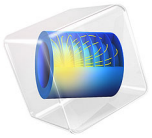

Lithium-Ion Battery Base Model in 1D

Introduction

This is a template base model containing the physics, geometry, and mesh of a lithium-ion battery.

The model is defined using the Lithium-Ion Battery interface, based on the Doyle–Fuller–Newman framework (Ref. 1). For a general introduction to the Lithium-Ion Battery interface, the user is recommended to first run the tutorial 1D Isothermal Lithium-Ion Battery, which is set up in a similar way.

This base model uses the global SOC and Initial Charge Distribution node to define the cell state-of-charge and initial charge inventory. The following tutorials, available in the Battery Design Module Application Library, make use of this base model:

- 1D Lithium-Ion Battery Drive-Cycle Monitoring, which demonstrates how to run the model using a time-dependent current load curve
- Lithium-Ion Battery Rate Capability, which uses the base model to perform a range of discharge simulations at different rates. By modifying the cross-sectional capacity of the cell, an energy-optimized cell is compared to a power-optimized cell in a Ragone plot.
- Lithium-Ion Battery Internal Resistance, which simulates a hybrid pulse power characterization (HPPC) test and makes a full analysis of the different roots of the various voltage losses in the cell.
- Diffusion-Induced Stress in a Lithium-Ion Battery, which adds stresses and strains to the particles and in the negative electrode, and analyzes the mechanical stress that the particles are subjected to during a current load.
- *Surrogate Model Training of a Battery Rate Capability Model*, which is an application that uses the base model to compute data for training a deep neural network function. The application can be used to investigate the effect of battery electrode parameters on the rate capability of the battery.

Model Definition

The model is defined in 1D along the through-layer direction between the metal current collector foils of a lithium jelly roll. The geometry thus consists of one negative porous electrode, one separator and one positive porous electrode domain.

In this tutorial, we will investigate a 21,700 battery where it is assumed that 90% of the internal volume is occupied by the active jelly roll (electrode, separator, and current collector layers). Because of the 1D geometry, the current load of the battery model is formulated as a current density boundary condition with the unit of A/m^2. The cell

current is calculated using a 1C current variable $I_{1C,\,cell}$ (A), which is provided by the SOC and Initial Charge Distribution node. To convert from cell current (A) to cell current density (A/m^2) on the jelly roll, the cell area is used. The cell area is computed as

$$A_{cell} = \frac{V_{cell}}{L_{cell}} \tag{1}$$

where the length L_{cell} of the cell is calculated as

$$L_{cell} = L_{neg} + L_{sep} + L_{pos} + L_{ccs}/2 \tag{2}$$

where L_{ccs} is the sum of the thicknesses of the positive and negative current collector foils in the jelly roll. The factor $1/2$ stems from the configuration of a typical jelly roll, where each metal foil is being coated on both sides by the same electrode layer.

MATERIALS

The battery model consists of the following materials:

- Negative electrode: Graphite (MCMB Li_xC_6)
- Positive electrode: NMC 111 ($Li_{1/3}Mn_{1/3}Co_{1/3}O_2$)
- Electrolyte: 1.0 M $LiPF_6$ in 3:7 EC:EMC

These materials are available from the Battery Material Library.

ELECTRODE THICKNESS BALANCING

The thickness of the positive electrode is set to 45 µm. The negative electrode thickness is calculated based on electrode balancing, using the following criteria:

- In order to avoid lithium plating during fast charging, the negative graphite electrode should have excess host capacity, so that an approximate negative electrode lithiation level of 80% is reached at 100% cell state of charge (SOC).
- In order to avoid dissolution of the active electrode material and other harmful side reactions, the positive electrode potential is limited to about 4.23 V at 100% SOC, corresponding to a positive electrode lithiation level of 10%.

Based on the maximum Li concentration ($c_{s,\,max}$) and volume fractions (ε_s) of the electrode materials, the thickness of the negative electrode may now be computed as

$$L_{neg} = \frac{(1-0.1)\varepsilon_{s,\,NMC} c_{s,\,max,NMC}}{0.8\varepsilon_{s,\,Gr} c_{s,\,max,Gr}} L_{pos}$$

PHYSICAL MODEL

The Lithium-Ion Battery interface, used for defining the model, accounts for:

- Electronic conduction in the electrodes
- Ionic charge transport in the electrodes and electrolyte or separator
- Material transport in the electrolyte, allowing for the introduction of the effects of concentration on the ionic conductivity and concentration overpotentials
- Material transport within the spherical particles that form the electrodes, defined on an extra (pseudo) dimension
- Butler–Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium (half cell) potentials.

This tutorial model uses the global SOC and Initial Charge Distribution node to define the cell state-of-charge and initial charge inventory. This node is activated by enabling Define cell state-of-charge (SOC) and initial charge inventory on the interface top node. In this model, the cell voltages at 0% and 100% SOC are set to be defined from operational potential limits, and the initial cell charge distribution is defined by an initial cell SOC parameter. The total initial charge inventory of the cell is defined by the positive electrode host capacity. A formation loss is added in order to reduce the initial charge inventory, assuming that some charge inventory has been irreversibly lost prior to the start of the simulation.

The Lithium-Ion Battery interface defines and solves for the solid lithium concentration in the electrode particles, individually for each electrode. Based on the lithium concentration, the degree of lithiation, SOL (dimensionless), then relates the solid concentration levels to the maximum concentration of lithium atoms that the electrode material can host:

$$\mathrm{SOL} = \frac{c_{\mathrm{s}}}{c_{s,\mathrm{max}}} \tag{3}$$

The individual degrees of lithiation for each electrode then in turns determine the local equilibrium potential for intercalation (the half cell potentials). During charge of a lithium-ion battery, c_{s} in the negative electrode will increase, whereas c_{s} in the positive electrode will decrease, with the rate being proportional to the battery current.

At open circuit of a fully relaxed cell, the cell voltage $E_{\mathrm{OCV,cell}}$ can be expressed as

$$E_{\mathrm{OCV,cell}} = E_{\mathrm{eq,pos}}(\mathrm{sol}_{\mathrm{pos}}) - E_{\mathrm{eq,neg}}(\mathrm{sol}_{\mathrm{neg}}) \tag{4}$$

where $E_{eq,pos}$ and $E_{eq,neg}$ (V) are the equilibrium potentials, expressed as functions of the degrees of lithiation SOL_{pos} and SOL_{neg} (1) of the positive and negative electrode materials, respectively, based on the average c_s variables of the corresponding electrode.

Unless the degrees of lithiation in the individual electrodes are coupled in some way, there exists an infinite number of combinations of values of SOL_{pos} and SOL_{neg} that fulfill the above equation. However, for an assembled battery cell, a change in SOL_{pos} will always result in a corresponding change in SOL_{neg}, and vice versa. The reason is that the total amount of lithium in the cell is conserved during cycling, resulting in a unique solution to the above equation.

In contrast to the individual electrode degrees of intercalation, which depend on the local concentrations of lithium, the state of charge (SOC) of a battery cell is typically defined on a global level as being proportional to the amount of charge passed when cycling between two corresponding open circuit voltage limits. The lower voltage limit corresponds to 0% SOC, and the upper voltage limit corresponds to 100% SOC. A cell state-of-charge variable is automatically calculated by the SOC and Initial Charge Distribution node.

Reference

1. M. Doyle, J. Newman, A.S. Gozdz, C.N. Schmutz, and J.M. Tarascon, "Comparison of Modeling Predictions with Experimental Data from Plastic Lithium Ion Cells," *J. Electrochem. Soc.*, vol. 143, no. 6, pp. 1890–1903, 1996.

Application Library path: `Battery_Design_Module/Lithium-Ion_Batteries,_Performance/lib_base_model_1d`

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 **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**.

GLOBAL DEFINITIONS

Parameters 1

Load the parameters from a text file.

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 `lib_base_model_1d_parameters.txt`.

ADD MATERIAL

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

Add some data for the electrolyte and the electrodes from the material library.

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** > **NMC 111, LiNi0.33Mn0.33Co0.33O2 (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.

GEOMETRY 1

Draw the model geometry by defining the individual thicknesses of the negative electrode, the separator and the positive electrode.

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 Selected**.

MATERIALS

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)

Now assign the previously added materials to the different domains of the geometry. Create selections at the same time to facilitate choosing the same domains later on.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** click **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.

2 Select Domain 2 only.

3 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

4 Click  **Create Selection**.

5 In the **Create Selection** dialog, type `Separator` in the **Selection name** text field.

6 Click **OK**.

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)

1 In the **Model Builder** window, click **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

3 Click  **Clear Selection**.

4 Select Domain 1 only.

5 Click  **Create Selection**.

6 In the **Create Selection** dialog, type `Negative Electrode` in the **Selection name** text field.

7 Click **OK**.

NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)

1 In the **Model Builder** window, click **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.

2 Select Domain 3 only.

3 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

4 Click **Create Selection**.

5 In the **Create Selection** dialog, type `Positive Electrode` in the **Selection name** text field.

6 Click **OK**.

LITHIUM-ION BATTERY (LIION)

Now start defining the physics. Use the **SOC and Initial Charge Distribution** node in order to calculate the initial charge distribution in the cell.

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 **Initial Cell Charge Distribution** section.

3 In the SOC_0 text field, type `soc_init`.

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_l text field, type `epsl_sep`.

Porous Electrode - Negative

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

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode - Negative` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Negative Electrode**.

4 Locate the **Electrolyte Properties** section. From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.

5 Locate the **Electrode Properties** section. In the σ_s text field, type `sigmas_neg`.

6 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `epss_neg`.

7 In the ε_l text field, type `epsl_neg`.

8 Locate the **Effective Transport Parameter Correction** section. From the **Electric conductivity** list, choose **No correction**.

Particle Intercalation 1

1 In the **Model Builder** window, click **Particle Intercalation 1**.

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

3 In the r_p text field, type `rp_neg`.

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 **Electrode Kinetics** section.

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_neg`.

Porous Electrode - Positive

1 In the **Model Builder** window, right-click **Porous Electrode - Negative** and choose **Duplicate**.

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode - Positive` in the **Label** text field.

3 Locate the **Domain Selection** section. 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 `epss_pos`.

6 In the ε_l text field, type `epsl_pos`.

Particle Intercalation 1

1 In the **Model Builder** window, expand the **Porous Electrode - Positive** node, then click **Particle Intercalation 1**.

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

3 In the r_p text field, type `rp_pos`.

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 **Electrode Kinetics** section.

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_pos`.

Electric Ground 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Electric Ground**, locate the **Boundary Selection** section.

4 Click **Create Selection**.

5 In the **Create Selection** dialog, type `Negative CC` in the **Selection name** text field.

6 Click **OK**.

Electrode Current Density 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current Density**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Electrode Current Density**, locate the **Boundary Selection** section.

4 Click **Create Selection**.

5 In the **Create Selection** dialog, type `Positive CC` in the **Selection name** text field.

6 Click **OK**.

7 In the **Settings** window for **Electrode Current Density**, locate the **Electrode Current Density** section.

8 In the $i_{n,s}$ text field, type `I_1C`.

GLOBAL DEFINITIONS

Default Model Inputs

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 (COMP1)

Load some variables definitions from a text file.

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** 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 `lib_base_model_1d_variables.txt`.

Point Probe 1 (point1)

1 In the **Definitions** toolbar, click **Probes** and choose **Point Probe**.

2 In the **Settings** window for **Point Probe**, type `E_cell` in the **Variable name** text field.

3 Locate the **Probe Type** section. From the **Type** list, choose **Integral**.

4 Locate the **Source Selection** section. From the **Selection** list, choose **Positive CC**.

5 Locate the **Expression** section. In the **Expression** text field, type `phis`.

6 Select the **Description** checkbox. In the associated text field, type `Cell voltage`.

7 Click to expand the **Table and Window Settings** section. Click **Add Table**.

RESULTS

In the **Model Builder** window, expand the **Results** node.

Cell Voltage Probe Data

1 In the **Model Builder** window, expand the **Results** > **Tables** node, then click **Table 1**.

2 In the **Settings** window for **Table**, type `Cell Voltage Probe Data` in the **Label** text field.

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 From the **Time unit** list, choose **h**.

4 In the **Output times** text field, type `range(0,0.1,0.9)`.