Model created in COMSOL Multiphysics 6.4

# Charge Transport Dynamics in Polyethylene

## *Introduction*

The study explores charge transport dynamics in polyethylene, a common solid dielectric insulation material. It employs a bipolar charge transport model to calculate the densities of electrons, holes, and their trapped counterparts. The simulation's outcomes for discharge current and space charge distribution closely match experimental measurements.

## *Model Definition*

The Electric Discharge interface is used to simulate the charge transport in polyethylene. The built-in bipolar transport model is used:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (\mathbf{w}_i n_i - D_i \nabla n_i) = R_i$$

where

$i = \mathrm{e, h, te, th}$

$z_{\mathrm{e,\ h,\ te,\ th}} = -1, +1, -1, +1$

$\mathbf{w}_i = z_i \mu_i \mathbf{E}$

$$R_{\mathrm{e}} = A_{\mathrm{e}} n_{\mathrm{te}} - B_{\mathrm{e}} n_{\mathrm{e}}\left(1 - \frac{n_{\mathrm{te}}}{n_{0,\mathrm{te}}}\right) - C_1 n_{\mathrm{e}} n_{\mathrm{th}} - C_3 n_{\mathrm{e}} n_{\mathrm{h}}$$

$$R_{\mathrm{h}} = A_{\mathrm{h}} n_{\mathrm{th}} - B_{\mathrm{h}} n_{\mathrm{h}}\left(1 - \frac{n_{\mathrm{th}}}{n_{0,\mathrm{th}}}\right) - C_2 n_{\mathrm{h}} n_{\mathrm{te}} - C_3 n_{\mathrm{e}} n_{\mathrm{h}}$$

$$R_{\mathrm{te}} = -A_{\mathrm{e}} n_{\mathrm{te}} + B_{\mathrm{e}} n_{\mathrm{e}}\left(1 - \frac{n_{\mathrm{te}}}{n_{0,\mathrm{te}}}\right) - C_0 n_{\mathrm{te}} n_{\mathrm{th}} - C_2 n_{\mathrm{h}} n_{\mathrm{te}}$$

$$R_{\mathrm{th}} = -A_{\mathrm{h}} n_{\mathrm{th}} + B_{\mathrm{h}} n_{\mathrm{h}}\left(1 - \frac{n_{\mathrm{th}}}{n_{0,\mathrm{th}}}\right) - C_0 n_{\mathrm{te}} n_{\mathrm{th}} - C_1 n_{\mathrm{e}} n_{\mathrm{th}}$$

$$A_{\mathrm{e}} = \nu_{\mathrm{te}} \exp\left(-\frac{e\varphi_{\mathrm{te}}}{k_B T}\right) \frac{n_{\mathrm{te}}}{n_{0,\mathrm{te}}}$$

$$A_{\mathrm{h}} = \nu_{\mathrm{th}} \exp\left(-\frac{e\varphi_{\mathrm{th}}}{k_B T}\right) \frac{n_{\mathrm{th}}}{n_{0,\mathrm{th}}}$$

where

- e, h, te, and th denote electrons, holes, trapped electrons, and trapped holes
- $n_i$ is the number density of the charge carrier (SI unit: $1/\mathrm{m}^3$)
- $\mathbf{E}$ is the electric field (SI unit: V/m)
- $z_i$ denotes the carrier charge (SI unit: 1)

- $\mu_i$ denotes the carrier mobility (SI unit: $m^2/(V{\cdot}s)$)
- $\mathbf{w}_i$ is the drift velocity in the electric field (SI unit: m/s)
- $D_i$ is the diffusion coefficient (SI unit: $m^2/s$)
- $R_i$ is the reaction rate (SI unit: $1/(m^3{\cdot}s)$)
- $A_e$ and $A_h$ are detrapping rate for trapped electrons and trapped holes (SI unit: 1/s)
- $B_e$ and $B_h$ are trapping rate for electrons and holes (SI unit: 1/s)
- $\nu_{te}$ and $\nu_{th}$ are attempt-to-escape frequency for trapped electrons and trapped holes (SI unit: 1/s)
- $\varphi_{te}$ and $\varphi_{th}$ are detrapping barrier height for trapped electrons and trapped holes (SI unit: V)
- $n_{0,te}$ and $n_{0,th}$ are density of deep traps for electrons and holes (SI unit: $1/m^3$)
- $k_B$ is the Boltzmann constant (SI unit: J/K)
- $T$ is the temperature (SI unit: K)
- $C_0$ is the trapped electron–trapped hole recombination coefficient (SI unit: $m^3/s$)
- $C_1$ is the electron–trapped hole recombination coefficient (SI unit: $m^3/s$)
- $C_2$ is the trapped electron–hole recombination coefficient (SI unit: $m^3/s$)
- $C_3$ is the electron–hole recombination coefficient (SI unit: $m^3/s$)

The above transport equations are fully coupled with Poisson's equation through the electric field and the space charge:

$$\nabla \cdot (\varepsilon_r \varepsilon_0 \mathbf{E}) = \rho$$

$$\rho = e\sum_i z_i n_i$$

## *Results and Discussion*

Figure 1 shows the distribution of the number density of electrons and holes at $t = 1$ s, 100 s, and 10,000 s under a 12 kV DC voltage (initial electric field 80 kV/mm). Figure 2 shows the evolution of the electric field, Figure 3 shows the total discharge current, and Figure 4 shows the dynamics of the space charge density.

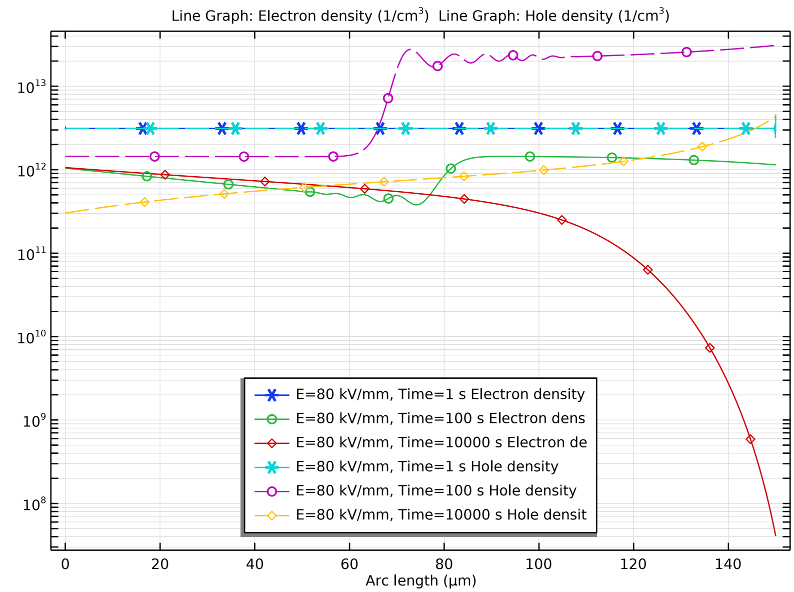


*Figure 1: Electron and hole number density at t = 1, 100, 10 000 s under 12 kV DC voltage.*

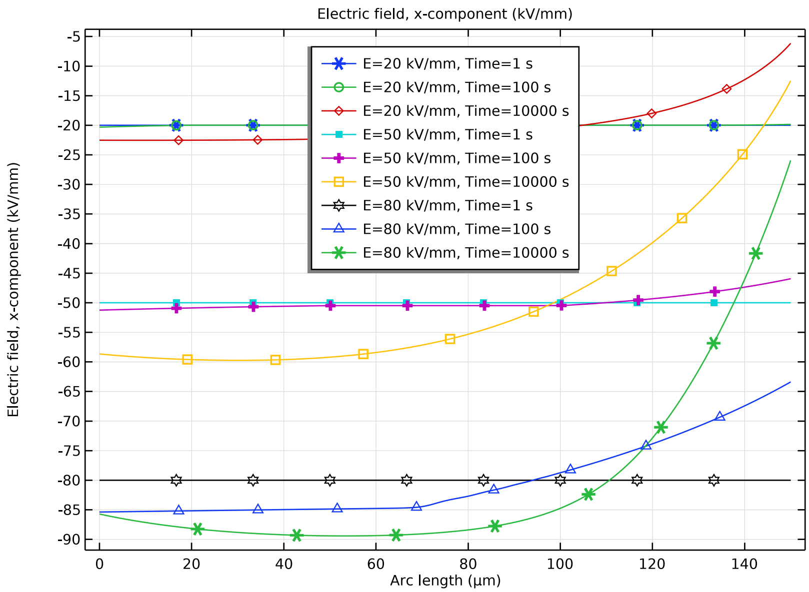


*Figure 2: The electric field distribution at t = 0, 100, 10 000 s.*

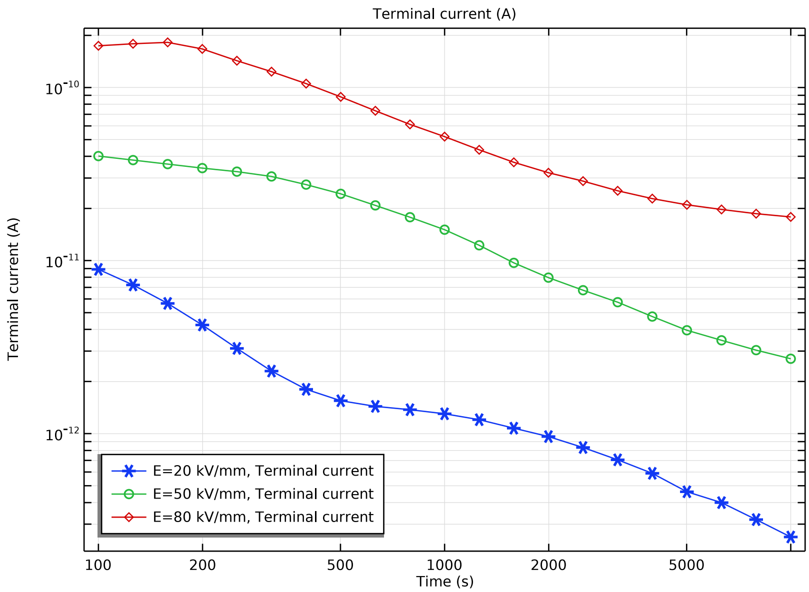


*Figure 3: The total current as a function of time.*

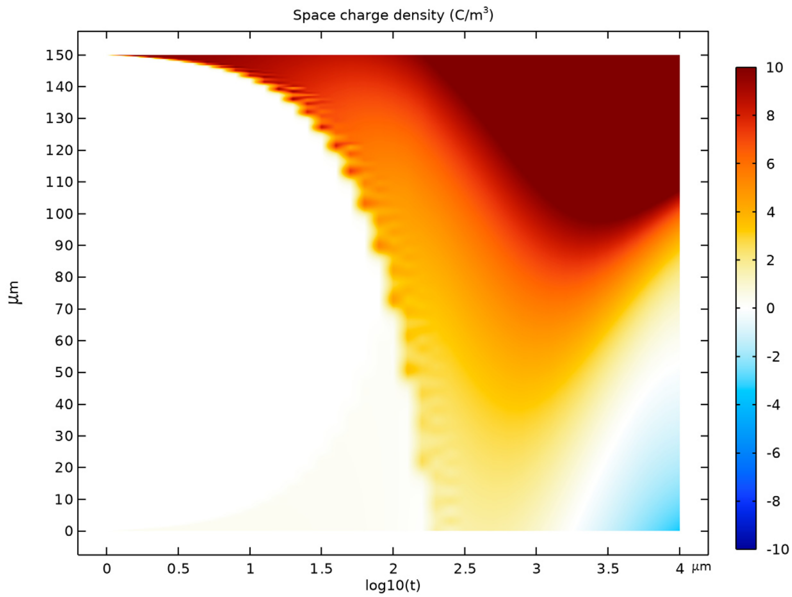


*Figure 4: The dynamics of space charge density where the x-axis is time in logarithmic scale and the y-axis is the thickness of the sample.*

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**Application Library path:** `Electric_Discharge_Module/Solid_Dielectrics/charge_transport_in_polyethylene`

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## *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 **1D**.

2 In the **Select Physics** tree, select **Electric Discharge** > **Electric Discharge (edis)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Time Dependent with Initialization**.

6 Click **Done**.

## 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 |
|---|---|---|---|
| d | 150[um] | 1.5E-4 m | Thickness |
| E | 20[kV/mm] | 2E7 V/m | Initial electric field |
| V0 | d*E | 3000 V | Applied voltage |

## GEOMETRY 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Geometry 1** node, then click **Geometry 1**.

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

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

### *Interval 1 (i1)*

1 Right-click **Geometry 1** and choose **Interval**.

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

3 In the table, enter the following settings:

| Coordinates (µm) |
|---|
| 0 |
| d |

4 Click **Build Selected**.

## ELECTRIC DISCHARGE (EDIS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electric Discharge (edis)**.

2 In the **Settings** window for **Electric Discharge**, locate the **Physical Model** section.

3 Clear the **Gas** checkbox.

4 Select the **Solid** checkbox.

5 Click the **Show More Options** button in the **Model Builder** toolbar.

6 In the **Show More Options** dialog, select **Physics** > **Stabilization** in the tree.

7 In the tree, select the checkbox for the node **Physics** > **Stabilization**.

8 Click **OK**.

9 In the **Settings** window for **Electric Discharge**, click to expand the **Inconsistent Stabilization** section.

10 Select the **Isotropic diffusion** checkbox.

11 In the $\delta_{id}$ text field, type `0.25`.

### ADD MATERIAL

1 In the **Materials** toolbar, click **Add Material** to open the **Add Material** window.

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

3 In the tree, select **Electric Discharge** > **Solids** > **Polyethylene**.

4 Right-click and choose **Add to Component 1 (comp1)**.

5 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

### ELECTRIC DISCHARGE (EDIS)

#### *Electrode 1*

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode**.

2 Select Boundary 1 only.

#### *Solid 1*

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

#### *Electrode 2*

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Electrode**, locate the **Terminal** section.

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

#### *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 $n_e$ text field, type `0.5[C/m^3]/e_const`.

**4** In the $n_h$ text field, type `0.5[C/m^3]/e_const`.

## MESH 1

### *Edge 1*

In the **Mesh** toolbar, click **Edge**.

### *Distribution 1*

**1** Right-click **Edge 1** and choose **Distribution**.

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

**3** From the **Distribution type** list, choose **Predefined**.

**4** In the **Number of elements** text field, type `1000`.

**5** In the **Element ratio** text field, type `5`.

**6** Select the **Symmetric distribution** checkbox.

**7** Click **Build All**.

## STUDY 1

### *Parametric Sweep*

**1** In the **Study** toolbar, click **Parametric Sweep**.

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

**3** Click **Add**.

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

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| E (Initial electric field) | 20 50 80 | kV/mm |

### *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 **Study Settings** section.

**3** In the **Output times** text field, type `10^{range(log10(1),1/10,log10(1e4))}`.

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

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

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

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

## RESULTS

### *Charge Carrier Density*

1. In the **Model Builder** window, expand the **Results** node.
2. Right-click **Results** and choose **1D Plot Group**.
3. In the **Settings** window for **1D Plot Group**, type `Charge Carrier Density` in the **Label** text field.
4. Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.
5. From the **Parameter selection (E)** list, choose **Last**.
6. From the **Time selection** list, choose **Interpolated**.
7. In the **Times (s)** text field, type `1 1e2 1e4`.
8. Locate the **Legend** section. From the **Position** list, choose **Lower middle**.

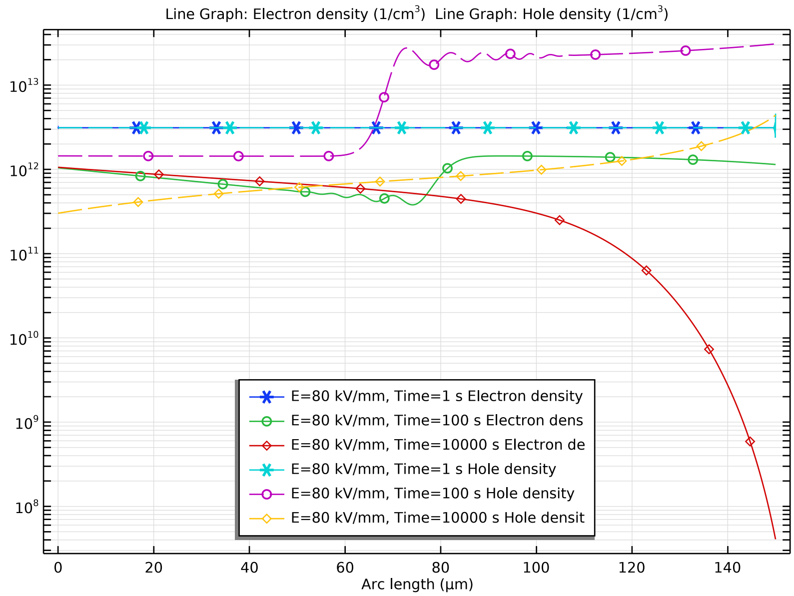
### *Line Graph 1*

1. Right-click **Charge Carrier Density** and choose **Line Graph**.
2. Select Domain 1 only.
3. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
4. In the **Expression** text field, type `edis.n_e`.
5. In the **Unit** field, type `1/cm^3`.
6. Click to expand the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.
7. From the **Positioning** list, choose **Interpolated**.
8. Click to expand the **Legends** section. Select the **Show legends** checkbox.
9. Find the **Include** subsection. Select the **Description** checkbox.

### *Line Graph 2*

1. Right-click **Line Graph 1** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3. In the **Expression** text field, type `edis.n_h`.
4. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
5. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle (reset)**.
6. Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

**7** In the **Charge Carrier Density** toolbar, click **Plot**.




### *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 **Legend** section. From the **Position** list, choose **Upper middle**.

**4** Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

**5** From the **Time selection** list, choose **Interpolated**.

**6** In the **Times (s)** text field, type `1 1e2 1e4`.

### *Line Graph 1*

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

**2** Select Domain 1 only.

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

**4** In the **Expression** text field, type `edis.Ex`.

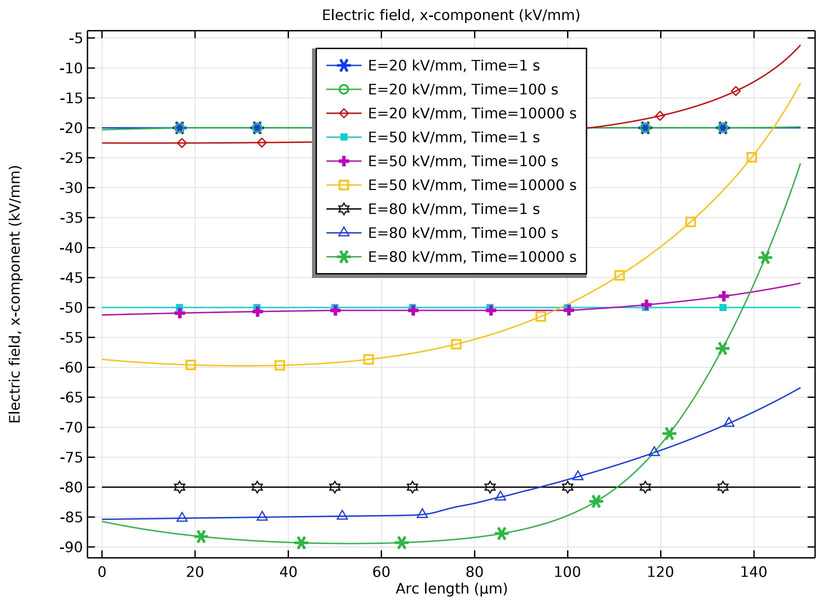
**5** In the **Unit** field, type `kV/mm`.

**6** Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

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

**8** Locate the **Legends** section. Select the **Show legends** checkbox.

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




*Discharge Current*

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

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

**3** Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

**4** From the **Time selection** list, choose **Interpolated**.

**5** In the **Times (s)** text field, type `10^{range(log10(100),1/10,log10(1e4))}`.

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

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

**8** Select the **y-axis log scale** checkbox.

*Global 1*

**1** Right-click **Discharge Current** and choose **Global**.

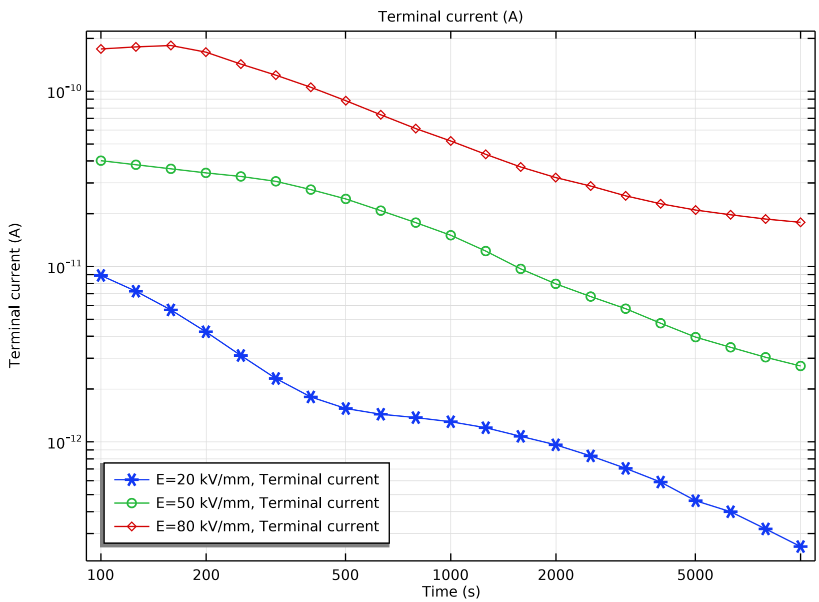
**2** In the **Settings** window for **Global**, locate the **y-Axis Data** section.

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

| Expression | Unit | Description |
|---|---|---|
| `edis.I0_1` | `A` | `Terminal current` |

**4** Click to expand the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

**5** In the **Discharge Current** toolbar, click **Plot**.




*Parametric Extrusion 1D 1*

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

**2** Right-click **Results** > **Datasets** and choose **More Datasets** > **Parametric Extrusion 1D**.

**3** In the **Settings** window for **Parametric Extrusion 1D**, locate the **Data** section.

**4** From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.

**5** From the **Parameter selection (E)** list, choose **Last**.

**6** Locate the **Settings** section. From the **Level transformation** list, choose **Expression**.

**7** In the **Transformation expression** text field, type `log10(level)`.

*Transformation 2D 1*

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

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

3 From the **Transformation type** list, choose **General**.

4 Find the **Base vectors** subsection. In row **x**, set **First** to `0`.

5 In row **x**, set **Second** to `1`.

6 In row **y**, set **First** to `1`.

7 In row **y**, set **Second** to `0`.

*Space Charge Density Dynamics*

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

2 In the **Settings** window for **2D Plot Group**, type `Space Charge Density Dynamics` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Transformation 2D 1**.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `log10(t)`.

6 Select the **y-axis label** checkbox. In the associated text field, type `\mu m`.

7 Clear the **Plot dataset edges** checkbox.

*Surface 1*

1 Right-click **Space Charge Density Dynamics** and choose **Surface**.

2 In the **Settings** window for **Surface**, click to expand the **Range** section.

3 Select the **Manual color range** checkbox.

4 In the **Minimum** text field, type `-10`.

5 In the **Maximum** text field, type `10`.

6 Locate the **Coloring and Style** section. From the **Color table** list, choose **Ranitomeya**.

**7** In the **Space Charge Density Dynamics** toolbar, click **Plot**.