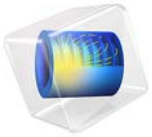

Lithium-Ion Battery Base Model in 1D

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 introduces a number of lithiation parameters which are used to define the relative balancing of the negative and positive electrodes, defining the degrees of lithiations in the individual electrodes at 0% and 100 % cell state of charge (SOC). This allows for a global SOC variable to be defined in the model, and for defining the initial lithiation levels of the electrodes based on an initial SOC parameter value. In addition, a cell cross-sectional capacity parameter is used to define the electrode thicknesses.

The following tutorials, available in the Battery Design 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 hybride 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.

Model Definition

GEOMETRY

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.

Given the 1D geometry, the capacity of the cell is defined per cross-sectional area as Ah/m^2, and the current boundary condition for the physical model is expressed as a current density (A/m^2). Conversion to and from total capacity and current (Ah and A) from and to areal capacity and current density (Ah/m^2 and A/m^2) can be done based on the layer thicknesses and an assumed active jelly roll volume. This is exemplified in the Lithium-Ion Battery Internal Resistance tutorial.

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.

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/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.

CELL STATE OF CHARGE DEFINITION BASED ON THE ELECTRODE DEGREES OF LITHIATION

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 concentrations, the degrees of lithiation, sol (dimensionless), then relates the solid concentration levels to the maximum concentrations of lithium atoms that the electrode materials can host.

$$\text{sol} = \frac{c_s}{c_{s,\max}} \tag{1}$$

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 $E_{OCV,cell}$ can be expressed as

$$E_{OCV,cell} = E_{eq,pos}(sol_{pos}) - E_{eq,neg}(sol_{neg}) \tag{2}$$

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 for values of sol_{pos} and sol_{neg} to fulfill the above equation. For an assembled battery cell however, a change in sol_{pos} will always result in a corresponding change in sol_{neg} and vice versa since the total amount of lithium in the cell 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 corresponding to 0% SOC and the upper voltage limit to 100% SOC.

To define the conversion between the global SOC and the local sol variables, the model makes use of the four lithiation parameters $sol_{pos,100}$, $sol_{neg,100}$, $sol_{pos,0}$ and $sol_{neg,0}$ for the degrees of lithiation in the positive and negative electrodes at 100 and 0% SOC, respectively. Generally, as a result of the negative electrode being lithiated during charge, and the positive electrode being delithiated, $sol_{neg,100} > sol_{neg,0}$ and $sol_{pos,0} > sol_{pos,100}$.

The four lithiation parameters will determine the open circuit voltage at 0% and 100% SOC of the cell according to

$$\begin{aligned} E_{OCV,cell,\ 0\%\ SOC} &= E_{eq,pos}(sol_{pos,0}) - E_{eq,neg}(sol_{neg,0}) \\ E_{OCV,cell,\ 100\%\ SOC} &= E_{eq,pos}(sol_{pos,\ 100}) - E_{eq,neg}(sol_{neg,\ 100}) \end{aligned} \tag{3}$$

What cell voltage, and in term what individual electrode voltages, should correspond a 0% and a 100% cell state of charge (SOC) is to a high degree an engineering decision, related mainly to durability constraints, since a too low cell voltage could result in, for instance, corrosion of the negative current collector, and a too high cell voltage could result in excessive SEI formation and/or lithium plating on the negative electrode, or degradation

of and/or electrolyte decomposition (gassing) on the positive electrode. As discussed in the next section, the lithiation parameters also determine the relative balancing of the host capacities and resulting electrode thicknesses of the cell.

The state-of-charge of the battery cell may now be defined either by the lithiation level in the negative or positive electrode as

$$\mathrm{SOC} = \frac{\mathrm{sol}_{\mathrm{pos}} - \mathrm{sol}_{\mathrm{pos},0}}{\mathrm{sol}_{\mathrm{pos},100} - \mathrm{sol}_{\mathrm{pos},0}} = \frac{\mathrm{sol}_{\mathrm{neg}} - \mathrm{sol}_{\mathrm{neg},0}}{\mathrm{sol}_{\mathrm{neg},100} - \mathrm{sol}_{\mathrm{neg},0}} \tag{4}$$

It should be noted that these definitions of SOC will only be equal and consistent as long as no parasitic (aging) side reactions occur in the cell, resulting in loss of either cyclable lithium and/or loss of electrode material available for lithium intercalation.

Conversely, we may express the degrees of lithiation based on the SOC as

$$\begin{aligned} \mathrm{sol}_{\mathrm{pos}} &= (\mathrm{sol}_{\mathrm{pos},100} - \mathrm{sol}_{\mathrm{pos},0})\mathrm{SOC} + \mathrm{sol}_{\mathrm{pos},0} \\ \mathrm{sol}_{\mathrm{neg}} &= (\mathrm{sol}_{\mathrm{neg},100} - \mathrm{sol}_{\mathrm{neg},0})\mathrm{SOC} + \mathrm{sol}_{\mathrm{neg},0} \end{aligned} \tag{5}$$

The above expression is used to set the initial solid concentration levels in the electrodes in the model, based on an initial SOC parameter.

ELECTRODE THICKNESSES BASED ON THE CELL CAPACITY

The parameter q_{cell} ($\mathrm{Ah/m^2}$) for the cross-sectional cell capacity of the battery when cycling between 0 and 100% SOC, together with the four degree of lithiation parameters described in the previous section, are used to define the electrode thicknesses.

We first define the host capacity of each electrode as

$$q_{\mathrm{host}} = Fc_{\mathrm{s,max}}\varepsilon_{\mathrm{s}}L \tag{6}$$

where F (C) is Faraday's constant, ε_{s} (dimensionless) the electrode volume fraction and L the electrode thickness.

We then note that each electrode needs to be able to accommodate q_{cell} when cycling between 0% and 100% SOC, resulting in

$$q_{\mathrm{cell}} = (\mathrm{sol}_{\mathrm{pos},0} - \mathrm{sol}_{\mathrm{pos},100})q_{\mathrm{host,pos}} = (\mathrm{sol}_{\mathrm{neg},100} - \mathrm{sol}_{\mathrm{neg},0})q_{\mathrm{host,pos}} \tag{7}$$

The individual electrode thicknesses may now be expressed as

$$L_{\text{pos}} = \frac{q_{\text{cell}}}{(\text{sol}_{\text{pos},0} - \text{sol}_{\text{pos},100})Fc_{s,\text{max,pos}}\varepsilon_{s,\text{pos}}}$$
$$L_{\text{neg}} = \frac{q_{\text{cell}}}{(\text{sol}_{\text{neg},100} - \text{sol}_{\text{neg},0})Fc_{s,\text{max,neg}}\varepsilon_{s,\text{neg}}} \quad (8)$$

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/lib_base_model_1d`

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.

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 **General Studies>Time Dependent**.

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 **Home** 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 **Home** 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 box, 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 box, 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 box, type `Positive Electrode` in the **Selection name** text field.
6. Click **OK**.

LITHIUM-ION BATTERY (LIION)

Now start defining the physics. Start with the separator.

Separator 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Lithium-Ion Battery (liion)** and choose **Separator**.

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

3 From the **Selection** list, choose **Separator**.

4 Locate the **Porous Matrix Properties** section. 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. From the σ_s list, choose **User defined**. In the associated 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 **Electrical 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 **Species Settings** section.

3 In the $c_{s,init}$ text field, type `cs_neg_init`.

4 Locate the **Particle Transport Properties** section. 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 $i_{0,ref}(T)$ 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 **Species Settings** section.

3 In the $c_{s,init}$ text field, type `cs_pos_init`.

4 Locate the **Particle Transport Properties** section. 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 $i_{0,ref}(T)$ 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 box, 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 box, 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`.

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 *phil* text field, type `-E_neg_init`.

Initial Values 2

1 Right-click **Component 1 (comp1)>Lithium-Ion Battery (liion)>Initial Values 1** and choose **Duplicate**.

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

3 From the **Selection** list, choose **Positive Electrode**.

4 Locate the **Initial Values** section. In the *phis* text field, type `E_cell_init`.

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** check box. 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 1: Time Dependent

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

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

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