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Oxygen Boltzmann Analysis

Introduction

The Boltzmann equation can be solved to validate sets of electron impact collision cross sections. In fact, sets of collision cross sections are traditionally inferred by solving a two-term approximation to the Boltzmann equation and comparing the results to swarm experiments. This model solves the Boltzmann equation in the two-term approximation and compares the computed drift velocity and the characteristic energy to experimental data.

Model Definition

The Boltzmann equation in the two-term approximation can be written as

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

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

$$W = -\gamma\varepsilon^2\sigma_\varepsilon - 3a\left(\frac{n_e}{N_n}\right)A_1 \tag{1}$$

and

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

For definitions of the quantities in the equations Equation 1 and Equation 2, 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:

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

and as $\varepsilon \to \infty$, $f \to 0$.

When the Boltzmann equation has been solved the drift velocity and characteristic energy for a given reduced electric field can be compared to experimental results. The drift velocity is defined as

$$w = \mu N\frac{E}{N_n}$$

where E/N_n is the reduced electric field and μN is the reduced electron mobility which for a DC electric field is

$$\mu N_n = -\left(\frac{\gamma}{3}\right)\int_0^\infty \frac{\varepsilon}{\sigma_m}\left(\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon .$$

The characteristic energy is defined as

$$E = \frac{DN_n}{\mu N_n}$$

where D is the electron diffusion coefficient

$$DN_n = -\left(\frac{\gamma}{3}\right)\int_0^\infty \frac{\varepsilon}{\sigma_m} f d\varepsilon$$

The experimental data comes from Ref. 2.

The EEDF is defined by how electrons gain energy from the electric field and lose (or gain) their energy in collisions with the background gas. The electron collisions are characterized by cross sections that need to be provided by the user. In this model, the background gas is molecular oxygen and the following electron impact collisions are considered (electron impact cross-sections are obtained from Ref. 3):

TABLE 1: TABLE OF COLLISIONS.

REACTION	FORMULA	TYPE	$\Delta\varepsilon$ (eV)
1	e+O2=>e+O2	Momentum	0
2	e+O2=>O+O	Attachment	0
3	e+O2=>e+O2(rot)	Excitation	0.02
4	e+O2=>e+O2(v=1)	Excitation	0.19
5	e+O2=>e+O2(v=1)	Excitation	0.19
6	e+O2=>e+O2(v=2)	Excitation	0.38
7	e+O2=>e+O2(v=2)	Excitation	0.38
8	e+O2=>e+O2(v=3)	Excitation	0.75
9	e+O2=>e+O2(v=3)	Excitation	0.75
10	e+O2=>e+O2(a1d)	Excitation	0.977
11	e+O2(a1d)=>e+O2	Superelastic	-0.977
12	e+O2=>e+O2(b1s)	Excitation	1.627
13	e+O2(b1s)=>e+O2	Superelastic	-1.627

TABLE 1: TABLE OF COLLISIONS.

REACTION	FORMULA	TYPE	Δε (eV)
14	e+O2=>e+O2(45)	Excitation	4.5
15	e+O2(45)=>e+O2	Superelastic	-4.5
16	e+O2=>e+O+O	Dissociation	6.0
17	e+O2=>e+O+O(1D)	Dissociation	8.4
18	e+O2=>e+O+O(1S)	Dissociation	9.97
19	e+O2=>e+O2+	Ionization	12.06

In a superelastic collision, the electrons gain energy from excited species. The mole fraction of each species is given in the table below and is estimated from typical discharge conditions that occur in a drift tube. The degree of ionization is set to 10^{-6}.

TABLE 2: TABLE OF MOLE FRACTIONS OF EACH SPECIES.

SPECIES	MOLE FRACTION
O2	0.99997
O2(a1d)	1.5E-5
O2(b1s)	1E-5
O2(45)	5E-6

Results and Discussion

Figure 1 plots EEDFs resulting from the solution of the Boltzmann equation in the two-term approximation for different values of the mean electron energy. The EEDF with lowest mean electron energy (2 eV blue line) has a very low population of electrons with energies above the ionization threshold. As the mean electron energy increases, the population of electrons with higher energy increases. This makes ionization processes more likely. Electron impact ionization is important as it is usually the primary mechanism for sustaining plasmas. Notice also that the EEDF is not linear on the log scale. This indicates that the EEDF is non-Maxwellian under these conditions.

The reduced electron transport properties are plotted in Figure 2. The transport properties have a much weaker dependence on the EEDF compared to rate or Townsend coefficients. The electron mobility and electron energy mobility decrease as the mean electron energy increases. The electron diffusivity and electron energy diffusivity increase as the mean electron energy increases. If the EEDF was Maxwellian the rate of change of the transport parameters would be such that the following relations would hold

$$D_e = \mu_e T_e, \mu_\varepsilon = \left(\frac{5}{3}\right)\mu_e, D_\varepsilon = \mu_\varepsilon T_e$$

In the case that the EEDF is non-Maxwellian, this relation does not necessarily hold true.

The electron drift velocity and the characteristic energy (ratio of the electron diffusivity and mobility) are macroscopic quantities that can be computed by integrating appropriate cross sections over computed EEDFs and compared directly with measurements from swarm experiments. Since the EEDF is very sensitive to the cross sections the comparison between the measured and computed drift velocity and the characteristic energy can be used to find a coherent set of cross sections.

The simulated and experimental drift velocity and characteristic energy are plotted in Figure 3 and Figure 4. The agreement between the two is good over a wide range of reduced electric fields, indicating that the cross section data is consistent with experimental measurements.

The fraction of power channeled into various reactions is shown in Figure 5. This is important in design of plasma sources because often the desired reactive species is known in advance. The plot gives an indication of what the target mean electron energy should be in order to channel as much of the available power into a specific reaction. Of course, the power channeled into ionization must be high enough to sustain the plasma.

The Townsend coefficients are plotted in Figure 6. The Townsend coefficients offer an alternative way of defining reaction rates. The reaction rate depends on the electron flux rather than the electron density. Townsend coefficients should be used when modeling DC discharges.

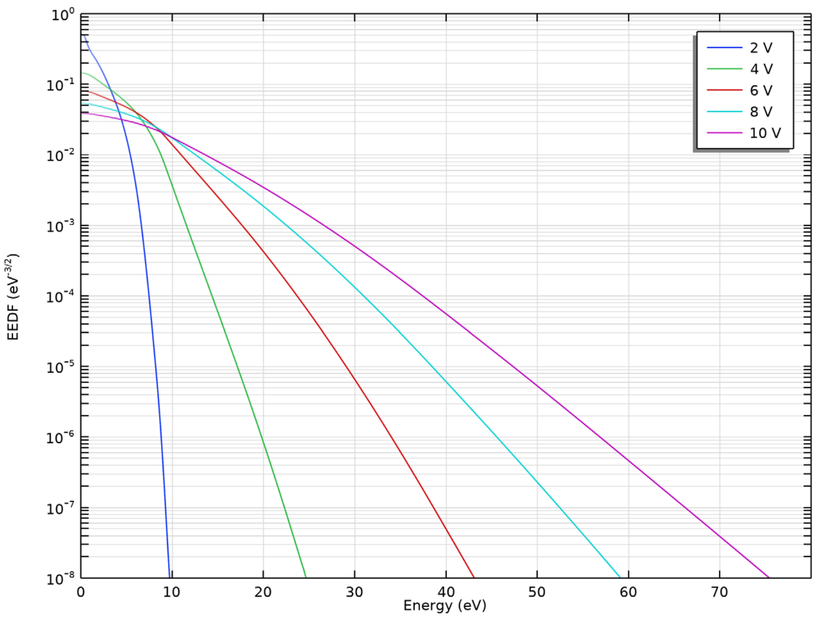

Figure 1: Plot of the EEDF for different values of the mean electron energy.

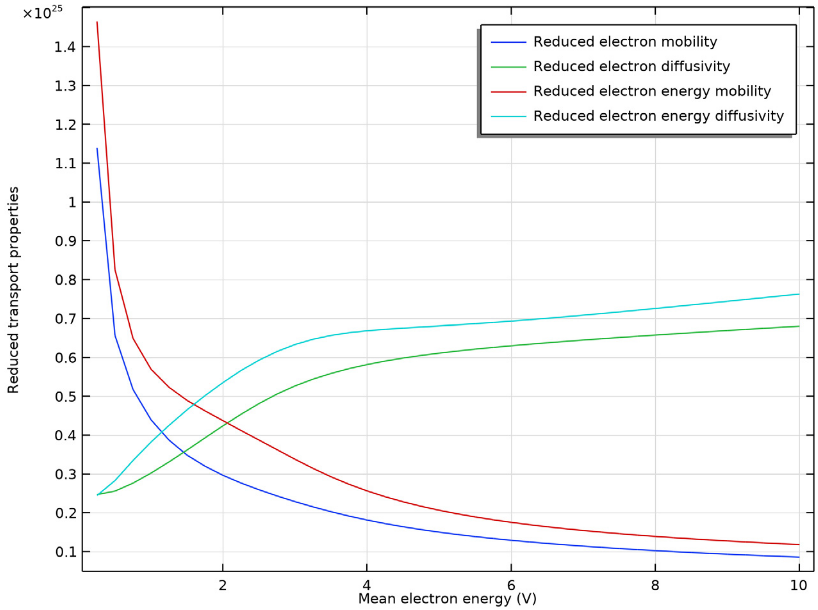

Figure 2: Reduced transport properties vs. mean electron energy.

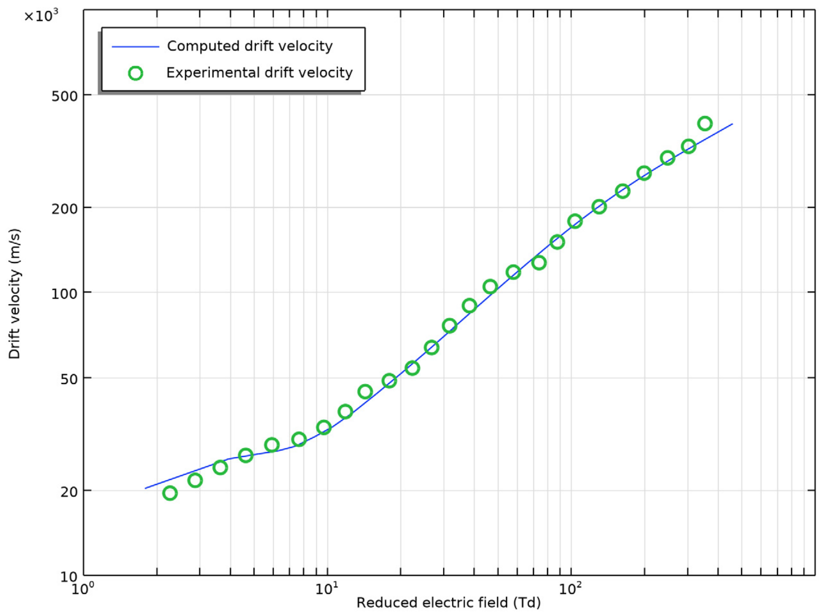

Figure 3: Computed and experimental drift velocity for oxygen.

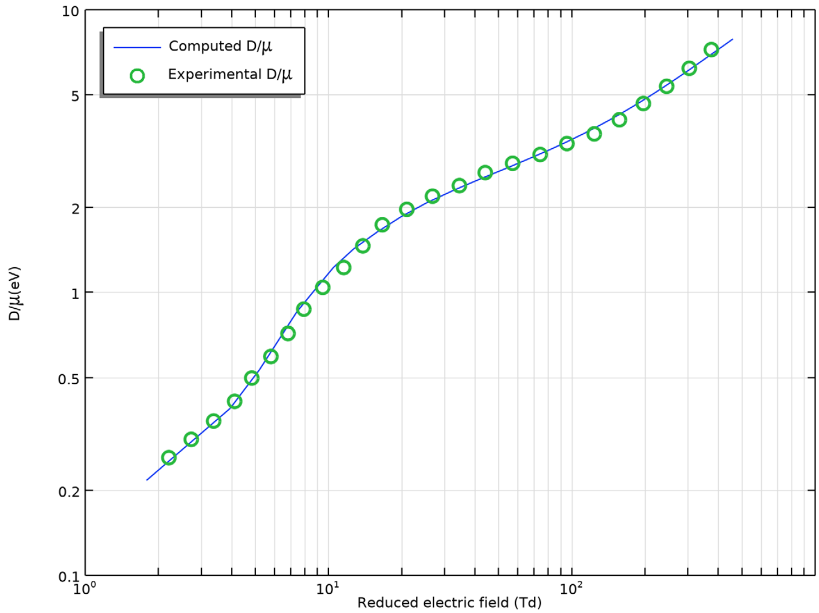

Figure 4: Computed and experimental D/μ *for different reduced electric fields.*

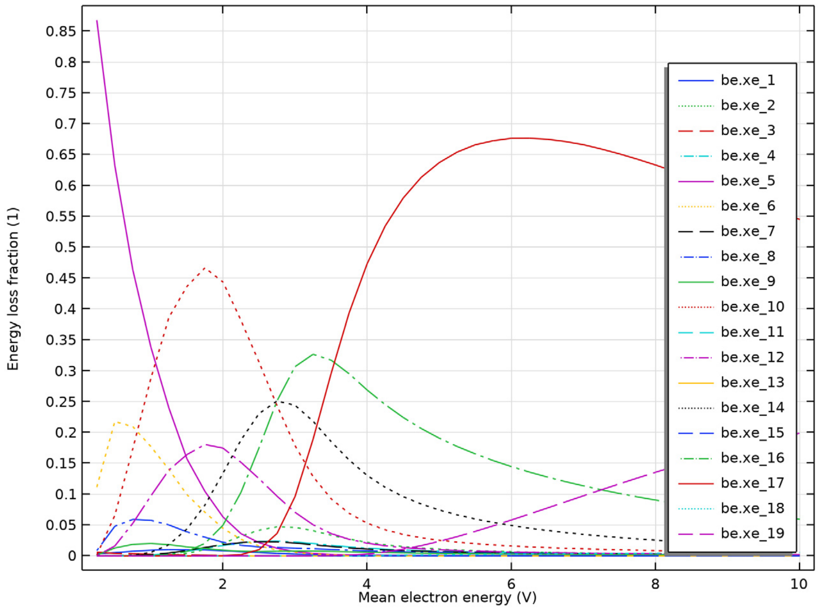

Figure 5: Plot of the fraction of the total power channeled into each reaction vs. mean electron energy.

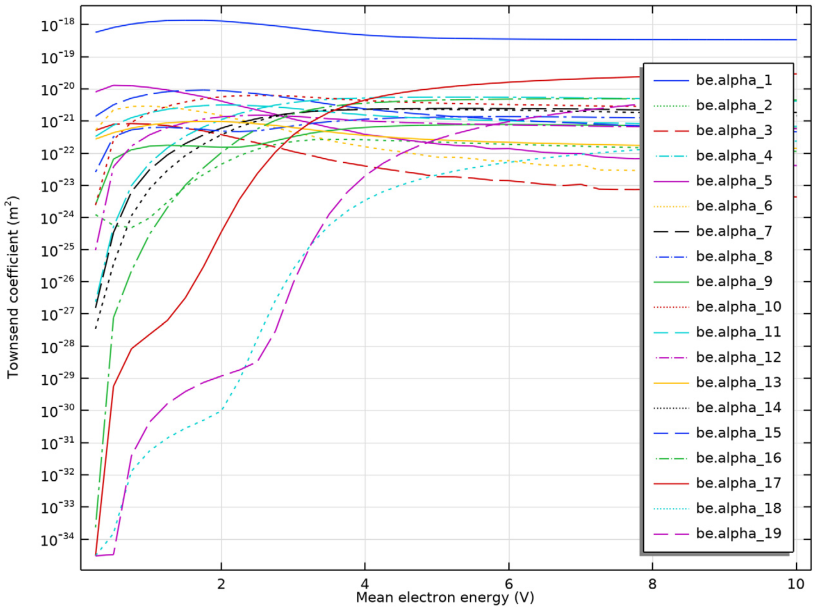

Figure 6: Townsend coefficients vs. mean electron energy for oxygen.

References

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.

2. J. Dutton, "A Survey of Electron Swarm Data", *J. Phys. Chem. Ref. Data*, vol. 4, pp. 577–866, 1975.

3. Morgan database, www.lxcat.net, retrieved 2017.

Application Library path: `Plasma_Module/Two-Term_Boltzmann_Equation/boltzmann_oxygen`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, Select the **Boltzmann Equation, Two-Term Approximation (be)** interface and the **Mean Energies** study.

2 click **0D**.

3 In the **Select Physics** tree, select **Plasma>Boltzmann Equation, Two-Term Approximation (be)**.

4 Click **Add**.

5 Click **Study**.

6 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Mean Energies**.

7 Click **Done**.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION (BE)

Select to solve the Boltzmann equation in the two-term approximation, include electron-electron collisions, and change the number of elements and the element ratio in the extra dimension.

Select also to automatically compute the maximum energy that the EEDF is solved for.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Boltzmann Equation, Two-Term Approximation (be)**.

2 In the **Settings** window for **Boltzmann Equation, Two-Term Approximation**, locate the **Electron Energy Distribution Function Settings** section.

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

4 Select the **Electron-electron collisions** check box.

5 In the N text field, type 500.

6 In the R text field, type 100.

7 Select the **Compute maximum energy** check box.

Import a set of electron impact cross sections for Oxygen.

Cross Section Import 1

1 In the **Physics** toolbar, click **Global** and choose **Cross Section Import**.

2 In the **Settings** window for **Cross Section Import**, locate the **Cross Section Import** section.

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `O2_xsecs.txt`.

5 Click **Import**.

Set the mole fraction of the different species, and choose which results are to be plotted.

Boltzmann Model 1

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

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

3 From the **Mole constrained species** list, choose **O2**.

4 In the table, enter the following settings:

Species	Mole fraction (1)
O2a1d	1.5e-5
O2b1s	1e-5
O245	5e-6

5 Locate the **Results** section. Find the **Generate the following default plots** subsection. Clear the **Mean electron energy** check box.

6 Clear the **Rate coefficients** check box.

7 Select the **Townsend coefficients** check box.

8 Select the **Energy loss fraction** check box.

Set mean electron energy to 0.25 eV since the simulation starts with that value.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the ε_0 text field, type `0.25[V]`.

Import experimental data for the electron drift velocity and the characteristic energy to later compare with the simulation results.

DEFINITIONS (COMP1)

Interpolation 1 (int1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global>Interpolation**.

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `O2_drift_velocity_expt.txt`.

5 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
t	Td

6 In the **Function** table, enter the following settings:

Function	Unit
int1	m/s

Interpolation 2 (int2)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global>Interpolation**.

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `O2_Te_expt.txt`.

5 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
t	Td

6 In the **Function** table, enter the following settings:

Function	Unit
int2	V

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

Prepare the study to sweep from 0.25 to 10 eV with steps of 0.25 eV.

STUDY 1

Step 1: Mean Energies

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

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

3 Click **Range**.

4 In the **Range** dialog box, type `0.25` in the **Start** text field.

5 In the **Step** text field, type `0.25`.

6 In the **Stop** text field, type `10`.

7 Click **Replace**.

Step 1: Mean Energies

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

2 In the **Home** toolbar, click **Compute**.

Look at the EEDFs, transport parameters, Townsend coefficients and energy loss fractions.

RESULTS

EEDF (be)

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

2 From the **Parameter selection (freq)** list, choose **From list**.

3 In the **Parameter values (freq (V))** list, choose **2**, **4**, **6**, **8**, and **10**.

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

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

6 In the **x maximum** text field, type `80`.

7 In the **y minimum** text field, type `1e-8`.

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

9 In the **EEDF (be)** toolbar, click **Plot**.

Transport Properties (be)

1 In the **Model Builder** window, click **Transport Properties (be)**.

2 In the **Transport Properties (be)** toolbar, click **Plot**.

Global 1

1 In the **Model Builder** window, expand the **Townsend Coefficients (be)** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click to expand the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

4 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** check box.

5 Select the **Expression** check box.

6 In the **Townsend Coefficients (be)** toolbar, click **Plot**.

Global 1

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

2 In the **Model Builder** window, expand the **Energy Loss Fraction (be)** node, then click **Global 1**.

3 In the **Settings** window for **Global**, locate the **Coloring and Style** section.

4 Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

5 Locate the **Legends** section. Find the **Include** subsection. Clear the **Description** check box.

6 Select the **Expression** check box.

7 In the **Energy Loss Fraction (be)** toolbar, click **Plot**.

Prepare the plots to compare the computed and measured drift velocity and characteristic energy as a function of the reduced electric field.

Drift velocity

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

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

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

4 In the **Label** text field, type `Drift velocity`.

5 Locate the **Plot Settings** section.

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

7 Select the **y-axis label** check box. In the associated text field, type `Drift velocity (m/s)`.

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

9 In the **x minimum** text field, type `1`.

10 In the **x maximum** text field, type `1e3`.

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

12 In the **y maximum** text field, type `1e6`.

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 **Drift velocity** 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
`be.w`	`m/s`	`Computed drift velocity`

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

5 In the **Expression** text field, type `be.EN`.

6 From the **Unit** list, choose **Td**.

Global 2

1 In the **Model Builder** window, right-click **Drift velocity** 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
`int1(be.EN)`	`m/s`	`Experimental drift velocity`

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

5 In the **Expression** text field, type `be.EN`.

6 From the **Unit** list, choose **Td**.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

8 From the **Width** list, choose **3**.

9 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

10 From the **Positioning** list, choose **Interpolated**.

11 In the **Number** text field, type `25`.

12 In the **Drift velocity** toolbar, click **Plot**.

Characteristic energy

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

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

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

4 In the **Label** text field, type `Characteristic energy`.

5 Locate the **Plot Settings** section.

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

7 Select the **y-axis label** check box. In the associated text field, type `D/\mu (eV)`.

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

9 In the **x minimum** text field, type `1`.

10 In the **x maximum** text field, type `1e3`.

11 In the **y minimum** text field, type `0.1`.

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

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 **Characteristic energy** 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**
`be.DeN/be.muN`	`V`	`Computed D/\mu`

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

5 In the **Expression** text field, type `be.EN`.

6 From the **Unit** list, choose **Td**.

Global 2

1 In the **Model Builder** window, right-click **Characteristic energy** 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**
`int2(be.EN)`	`V`	`Experimental D/\mu`

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

5 In the **Expression** text field, type `be.EN`.

6 From the **Unit** list, choose **Td**.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

8 From the **Width** list, choose **3**.

9 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

10 From the **Positioning** list, choose **Interpolated**.

11 In the **Number** text field, type `25`.

12 In the **Characteristic energy** toolbar, click **Plot**.