



Model created in COMSOL Multiphysics 6.4

# 1D Lithium-Ion Battery Model for the SEI Formation Tutorial

## *Introduction*

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This is a template model containing the physics, geometry, and mesh of a lithium-ion battery (without any SEI (solid-electrolyte-interface) reactions or mechanisms added). The [SEI Formation in a Lithium-Ion Battery](#) application available in the Application Library makes use of this model setup.

The battery cell model is created using the Lithium-Ion Battery interface. A more detailed description on how to set up this type of model can be found in the model example [1D Isothermal Lithium-Ion Battery](#).

## *Model Definition*

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The model is set up for a graphite/NCA battery cell. The materials are available from the Battery material library and mainly default settings are selected. The model domains consist of:

- Negative porous electrode: Graphite (MCMB  $\text{Li}_x\text{C}_6$ ) active material
- Separator
- Positive porous electrode: NCA ( $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ ) active material
- Electrolyte: 1.0 M  $\text{LiPF}_6$  in EC:EMC (3:7 by weight)

The Lithium-Ion Battery interface accounts for:

- Electronic conduction in the electrodes
- Ionic charge transport in the electrodes and electrolyte/separator
- Material transport in the electrolyte, allowing for the introduction of the effects of concentration on ionic conductivity and concentration overpotential
- Material transport within the spherical particles that form the electrodes
- Butler–Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium potential

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**Application Library path:** Battery\_Design\_Module/Lithium-Ion\_Batteries, Aging\_and\_Abuse/sei\_formation\_seed


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## Modeling Instructions




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

### NEW

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

### MODEL WIZARD


- 1 In the **Model Wizard** window, click  **ID**.
- 2 In the **Select Physics** tree, select **Electrochemistry** > **Batteries** > **Lithium-Ion Battery (liion)**.
- 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**.

### ROOT

Add the model parameters from a text file.

### 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 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `sei_formation_parameters.txt`.

### GEOMETRY 1

#### *Interval 1 (i1)*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.
- 2 In the **Settings** window for **Interval**, locate the **Interval** section.
- 3 From the **Specify** list, choose **Interval lengths**.

4 In the table, enter the following settings:



Lengths (m)
L_neg
L_sep
L_pos

5 Click  **Build All Objects**.

## MATERIALS

Load the materials from the material library.


### 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 **Battery > Electrolytes > LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery)**.
- 4 Right-click and choose **Add to Component 1 (comp1)**.
- 5 In the tree, select **Battery > Electrodes > Graphite, LixC6 MCMB (Negative, Li-ion Battery)**.
- 6 Right-click and choose **Add to Component 1 (comp1)**.
- 7 In the tree, select **Battery > Electrodes > NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery)**.
- 8 Right-click and choose **Add to Component 1 (comp1)**.
- 9 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.


### DEFINITIONS

Explicit selections are made in the model geometry.


#### *Negative Electrode*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Negative Electrode in the **Label** text field.
- 3 Select Domain 1 only.

#### *Separator*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Separator in the **Label** text field.
- 3 Select Domain 2 only.

### *Positive Electrode*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Positive Electrode in the **Label** text field.
- 3 Select Domain 3 only.

### **LITHIUM-ION BATTERY (LIION)**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lithium-Ion Battery (liion)**.
- 2 In the **Settings** window for **Lithium-Ion Battery**, locate the **Cross-Sectional Area** section.
- 3 In the  $A_c$  text field, type  $A_{cell}$ .
- 4 Locate the **Cell Settings** section. Select the **Define cell state of charge (SOC) and initial charge inventory** checkbox.

### *SOC and Initial Charge Distribution 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Lithium-Ion Battery (liion)** click **SOC and Initial Charge Distribution 1**.
- 2 In the **Settings** window for **SOC and Initial Charge Distribution**, locate the **State-of-Charge Definition** section.
- 3 From the list, choose **User defined**. In the  $E_{cell}^{0\%SOC}$  text field, type  $E_{cell\_0SOC}$ .
- 4 In the  $E_{cell}^{100\%SOC}$  text field, type  $E_{cell\_100SOC}$ .
- 5 Locate the **Initial Cell Charge Distribution** section. From the **Define by** list, choose **Cell voltage**.
- 6 In the  $E_{cell,0}$  text field, type  $E_{min}$ .

### *Negative Electrode Domain Selection 1*

- 1 In the **Model Builder** window, click **Negative Electrode Domain Selection 1**.
- 2 In the **Settings** window for **Negative Electrode Domain Selection**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Negative Electrode**.


### *Positive Electrode Domain Selection 1*

- 1 In the **Model Builder** window, click **Positive Electrode Domain Selection 1**.
- 2 In the **Settings** window for **Positive Electrode Domain Selection**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Positive Electrode**.

### Separator 1

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Lithium-Ion Battery (liion)** click **Separator 1**.
- 2 In the **Settings** window for **Separator**, locate the **Porous Matrix Properties** section.
- 3 In the  $\epsilon_1$  text field, type `eps1_sep`.
- 4 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the  $f_1$  text field, type `eps1_sep^brug1_sep`.
- 5 From the **Diffusion** list, choose **User defined**. In the  $f_{D1}$  text field, type `eps1_sep^brug1_sep`.

### Porous Electrode 1

- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.
- 2 In the **Settings** window for **Porous Electrode**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Negative Electrode**.
- 4 Locate the **Electrode Properties** section. In the  $\sigma_s$  text field, type `sigmas_neg`.
- 5 Locate the **Porous Matrix Properties** section. In the  $\epsilon_s$  text field, type `eps_s_neg`.
- 6 In the  $\epsilon_1$  text field, type `eps1_neg`.

### Particle Intercalation 1

- 1 In the **Model Builder** window, click **Particle Intercalation 1**.
- 2 In the **Settings** window for **Particle Intercalation**, locate the **Material** section.
- 3 From the **Particle material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.
- 4 Locate the **Particle Transport Properties** section. In the  $r_p$  text field, type `rp_neg`.
- 5 Click to expand the **Particle Discretization** section. In the  $N_{el}$  text field, type 5.
- 6 Select the **Fast assembly in particle dimension** checkbox.

### Porous Electrode Reaction 1

- 1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Material** section.
- 3 From the **Material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.
- 4 Locate the **Electrode Kinetics** section. In the  $i_{0,ref}(T)$  text field, type `i0ref_neg`.

### Porous Electrode 2

- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.

- 2 In the **Settings** window for **Porous Electrode**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Positive Electrode**.
- 4 Locate the **Electrode Properties** section. In the  $\sigma_s$  text field, type `sigmas_pos`.
- 5 Locate the **Porous Matrix Properties** section. In the  $\epsilon_s$  text field, type `eps_s_pos`.
- 6 In the  $\epsilon_l$  text field, type `eps_l_pos`.
- 7 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the  $f_l$  text field, type `liion.eps_l^brugl_pos`.
- 8 From the **Diffusion** list, choose **User defined**. In the  $f_{Dl}$  text field, type `liion.eps_l^brugl_pos`.

#### *Particle Intercalation I*

- 1 In the **Model Builder** window, click **Particle Intercalation I**.
- 2 In the **Settings** window for **Particle Intercalation**, locate the **Material** section.
- 3 From the **Particle material** list, choose **NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3)**.
- 4 Locate the **Particle Transport Properties** section. In the  $r_p$  text field, type `rp_pos`.
- 5 Locate the **Particle Discretization** section. In the  $N_{el}$  text field, type 3.
- 6 Select the **Fast assembly in particle dimension** checkbox.

#### *Porous Electrode Reaction I*

- 1 In the **Model Builder** window, click **Porous Electrode Reaction I**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Material** section.
- 3 From the **Material** list, choose **NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3)**.
- 4 Locate the **Electrode Kinetics** section. In the  $i_{0,ref}(T)$  text field, type `i0ref_pos`.

#### *Electric Ground I*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Ground**.
- 2 Select Boundary 1 only.

## **GLOBAL DEFINITIONS**

#### *Default Model Inputs*




Set up the temperature value used in the entire model.

- 1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.


- 2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.
- 3 In the tree, select **General > Temperature (K) - minput.T**.
- 4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type T.

## DEFINITIONS

### *Piecewise 1 (pw1)*

- 1 In the **Definitions** toolbar, click  **Piecewise**.
- 2 In the **Settings** window for **Piecewise**, type K in the **Function name** text field.
- 3 Locate the **Definition** section. From the **Smoothing** list, choose **Continuous function**.
- 4 Find the **Intervals** subsection. Click  **Load from File**.
- 5 Browse to the model's Application Libraries folder and double-click the file sei\_formation\_piecewise.txt.
- 6 Click  **Plot**.

### *Variables 1*

- 1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file sei\_formation\_variables.txt.

## STUDY 1

### *Step 2: Time Dependent*

- 1 In the **Model Builder** window, under **Study 1** 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 range(0,180,t\_cycling).