to compute the rate coefficients over a wide range of mean electron energies for different degrees of ionization.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION

Boltzmann Model 1

1 In the **Model Builder** window, under **Model 1>Boltzmann Equation, Two-Term Approximation** click **Boltzmann Model 1**.

2 In the **Boltzmann Model** settings window, locate the **Boltzmann Settings** section.

3 In the β edit field, type `beta`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} edit field, type `1`.

5 In the x_{Ars} edit field, type `0`.

ROOT

In the **Model Builder** window, right-click the root node and choose **Add Study**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Find the **Studies** subsection. In the tree, select **Preset Studies>Mean Energies**.

3 Click **Finish**.

STUDY 4

Step 1: Mean Energies

1 In the **Model Builder** window, under **Study 4** click **Step 1: Mean Energies**.

2 In the **Mean Energies** settings window, locate the **Study Settings** section.

3 In the **Mean energies** edit field, type `range(2,0.5,10)`.

Parametric Sweep

1 In the **Model Builder** window, right-click **Study 4** and choose **Parametric Sweep**.

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2 In the **Parametric Sweep** settings window, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

PARAMETER NAMES	PARAMETER VALUE LIST
beta	1e-6 1e-5 1e-4 1e-3 1e-2

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

6 In the **Study** settings window, locate the **Study Settings** section.

7 Clear the **Generate default plots** check box.

8 Click the **Compute** button.

RESULTS

1D Plot Group 10

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

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

3 From the **Data set** list, choose **Solution 5**.

4 Right-click **Results>1D Plot Group 10** and choose **Global**.

5 In the **Global** settings window, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Boltzmann Equation, Two-Term Approximation>Rate coefficients>Rate coefficient (be.k_4)**.

6 In the **Model Builder** window, under **Results>1D Plot Group 10** click **Global 1**.

7 In the **Global** settings window, locate the **x-Axis Data** section.

8 From the **Axis source data** list, choose **Inner solutions**.

9 Click to expand the **Legends** section. Find the **Include** subsection. Select the **Expression** check box.

10 Clear the **Description** check box.

11 Click the **Plot** button.

12 In the **Global** settings window, locate the **Legends** section.

13 Find the **Include** subsection. Select the **Expression** check box.

14 Clear the **Description** check box.

15 In the **Model Builder** window, click **1D Plot Group 10**.

16 In the **1D Plot Group** settings window, locate the **Axis** section.

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

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

19 Click the **Plot** button.

20 Locate the **Plot Settings** section. Select the **x-axis label** check box.

21 In the associated edit field, type `Mean electron energy (eV)`.

22 Select the **y-axis label** check box.

23 In the associated edit field, type `Ionization rate coefficient (m<sup>3</sup>/s)`.

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

25 In the **y minimum** edit field, type `10^(-21)`.

26 In the **y maximum** edit field, type `10^(-14)`.

27 Click the **Plot** button.

Next, use the parametric sweep feature to compute the rate coefficients over a wide range of mean electron energies for different mole fractions of excited argon.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION

Boltzmann Model 1

1 In the **Model Builder** window, under **Model 1>Boltzmann Equation, Two-Term Approximation** click **Boltzmann Model 1**.

2 In the **Boltzmann Model** settings window, locate the **Boltzmann Settings** section.

3 In the β edit field, type `0`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} edit field, type `1-beta`.

5 In the x_{Ars} edit field, type `beta`.

ROOT

In the **Model Builder** window, right-click the root node and choose **Add Study**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Find the **Studies** subsection. In the tree, select **Preset Studies>Mean Energies**.

3 Click **Finish**.

STUDY 5

Step 1: Mean Energies

1 In the **Model Builder** window, under **Study 5** click **Step 1: Mean Energies**.

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2 In the **Mean Energies** settings window, locate the **Study Settings** section.

3 In the **Mean energies** edit field, type `range(2,0.5,10)`.

Parametric Sweep

1 In the **Model Builder** window, right-click **Study 5** and choose **Parametric Sweep**.

2 In the **Parametric Sweep** settings window, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

PARAMETER NAMES	PARAMETER VALUE LIST
beta	`0 1e-5 1e-4 1e-3`

5 In the **Model Builder** window, click **Study 5**.

6 In the **Study** settings window, locate the **Study Settings** section.

7 Clear the **Generate default plots** check box.

8 Click the **Compute** button.

RESULTS

1D Plot Group 11

1 In the **Model Builder** window, under **Results** right-click **1D Plot Group 10** and choose **Duplicate**.

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

3 From the **Data set** list, choose **Solution 7**.

4 Click the **Plot** button.

Finally, compute the EEDF for a mean electron energy of 2.15 eV for different reduced angular frequencies.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION

1 In the **Model Builder** window, under **Model 1** click **Boltzmann Equation, Two-Term Approximation**.

2 In the **Boltzmann Equation, Two-Term Approximation** settings window, locate the **Boltzmann Properties** section.

3 From the **Oscillating field** list, choose **On**.

Boltzmann Model 1

1 In the **Model Builder** window, under **Model 1>Boltzmann Equation, Two-Term Approximation** click **Boltzmann Model 1**.

2 In the **Boltzmann Model** settings window, locate the **Boltzmann Settings** section.

3 In the ω/N edit field, type `beta`.

4 Locate the **Mole Fraction Settings** section. In the x_{Ar} edit field, type `1`.

5 In the x_{Ars} edit field, type `0`.

ROOT

In the **Model Builder** window, right-click the root node and choose **Add Study**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Find the **Studies** subsection. In the tree, select **Preset Studies>Mean Energies**.

3 Click **Finish**.

STUDY 6

Step 1: Mean Energies

1 In the **Model Builder** window, under **Study 6** click **Step 1: Mean Energies**.

2 In the **Mean Energies** settings window, locate the **Study Settings** section.

3 In the **Mean energies** edit field, type `2.15`.

Parametric Sweep

1 In the **Model Builder** window, right-click **Study 6** and choose **Parametric Sweep**.

2 In the **Parametric Sweep** settings window, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

PARAMETER NAMES	PARAMETER VALUE LIST
beta	`0 1e-13 2e-13`

5 Right-click **Study 6** and choose **Compute**.

RESULTS

Click the **Zoom Extents** button on the Graphics toolbar.

EEDF (be) 3

1 In the **Model Builder** window, under **Results** click **EEDF (be) 3**.

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

3 From the **Data set** list, choose **Solution 8**.

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

5 Select the **Manual axis limits** check box.

6 In the **x minimum** edit field, type `0`.

7 In the **x maximum** edit field, type `20`.

8 In the **y minimum** edit field, type `10^(-8)`.

9 In the **y maximum** edit field, type `1`.

10 Click the **Plot** button.

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