Created in COMSOL Multiphysics 5.6

Drift Diffusion Tutorial

Introduction

The foundation of the *COMSOL Multiphysics Plasma Module* is the Drift Diffusion interface, which describes the transport of electrons in an electric field. The Drift Diffusion interface solves a pair of reaction/convection/diffusion equations, one for the electron density and the other for the electron energy density. The mean electron energy is computed by dividing the electron energy density by the electron number density.

Model Definition

This tutorial example computes the electron number density and mean electron energy in a drift tube. Electrons are released due to thermionic emission on the left boundary with an assumed mean electron energy. The electrons are then accelerated toward the right boundary due to an imposed external electric field that is oriented in the opposite direction from the electron drift velocity:

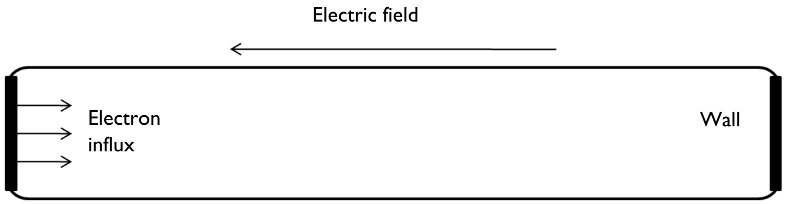

Figure 1: In the drift tube the electrons enter the left boundary and are accelerated by the electric field toward the wall.

MODEL EQUATIONS

A simple model is set up to test the Drift Diffusion interface. The equations solved are, for the electron number density:

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e \tag{1}$$

where

$$\Gamma_e = -(\mu_e \bullet \mathbf{E})n_e - \mathbf{D}_e \bullet \nabla n_e \tag{2}$$

and, n_e denotes the electron density ($1/\mathrm{m}^3$), R_e is the electron rate expression ($1/(\mathrm{m}^3 \cdot \mathrm{s})$), μ_e is the electron mobility which is either a scalar or tensor ($\mathrm{m}^2/(\mathrm{V} \cdot \mathrm{s})$), $\mathbf{E}$ is the electric field (V/m), and D_e is the electron diffusivity, which is either a scalar or a tensor. The first term on the right side of Equation 2 represents migration of electrons due to an electric field. The second term on the right side of Equation 2 represents diffusion of electrons from regions of high electron density to low electron density.

An equation for the electron energy density is solved in conjunction with Equation 1. The equation is:

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot \Gamma_\varepsilon + \mathbf{E} \cdot \Gamma_e = R_\varepsilon \tag{3}$$

where

$$\Gamma_\varepsilon = -(\mu_\varepsilon \bullet \mathbf{E})n_\varepsilon - \mathbf{D}_\varepsilon \bullet \nabla n_\varepsilon$$

Here, n_ε is the electron energy density (V/m^3), R_ε is the energy loss/gain due to inelastic collisions (V/(m^3·s)), μ_ε is the electron energy mobility (m^2/(V·s)), **E** is the electric field (V/m), and D_ε is the electron energy diffusivity (m^2/s). The subscript ε refers to electron energy. The third term on the left side of Equation 3 represents heating of the electrons due to an external electric field. Note that this term can either be a heat source or a heat sink depending on whether the electrons are drifting in the same direction as the electric field or not. For a Maxwellian electron energy distribution function, the following relationships hold:

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

where T_e is the electron "temperature". So, given the electron mobility, the other transport properties required can be computed. The electron "temperature" is a function of the mean electron energy, $\bar{\varepsilon}$, which is defined as:

$$\bar{\varepsilon} = \frac{n_\varepsilon}{n_e}$$

and then:

$$T_e = \left(\frac{2}{3}\right)\bar{\varepsilon}$$

SOURCE COEFFICIENTS

The electron source term, R_e is the sum of the electron impact reaction rates that make up the plasma chemistry. The electron energy loss due to inelastic collisions, R_ε is a function of the electron impact reaction rates multiplied by the energy loss corresponding to each reaction. Mathematically, the electron source is defined as:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where x_j is the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (m^3/s), and N_n is the total neutral number density ($1/\mathrm{m}^3$). The energy loss is defined as:

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

where $\Delta\varepsilon_j$ is the energy loss from reaction j (V).

An influx of electron due to thermionic emission is specified on the left boundary. The electrons that are emitted from the surface are then accelerated toward the wall by the electric field. The acceleration leads to an increase in the mean electron energy and subsequently ionization occurs. This creates new electrons, which are ultimately lost into a wall opposite the emitting surface. The gain of electrons due to ionization is included in the model by assuming the drift tube contains argon. This example assumes that the mole fraction of electronically excited argon atoms and argon ions is very small. This means that you do not solve additional equations for the mole fractions of these two species. The following reactions are included in the model:

TABLE 1: TABLE OF COLLISIONS AND REACTIONS MODELED.

REACTION	**FORMULA**	**TYPE**	$\Delta\varepsilon(\mathrm{eV})$	**A**	**B**	**E**
1	e+Ar=>e+Ar	Elastic	0	1.99E-014	0.93	0.41
2	e+Ar=>e+Ars	Excitation	11.5	8.77E-015	0.62	18.16
3	e+Ar=>2e+Ar+	Ionization	15.8	2.15E-014	0.49	24.75

The rate constants for these reactions are given in Arrhenius form:

$$k_j = A T_e^B \exp(-E/T_e)$$

The rate constants are computed from cross-section data for each reaction assuming a Maxwellian electron energy distribution function.

Results and Discussion

The electron density is plotted in Figure 2. The peak electron density occurs close to the far wall. The peak electron density is five times higher than the electron density on the left wall due to new electrons being created through ionization.

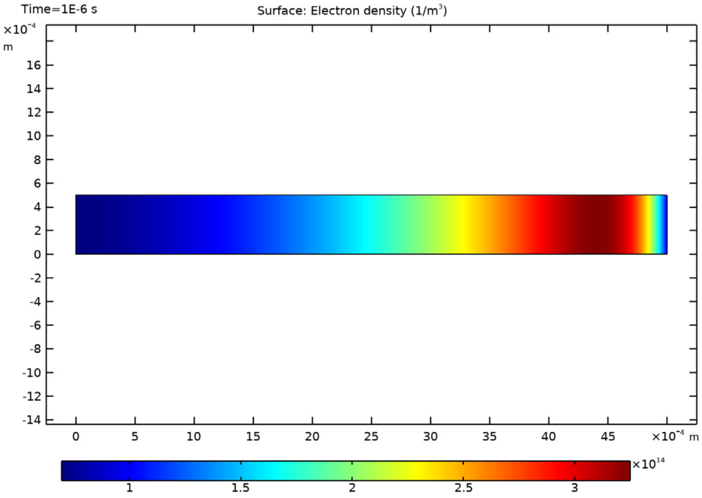

Figure 2: Plot of the electron density in the drift tube.

Because there are no variations in the solution in the y-direction it can be more convenient to create a 1D data set in the x-direction and plot various quantities versus the x-axis. Figure 3 plots the electron density as a function of the x-direction. The electron “temperature” is plotted in Figure 4. On the left wall the electron “temperature” is fixed to 2 eV. The temperature steadily increases over a narrow region. This is because there is a strong drift velocity in the opposite direction to the electric field. As the electron temperature increases, so do the rate constants, which are responsible for creating new electrons. The increase in electron temperature also has a significant effect on the number of inelastic collisions that occur in the tube. After the initial rise in electron temperature, the electron temperature remains constant until close to the far wall. In this region the Joule heating caused by the electron drift velocity in the opposite direction to the electric field is balanced by the energy loss due to inelastic collisions.

The highly nonlinear behavior in such a simple example showcases the fact that very complicated dynamics occur in even the simplest of plasmas.

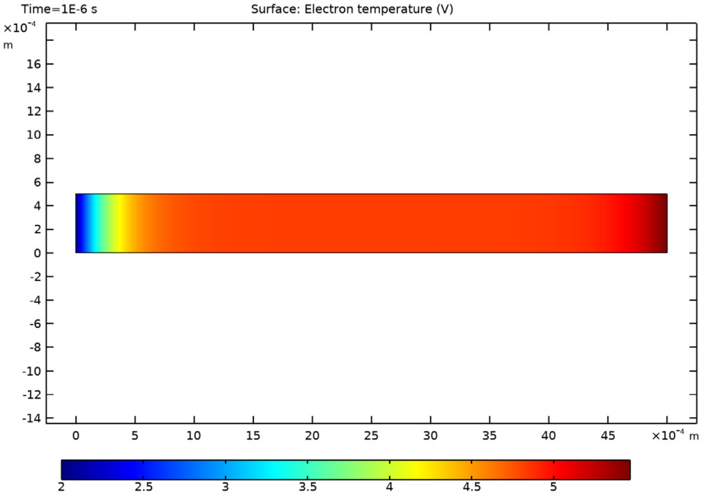

Figure 3: Plot of the electron "temperature" across the drift tube.

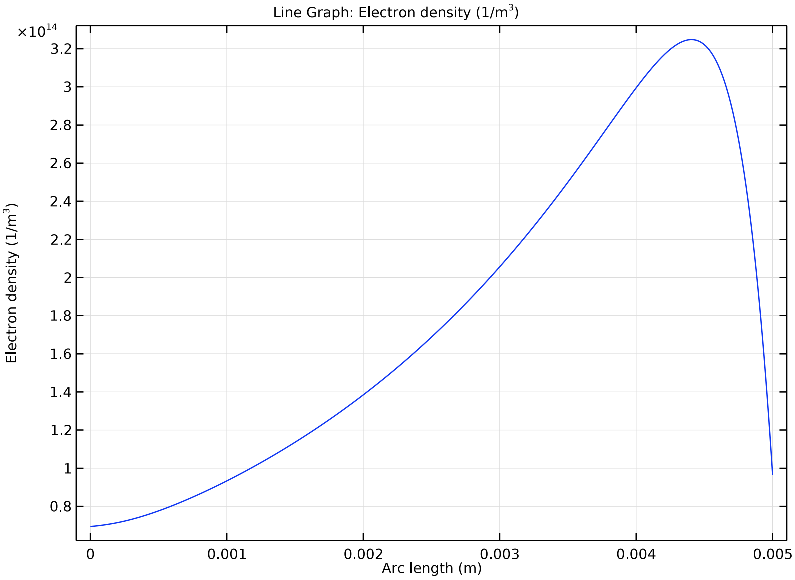

Figure 4: Cross section plot of electron density across the drift tube.

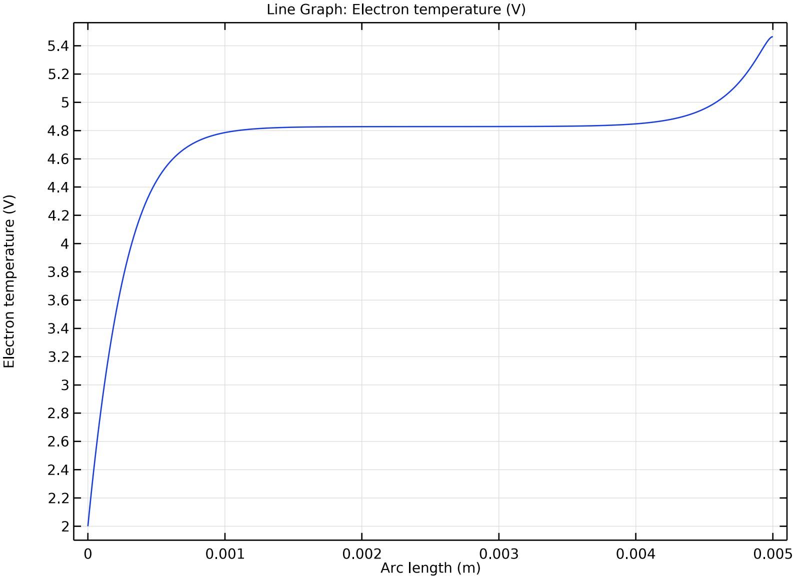

Figure 5: Cross plot of the electron temperature across the drift tube.

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 Sci. Technol.*, vol. 14, pp. 722–733, 2005.

Application Library path: `Plasma_Module/Direct_Current_Discharges/drift_diffusion_tutorial`

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**.
2. In the **Select Physics** tree, select **Plasma>Species Transport>Drift Diffusion (dd)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **General Studies>Time Dependent**.
6. Click **Done**.

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 `5E-3`.
4. In the **Height** text field, type `5E-4`.

   Now add a table of expressions for the external electric field, temperature, pressure, and the electron impact reactions occurring in the drift tube. You also define the influx of electrons due to thermionic emission. The influx of electrons and the external electric field are both ramped up from an initial value of zero to aid convergence at early timesteps.

DEFINITIONS

Variables 1

1 In the **Home** toolbar, click a= **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
ramp	tanh(1E7[1/s]*t)		Ramp function
T	300[K]	K	Gas temperature
p	10[torr]	Pa	Gas pressure
Nn0	p/k_B_const/T	1/m^3	Neutral number density
k1	1.993039e-014*dd.Te^0.93*exp(-0.41/dd.Te)		Elastic rate coefficient
k2	8.773932e-015*dd.Te^0.62*exp(-18.16/dd.Te)		Excitation rate coefficient
k3	2.153106e-014*dd.Te^0.49*exp(-24.75/dd.Te)		Ionization rate coefficient
r1	k1*dd.Nn*dd.ne		Elastic collision reaction rate
r2	k2*dd.Nn*dd.ne		Electronic excitation reaction rate
r3	k3*dd.Nn*dd.ne		Ionization reaction rate
de1	0[V]	V	Energy loss, elastic collision
de2	11.56[V]	V	Energy loss, electronic excitation
de3	15.8[V]	V	Energy loss, ionization
Re	r3		Electron production rate
Sen	-e_const*(r1*de1+r2*de2+r3*de3)		Collisional power loss
Ex	-d(V,x)	V/m	Electric field
V	-100[V]*ramp* (0.005[m]-x)/0.005[m]	V	Electric potential

Name	Expression	Unit	Description
`Ain`	`0.5E-3^2[m^2]`	m^2	Wall area
`I`	`2E-6[A]`	A	Thermal emission current
`influx`	`I/Ain/e_const*ramp`	$1/(m^2\cdot s)$	Electron influx
`mueN`	`4E24[1/(m*V*s)]`	$1/(V\cdot m\cdot s)$	Reduced electron mobility

DRIFT DIFFUSION (DD)

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Drift Diffusion (dd)**.
2. In the **Settings** window for **Drift Diffusion**, locate the **Electron Properties** section.
3. Select the **Use reduced electron transport properties** check box.

Drift Diffusion Model 1

1. In the **Model Builder** window, under **Component 1 (comp1)>Drift Diffusion (dd)** click **Drift Diffusion Model 1**.
2. In the **Settings** window for **Drift Diffusion Model**, locate the **Model Inputs** section.
3. In the N_n text field, type `Nn0`.
4. In the V text field, type `V`.
5. In the S_{en} text field, type `Sen`.
6. Locate the **Electron Density and Energy** section. In the $\mu_e N_n$ text field, type `mueN`.

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 $n_{e,0}$ text field, type `1E16`.
4. In the ε_0 text field, type `3`.

Electron Production Rate 1

1. In the **Physics** toolbar, click **Domains** and choose **Electron Production Rate**.
2. Select Domain 1 only.
3. In the **Settings** window for **Electron Production Rate**, locate the **Electron Production Rate** section.
4. In the R_e text field, type `Re`.

Wall 1

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

2. In the **Settings** window for **Wall**, locate the **General Wall Settings** section.
3. Select the **Include migration effects** check box.
4. Select Boundary 4 only.

Electron Density and Energy 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Electron Density and Energy**.
2. Select Boundary 1 only.
3. In the **Settings** window for **Electron Density and Energy**, locate the **Electron Density and Energy** section.
4. Select the **Fix mean electron energy** check box.

Wall 2

1. In the **Physics** toolbar, click **Boundaries** and choose **Wall**.
2. Select Boundary 1 only.
3. In the **Settings** window for **Wall**, locate the **Electron Density Wall Settings** section.
4. In the $\Gamma_t \cdot \mathbf{n}$ text field, type `influx`.
5. Locate the **Electron Energy Wall Settings** section. Clear the **Use wall for electron energy** check box.

   The above boundary conditions applied to boundary 1 means that the mean electron energy will be fixed at 3 electron volts and there will be an influx of electrons resulting in a net current influx of 2E-6 amps.

   When you create the mesh you want to use a finer mesh close to the walls so that the sharp gradients in the electron density and electron energy density are adequately resolved. You accomplish this by using a graded mapped mesh.

MESH 1

Mapped 1

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

Distribution 1

1. In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.
2. Select Boundaries 2 and 3 only.
3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. From the **Distribution type** list, choose **Predefined**.
5. In the **Number of elements** text field, type `200`.

6. In the **Element ratio** text field, type `5`.
7. From the **Growth formula** list, choose **Geometric sequence**.
8. Select the **Symmetric distribution** check box.

Size

1. In the **Model Builder** window, click **Size**.
2. In the **Settings** window for **Size**, locate the **Element Size** section.
3. From the **Predefined** list, choose **Extra fine**.
4. Click **Build All**.

   The mean electron energy and electron density can change on a subnanosecond time scale. The electron density and mean electron energy reach their steady state values very quickly so it is only necessary to solve the problem for 1 microsecond.

STUDY 1

Step 1: Time Dependent

1. In the **Model Builder** window, under **Study 1** 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`.
4. Click **Range**.
5. In the **Range** dialog box, choose **Number of values** from the **Entry method** list.
6. In the **Start** text field, type `-8`.
7. In the **Stop** text field, type `-6`.
8. In the **Number of values** text field, type `100`.
9. From the **Function to apply to all values** list, choose **exp10(x)** – **Exponential function (base 10)**.
10. Click **Add**.
11. In the **Home** toolbar, click **Compute**.

RESULTS

Electron Density (dd)

1. In the **Settings** window for **2D Plot Group**, click to expand the **Window Settings** section.
2. Locate the **Color Legend** section. From the **Position** list, choose **Bottom**.
3. Click the **Zoom Extents** button in the **Graphics** toolbar.
4. In the **Electron Density (dd)** toolbar, click **Plot**.

Electron Temperature (dd)

1. In the **Model Builder** window, click **Electron Temperature (dd)**.
2. In the **Settings** window for **2D Plot Group**, locate the **Color Legend** section.
3. From the **Position** list, choose **Bottom**.
4. Click the **Zoom Extents** button in the **Graphics** toolbar.
5. In the **Electron Temperature (dd)** toolbar, click **Plot**.

Cut Line 2D 1

1. In the **Results** toolbar, click **Cut Line 2D**.
2. Click the **Zoom Extents** button in the **Graphics** toolbar.
3. In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.
4. In row **Point 1**, set **Y** to `2.5e-4`.
5. In row **Point 2**, set **Y** to `2.5e-4` and **x** to `5-3`.
6. Click **Plot**.

1D Plot Group 3

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 **Cut Line 2D 1**.
4. From the **Time selection** list, choose **Last**.

Line Graph 1

1. Right-click **1D Plot Group 3** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1 (comp1)>Drift Diffusion> Electron density>dd.ne - Electron density - 1/m^3**.
3. In the **1D Plot Group 3** toolbar, click **Plot**.

1D Plot Group 4

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 **Data** section.
3. From the **Dataset** list, choose **Cut Line 2D 1**.
4. From the **Time selection** list, choose **Last**.

Line Graph 1

1. Right-click **1D Plot Group 4** and choose **Line Graph**.

2. In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Component 1 (comp1)>Drift Diffusion>Electron energy density>dd.Te - Electron temperature - V**.
3. In the **1D Plot Group 4** toolbar, click **Plot**.