



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

Introduction

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

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 Li_xC_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 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

Application Library path: Battery_Design_Module/Lithium-Ion_Batteries, Aging_and_Abuse/sei_formation_seed




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  **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 I

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

Interval I (i1)

- 1 In the **Model Builder** window, under **Component I (comp1)** right-click **Geometry I** 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 ϵ_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 σ_s text field, type `sigmas_neg`.
- 5 Locate the **Porous Matrix Properties** section. In the ϵ_s text field, type `eps_s_neg`.
- 6 In the ϵ_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 σ_s text field, type `sigmas_pos`.
- 5 Locate the **Porous Matrix Properties** section. In the ϵ_s text field, type `eps_s_pos`.
- 6 In the ϵ_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 I (pwI)

- 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 I

- 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 I

Step 2: Time Dependent

- 1 In the **Model Builder** window, under **Study I** 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).