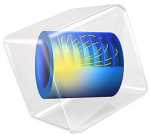


Model created in COMSOL Multiphysics 6.4

# Electric Discharge with Self-Defined Discharge Chemistry

## *Introduction*

The example shows how to generate a discharge model from the Reaction Engineering interface with a self-defined discharge chemistry. It reproduces the library model Double-Headed Streamer in Parallel-Plate Electrodes. The model investigates a double-headed streamer between parallel-plate electrodes. Initially, a cluster of electrons is positioned between two electrodes spaced 1 cm apart, subject to a 52 kV voltage, creating a background electric field of 52 kV/cm. Negative and positive streamers propagate toward the electrodes, exhibiting electric field and electron density consistent with simulation results in Ref. 1.

## *Model Definition*

The discharge model is generated from the Reaction Engineering interface with a self-defined discharge chemistry. For more details about the physical model, see Double-Headed Streamer in Parallel-Plate Electrodes.

## *Results and Discussion*

The results in this section are for a double-headed streamer propagating in a background gas kept at a constant density as obtained by the ideal gas law at atmospheric pressure and at a temperature of 293.15 K.

Figure 1 plots the $z$-component of the electric field for several instants during the streamer simulation. Figure 2 shows the electron density distribution at 2.5 ns. These results agree

with that from the model Double-Headed Streamer in Parallel-Plate Electrodes and that from Ref. 1.

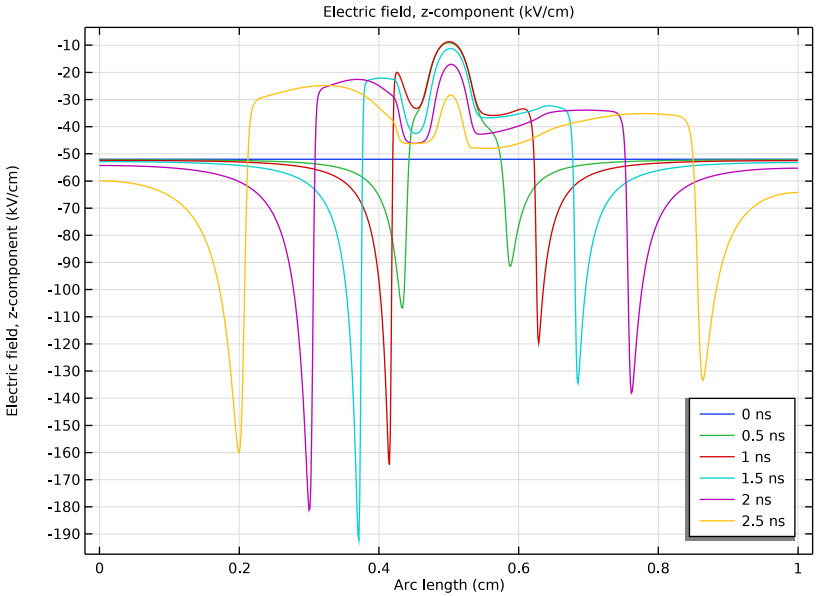



*Figure 1: Spatial distribution along the axis of symmetry of the z-component of the electric field for several time instants during the streamer propagation. Compare with figure 7 of* Ref. 1.

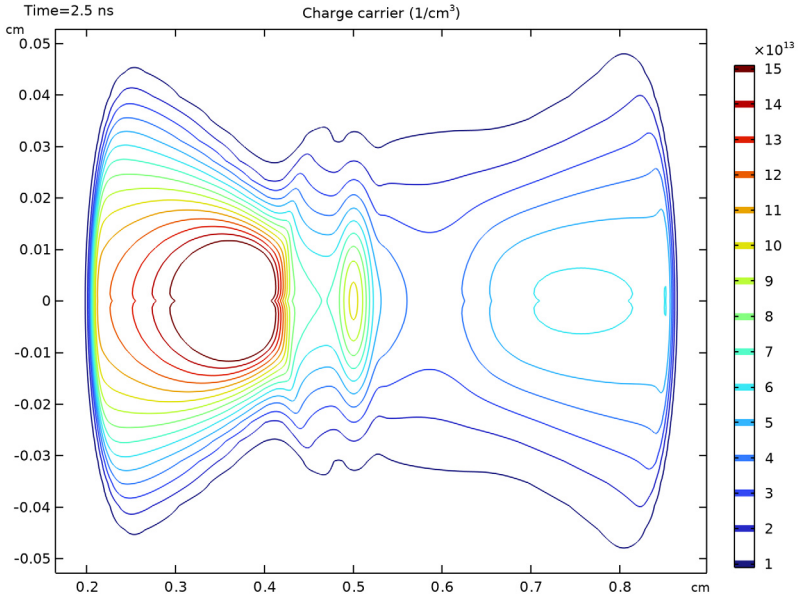



*Figure 2: Contours of the electron number density at 2.5 ns. Compare with figure 6 of* Ref. 1.

## *Reference*

1. D. Bessières, J. Paillol, A. Bourdon, P. Segur, and E. Marode, "A new one-dimensional moving mesh method applied to the simulation of streamer discharges," *J. Phys. D: Appl. Phys.*, vol. 40, pp. 6559–6570, 2007.

**Application Library path:** `Electric_Discharge_Module/Streamer_Discharges/double_headed_streamer_discharge_chemistry`

## *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 **0D**.

2 In the **Select Physics** tree, select **Chemical Species Transport** > **Reaction Engineering (re)**.

3 Click **Add**.

4 Click **Study**.

5 Click **Done**.

## REACTION ENGINEERING (RE)

*Reaction 1*

1 In the **Reaction Engineering** toolbar, click **Reaction**.

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

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

4 Click **Apply**.

5 Locate the **Rate Constants** section. In the $k^{\mathrm{f}}$ text field, type `0`.

*Species: e*

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

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

3 In the $z$ text field, type `-1`.

*Species: M*

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

2 In the **Settings** window for **Species**, locate the **Constant Concentration/Activity** section.

3 Select the **Keep concentration/activity constant** checkbox.

*Initial Values 1*

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

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

3 In the table, enter the following settings:

| Species | Concentration (mol/m^3) |
|---|---|
| M | cM |

*Species: p*

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

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

3 In the *z* text field, type 1.

*Generate Space-Dependent Model 1*

1 In the **Reaction Engineering** toolbar, click **Generate Space-Dependent Model**.

2 In the **Settings** window for **Generate Space-Dependent Model**, locate the **Component Settings** section.

3 From the **Component to use** list, choose **2Daxi: New**.

4 Locate the **Physics Interfaces** section. Find the **Chemical species transport** subsection. From the list, choose **Transport of Charge Carriers: New**.

5 Select the **Electrostatics** checkbox.

6 Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

### COMPONENT 2 (COMP2)

In the **Model Builder** window, expand the **Component 2 (comp2)** node.

### GEOMETRY 1 (2DAXI)

1 In the **Model Builder** window, expand the **Component 2 (comp2)** > **Geometry 1 (2Daxi)** node, then click **Geometry 1 (2Daxi)**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **cm**.

*Rectangle 1 (r1)*

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, click to expand the **Layers** section.

3 Clear the **Layers on bottom** checkbox.

4 Select the **Layers to the left** checkbox.

5 In the table, enter the following settings:

| Layer name | Thickness (cm) |
|---|---|
| Layer 1 | 0.06 |

6 Click **Build All Objects**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

## ELECTROSTATICS (ES)

*Space Charge Density 1*

1 In the **Model Builder** window, expand the **Component 2 (comp2)** > **Electrostatics (es)** node, then click **Space Charge Density 1**.

2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

3 Click the  **Select All** button in the **Graphics** toolbar.

## GLOBAL DEFINITIONS

*Parameters 1*

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

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

3 In the table, enter the following settings:

| Name | Expression | Value | Description |
|---|---|---|---|
| P | 1[atm] | 1.0133E5 Pa | Gas pressure |
| mu | 2.9e5/(P/1[Torr])*1[cm^2/V/s] | 0.038158 m²/(V·s) | Electron mobility |
| cM | P/R_const/300[K] | 40.622 mol/m³ | Gas molar concentration |
| V0 | 52[kV] | 52000 V | Applied voltage |

*Analytic 1 (an1)*

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

2 In the **Settings** window for **Analytic**, type `alphaFun` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `5.7*P/1[Torr]*exp(-260*P/1[Torr]/x)`.

4 Locate the **Units** section. In the **Function** text field, type `cm^-1`.

5 In the table, enter the following settings:

| Argument | Unit |
|---|---|
| x | V/cm |

## CHEMISTRY (CHEM)

*1: e + M => p + 2 e*

1 In the **Model Builder** window, expand the **Component 2 (comp2)** > **Chemistry (chem)** node, then click **1: e + M => p + 2 e**.

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

3 In the $k^f$ text field, type `alphaFun(es.normE)*mu*es.normE/cM`.

*Species: e*

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

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

3 In the $M$ text field, type `5.5e-7[kg/mol]`.

*Species: M (Constant)*

1 In the **Model Builder** window, click **Species: M (Constant)**.

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

3 In the $M$ text field, type `0.029[kg/mol]`.

*Species: p*

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

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

3 In the $M$ text field, type `0.029[kg/mol]`.

### ELECTROSTATICS (ES)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Electrostatics (es)**.

2 In the **Settings** window for **Electrostatics**, click to expand the **Discretization** section.

*Ground 1*

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

2 Select Boundaries 2 and 5 only.

*Electric Potential 1*

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

2 Select Boundaries 3 and 6 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the $V_0$ text field, type `V0`.

### DEFINITIONS (COMP2)

*Variables 1*

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Definitions** and choose **Variables**.

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

**3** In the table, enter the following settings:

| Name | Expression | Unit | Description |
|---|---|---|---|
| n0 | (1e8+1e14*exp(-((z/(1[cm])-0.5)/0.027)^2-(r/(1[cm]))/0.021)^2))[cm^-3] | 1/m³ | Initial condition |

### TRANSPORT OF CHARGE CARRIERS (TCC)

*Initial Values 1*

**1** In the **Model Builder** window, expand the **Component 2 (comp2)** > **Transport of Charge Carriers (tcc)** node, then click **Initial Values 1**.

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

**3** In the $n_{ne}$ text field, type `n0`.

**4** In the $n_{np}$ text field, type `n0`.

*Transport Properties 1*

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

**2** In the **Settings** window for **Transport Properties**, locate the **Drift** section.

**3** In the $\mu_{ne}$ text field, type `mu`.

**4** In the $\mu_{np}$ text field, type `0`.

**5** Locate the **Diffusion** section. In the $D_{np}$ text field, type `0`.

**6** From the list, choose **Diagonal**.

**7** Specify the $D_{ne}$ matrix as

| | |
|---|---|
| 1800[cm^2/s] | 0 |
| 0 | 2190[cm^2/s] |

### MESH 1

*Mapped 1*

**1** In the **Mesh** toolbar, click  **Mapped**.

**2** In the **Settings** window for **Mapped**, locate the **Domain Selection** section.

**3** From the **Geometric entity level** list, choose **Domain**.

**4** Select Domain 1 only.

*Distribution 1*

1 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 20.

6 In the **Element ratio** text field, type 10.

7 Select the **Reverse direction** checkbox.

*Distribution 2*

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1 and 4 only.

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

4 In the **Number of elements** text field, type 800.

*Free Triangular 1*

1 In the **Mesh** toolbar, click  **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click  **Build All**.

## STUDY 1

*Step 2: Time Dependent*

In the **Study** toolbar, click  **Time Dependent**.

*Step 1: Stationary*

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

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the **Solve for** column of the table, under **Component 2 (comp2)**, clear the checkboxes for **Chemistry (chem)** and **Transport of Charge Carriers (tcc)**.

*Step 2: Time Dependent*

1 In the **Model Builder** window, click **Step 2: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 In the **Solve for** column of the table, clear the checkbox for **Component 1 (comp1)**.

4 Locate the **Study Settings** section. From the **Time unit** list, choose **ns**.

5 In the **Output times** text field, type `range(0,0.5,2.5)`.

*Solution 1 (sol1)*

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

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

3 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Stationary Solver 1** node.

4 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Dependent Variables 1** node, then click **Electric Potential (comp2.V)**.

5 In the **Settings** window for **Field**, locate the **Scaling** section.

6 From the **Method** list, choose **Manual**.

7 In the **Scale** text field, type `1e3`.

8 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Dependent Variables 2** node, then click **Electric Potential (comp2.V)**.

9 In the **Settings** window for **Field**, locate the **Scaling** section.

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

11 In the **Scale** text field, type `1e3`.

12 In the **Model Builder** window, under **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** click **Time-Dependent Solver 1**.

13 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

14 From the **Maximum step constraint** list, choose **Constant**.

15 In the **Maximum step** text field, type `0.01[ns]`.

16 From the **Maximum BDF order** list, choose **3**.

17 From the **Minimum BDF order** list, choose **2**.

18 Find the **Algebraic variable settings** subsection. From the **Error estimation** list, choose **Exclude algebraic**.

19 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Time-Dependent Solver 1** node, then click **Direct 1**.

20 In the **Settings** window for **Direct**, locate the **General** section.

21 From the **Solver** list, choose **PARDISO**.

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

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

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

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

## RESULTS

### *Electric Field*

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution 1 (2) (sol1)**.

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

### *Line Graph 1*

1 Right-click **Electric Field** and choose **Line Graph**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

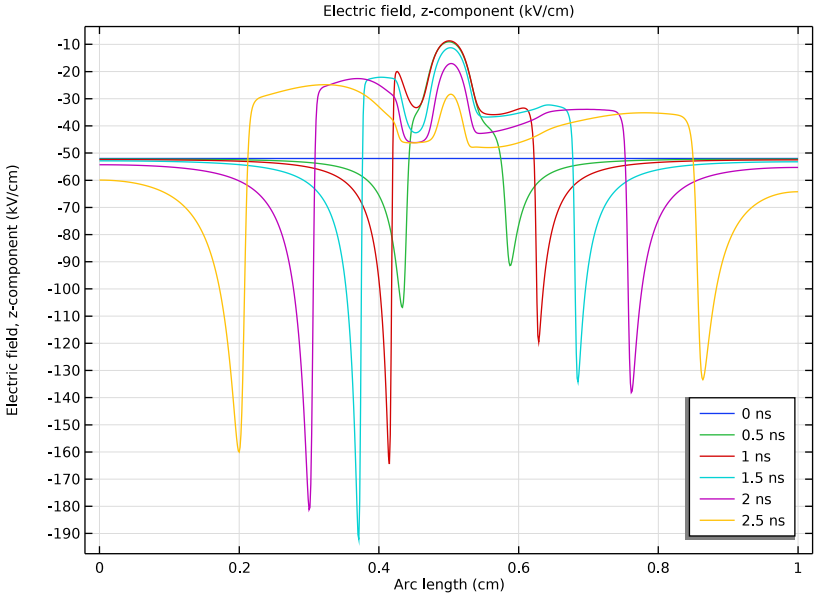
4 In the **Expression** text field, type `es.Ez`.

5 In the **Unit** field, type `kV/cm`.

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

7 In the **Electric Field** toolbar, click **Plot**.

8 Click the **Zoom Extents** button in the **Graphics** toolbar.



*2D Plot Group 2*

In the **Results** toolbar, click **2D Plot Group**.

*Mirror 2D 1*

In the **Results** toolbar, click **More Datasets** and choose **Mirror 2D**.

*Electron Density*

1. In the **Model Builder** window, under **Results** click **2D Plot Group 2**.
2. In the **Settings** window for **2D Plot Group**, type `Electron Density` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Mirror 2D 1**.

*Contour 1*

1. Right-click **Electron Density** and choose **Contour**.
2. In the **Settings** window for **Contour**, locate the **Expression** section.
3. In the **Unit** field, type `1/cm^3`.
4. Locate the **Levels** section. From the **Entry method** list, choose **Levels**.
5. In the **Levels** text field, type `range(1.0e13,1.0e13,1.5e14)`.

*Electron Density*

1. In the **Model Builder** window, click **Electron Density**.
2. In the **Settings** window for **2D Plot Group**, locate the **Plot Settings** section.
3. Clear the **Plot dataset edges** checkbox.
4. From the **View** list, choose **View 1**.
5. Click **Go to Source**.

### DEFINITIONS (COMP2)

*Axis*

1. Click the **Zoom Extents** button in the **Graphics** toolbar.
2. In the **Model Builder** window, expand the **View 1** node, then click **Axis**.
3. In the **Settings** window for **Axis**, locate the **Axis** section.
4. In the ***r* minimum** text field, type `0`.
5. In the ***r* maximum** text field, type `0.06`.
6. In the ***z* minimum** text field, type `0`.
7. In the ***z* maximum** text field, type `1`.
8. From the **View scale** list, choose **Automatic**.

## RESULTS

### *Transformation 1*

1 In the **Model Builder** window, right-click **Contour 1** and choose **Transformation**.

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

3 Select the **Rotate** checkbox.

4 In the **Angle** text field, type `-90`.

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

6 Click the **Zoom Extents** button in the **Graphics** toolbar.