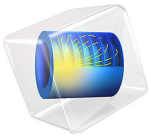

Lithium-Ion Battery Seed

Introduction

This is a template model containing the physics, geometry and mesh of a lithium-ion battery. The Lithium-Ion Battery Rate Capability, Lithium-Ion Battery Internal Resistance, 1D Lithium-Ion Battery Drive-Cycle Monitoring, and Diffusion-Induced Stress in a Lithium-Ion Battery applications available in the Applications Library make use of this model setup. Note that the former three applications belong to the category of battery management models.

This model setup is done using the Lithium-Ion Battery interface and incorporates mainly default physical properties. The material properties are taken from the Battery Material Library. As input, you only need to decide upon which initial cell voltage (or initial cell SOC), battery capacity, and thickness of electrodes and separator you want.

Model Definition

The model is set up for a graphite/LMO 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 and electronic conductor.
- Separator.
- Positive porous electrode: LMO ($LiMn_2O_4$) active material, electronic conductor, and filler.
- Electrolyte: 1.0 M $LiPF_6$ in EC:DEC (1:1 by weight)

This battery cell assembly gives a cell voltage around 4 V, depending on the state-of-charge (SOC) of the cell.

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.

An example of parameters that you set on your own for running the model is tabulated in Table 1. The values are selected for a typical 12 Ah graphite/LMO battery cell.

TABLE 1: PARAMETERS NEEDED TO BE SET BY THE USER.

PARAMETER	VALUE	DESCRIPTION
Q_B	12 Ah	Battery capacity
Ecell_init	3.9 V	Initial battery voltage
L_neg	30 µm	Thickness negative electrode
L_pos	55 µm	Thickness positive electrode
L_sep	30 µm	Thickness separator

This example utilizes the Initial Cell Charge Distribution global feature. This allows you to set the initial cell voltage (or initial cell state-of-charge (SOC)) as a model input. The feature computes the lithium concentrations (in the case of lithium-ion batteries) in the active electrode materials, c_s, and balances the electrodes in the cell to each other. For further reading on this feature, see the *Initial Cell Charge Distribution* section in the *Battery Design Module User's Guide*.

The next section contains a discussion that applies only to the battery management category of models (mentioned above), in which this template model has been used.

Battery Management

This application example is useful for investigation of the following in lithium-ion batteries under isothermal conditions:

- Voltage,
- polarization (voltage drop),
- internal resistance,
- state-of-charge (SOC), and
- rate capability.

Note that one can always make the system nonisothermal with a Heat Transfer interface. In this manner, a sixth property, temperature, may be added to the list above.

Some of the listed properties play an important part in battery management systems (BMS) in, for instance, electric and hybrid electric vehicles (see Figure 1). The more

properties that can be monitored accurately, the easier it is to manage the battery in order to maximize energy output and lifetime, and to guarantee safety.

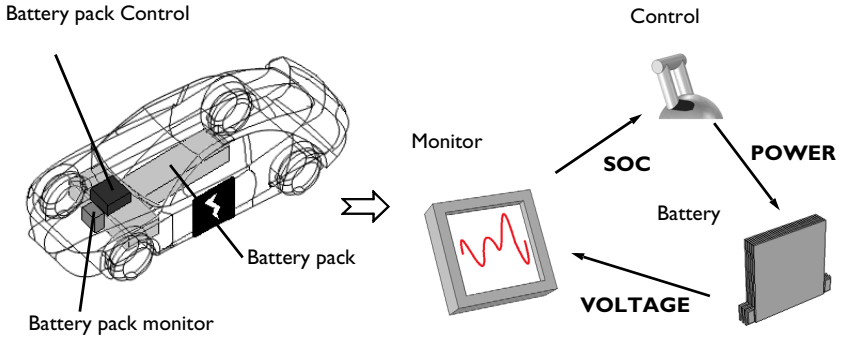

Figure 1: Electric vehicle with key components within the battery management system visualized. As the flowchart shows to the right, the battery voltage is often monitored and from this the SOC is either computed or determined from empirical data. The information from the monitor determines how the control unit will regulate the battery.

For battery manufacturers, the same properties can be considered when optimizing the design of the battery, for example choice of materials and thickness of electrodes.

Several useful variables are available with the battery management models. For the SOCs of the electrodes, both "coulombic" and "at load" are defined in the Lithium-Ion Battery interface. The "coulombic" in contrast to "at load" omits the impact of any polarization in the battery. This means that the "coulombic" type is based on the average concentration in the particle and the "load" on the particle surface concentration.

SOC, coulombic, in each electrode:

$$\mathrm{SOC} = \frac{\int_{\Omega_{\mathrm{electrode}}} c_{s,\mathrm{avg}} \mathrm{d}\Omega}{\int_{\Omega_{\mathrm{electrode}}} c_{s,\mathrm{max}} \mathrm{d}\Omega} \tag{1}$$

SOC, at load, in each electrode:

$$\mathrm{SOC}_l = \frac{\int_{\Omega_{\mathrm{electrode}}} c_{s,\mathrm{surf}} \mathrm{d}\Omega}{\int_{\Omega_{\mathrm{electrode}}} c_{s,\mathrm{max}} \mathrm{d}\Omega} \tag{2}$$

The cell SOC can likewise by either “coulombic” or “at load”. The cell SOC, coulombic, is computed in the model as:

$$\mathrm{SOC}_{\mathrm{cell}} = \frac{\int_{\Omega_{\mathrm{neg}}} c_{s,\mathrm{avg,cycl}} F \varepsilon_s \mathrm{d}\Omega}{\int_{\Omega_{\mathrm{neg}}} c_{s,\mathrm{avg,cycl}} F \varepsilon_s \mathrm{d}\Omega + \int_{\Omega_{\mathrm{pos}}} c_{s,\mathrm{avg,cycl}} F \varepsilon_s \mathrm{d}\Omega} \tag{3}$$

where the average cyclable lithium concentration in the electrode particles is inserted which is defined as:

$$c_{s,\mathrm{avg,cycl}} = c_{s,\mathrm{avg,electrode}} - \mathrm{soc}_{\mathrm{min}} c_{s,\,\mathrm{max}} \tag{4}$$

Cell SOC, at load, is computed as:

$$\mathrm{SOC}_{\mathrm{cell},\,l} = \frac{\int_{\Omega_{\mathrm{neg}}} c_{s,\mathrm{surf,cycl}} F \varepsilon_s \mathrm{d}\Omega}{\int_{\Omega_{\mathrm{neg}}} c_{s,\mathrm{surf,cycl}} F \varepsilon_s \mathrm{d}\Omega + \int_{\Omega_{\mathrm{pos}}} c_{s,\mathrm{surf,cycl}} F \varepsilon_s \mathrm{d}\Omega} \tag{5}$$

where the cyclable lithium concentration at the surface of the electrode particles is inserted which is defined as:

$$c_{s,\mathrm{surf,cycl}} = c_{s,\mathrm{surf}} - \mathrm{soc}_{\mathrm{min}} c_{s,\,\mathrm{max}} \tag{6}$$

The SOC definitions are furthermore used to compute the coulombic or at load open-circuit potential of each electrode and the corresponding open-circuit cell voltages.

Additionally, the model also sets up the local potential in the solid and electrolyte phases to calculate the cell voltage, E_{cell}, and the potential of each electrode, E, during load, as shown in Equation 7 and Equation 8.

$$E_{\mathrm{cell}} = \varphi_S\big|_{\mathrm{cc\ pos}} \tag{7}$$

$$E = \varphi_S\big|_{\mathrm{cc}} - \varphi_L\big|_{\mathrm{sep}} \tag{8}$$

Here, “cc” denotes the current collector boundary and “sep” the separator boundary.

The total polarization is determined in the model as well. It is calculated as the difference between the cell voltage and open-circuit cell voltage (coulombic).

$$\Delta V = E_{\text{cell}} - E_{\text{OCV, cell}}(\text{SOC}) \tag{9}$$

In the same way, the electrodes' polarization can be obtained as the difference between the electrode potential and open-circuit potential (coulombic).

Study Settings

In order for the Initial Cell Charge Distribution feature to function a Current Distribution Initialization study step is required.

Reference

1. M. Doyle, and Y. Fuentes, "Computer Simulations of a Lithium-Ion Polymer Battery and Implications for Higher Capacity Next-Generation Battery Designs," *J. Electrochem. Soc.*, vol. 150, no. 6, pp. A706–A713, 2003.

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/li_battery_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 **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**. This study step automatically computes the initial potentials in the cell.

6 Click **Done**.

GLOBAL DEFINITIONS

This model mainly uses the input of default parameters. However, the battery capacity and its initial voltage, together with the thicknesses of the electrodes and the separator are required to be set.

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
Q_B	12[Ah]	43200 C	Battery capacity
Ecell_init	3.90[V]	3.9 V	Initial cell voltage

ADD MATERIAL

The model has a graphite negative electrode, a LMO positive electrode, and a LiPF6 1:1 EC:DEC electrolyte. Import the materials from the Battery Material Library.

1 In the **Home** 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 1:1 EC:DEC (Liquid, Li-ion Battery)**.

4 Click the right end of the **Add to Component** split button in the window toolbar.

5 From the menu, choose **Add to Global Materials**.

6 In the tree, select **Battery>Electrodes>Graphite, LixC6 MCMB (Negative, Li-ion Battery)**.

7 Click the right end of the **Add to Component** split button in the window toolbar.

8 From the menu, choose **Add to Global Materials**.

9 In the tree, select **Battery>Electrodes>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery)**.

10 Click the right end of the **Add to Component** split button in the window toolbar.

11 From the menu, choose **Add to Global Materials**.

12 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

DEFINITIONS

Cell voltage probe

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

2 In the **Settings** window for **Global Variable Probe**, type `Cell voltage probe` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `Ecell`.

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)
30e-6
30e-6
55e-6

5 Click **Build Selected**.

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 Select Domain 2 only.

3 In the **Settings** window for **Explicit**, type `Separator` in the **Label** text field.

Positive electrode

1 In the **Definitions** toolbar, click **Explicit**.

2 Select Domain 3 only.

3 In the **Settings** window for **Explicit**, type `Positive electrode` in the **Label** text field.

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `negative` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **Negative electrode**.

Integration 2 (intop2)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `positive` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **Positive electrode**.

Integration 3 (intop3)

Select the end-terminal boundary, that is, the positive electrode current collector, along with the rest of the electrode boundaries.

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `pos_cc` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

Integration 4 (pos_cc2)

1 Right-click **Integration 3 (intop3)** and choose **Duplicate**.

2 In the **Settings** window for **Integration**, type `neg_cc` in the **Operator name** text field.

3 Select Boundary 1 only.

Integration 5 (neg_cc2)

1 Right-click **Integration 4 (pos_cc2)** and choose **Duplicate**.

2 In the **Settings** window for **Integration**, type `neg_sep` in the **Operator name** text field.

3 Select Boundary 2 only.

Integration 6 (neg_sep2)

1 Right-click **Integration 5 (neg_cc2)** and choose **Duplicate**.

2 In the **Settings** window for **Integration**, type `pos_sep` in the **Operator name** text field.

3 Select Boundary 3 only.

MATERIALS

Material Link 1 (matlnk1)

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **More Materials>Material Link**.

Material Link 2 (matlnk2)

1 Right-click **Materials** and choose **More Materials>Material Link**.

2 In the **Settings** window for **Material Link**, locate the **Link Settings** section.

3 From the **Material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

Material Link 3 (matlnk3)

1 Right-click **Materials** and choose **More Materials>Material Link**.

2 In the **Settings** window for **Material Link**, locate the **Link Settings** section.

3 From the **Material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat3)**.

LITHIUM-ION BATTERY (LIION)

Add the three typical battery domains in the Lithium-Ion Battery interface: a negative porous electrode, a positive porous electrode, and a separator.

Porous Electrode 1

For the negative electrode, select material properties where possible. Change the negative electrode particle radius. The initial concentration of lithium in graphite is calculated further on.

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Lithium-Ion Battery (liion)** 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 **Electrolyte Properties** section. From the **Electrolyte material** list, choose **Material Link 1 (matlnk1)**.

5 Locate the **Electrode Properties** section. From the **Electrode material** list, choose **Material Link 2 (matlnk2)**.

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 **Material Link 2 (matlnk2)**.

4 Locate the **Particle Transport Properties** section. In the r_p text field, type `2e-6[m]`.

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 **Material Link 2 (matlnk2)**.

Porous Electrode 2

Select material properties for the positive electrode as well. Change the positive electrode particle radius. The initial concentration of lithium in LMO is calculated further on.

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 **Electrolyte Properties** section. From the **Electrolyte material** list, choose **Material Link 1 (matlnk1)**.
5. Locate the **Electrode Properties** section. From the **Electrode material** list, choose **Material Link 3 (matlnk3)**.

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 **Material Link 3 (matlnk3)**.
4. Locate the **Particle Transport Properties** section. In the r_p text field, type `2e-6[m]`.

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 **Material Link 3 (matlnk3)**.

Separator 1

Since a liquid electrolyte is chosen, the battery model requires a separator.

1. In the **Physics** toolbar, click **Domains** 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 **Electrolyte Properties** section. From the **Electrolyte material** list, choose **Material Link 1 (matlnk1)**.

Select the global feature Initial Cell Charge Distribution to allow either cell voltage or cell state-of-charge initially as input. The feature computes the initial lithium concentration in the electrode materials and balances the electrodes by computing the electrode material volume fraction in each electrode.

Initial Cell Charge Distribution 1

1 In the **Physics** toolbar, click **Global** and choose **Initial Cell Charge Distribution**.

Since it is a lithium-ion battery chemistry with a negative carbon electrode, the default fractions in the Battery Cell Electrode Balancing section can be kept.

2 In the **Settings** window for **Initial Cell Charge Distribution**, locate the **Battery Cell Parameters** section.

3 In the $E_{\text{cell,0}}$ text field, type `Ecell_init`.

4 In the $Q_{\text{cell,0}}$ text field, type `Q_B`.

Negative Electrode Selection 1

Select which model domains that represent the negative and positive electrode, respectively.

1 In the **Model Builder** window, expand the **Initial Cell Charge Distribution 1** node, then click **Negative Electrode Selection 1**.

2 Select Domain 1 only.

Positive Electrode Selection 1

1 In the **Model Builder** window, click **Positive Electrode Selection 1**.

2 Select Domain 3 only.

Porous Electrode 1

To balance the electrodes in the cell and optimize the electrode material usage for the electrodes, revisit the Porous Electrode nodes and enter the electrode material volume fractions computed by the Initial Cell Charge Distribution feature.

1 In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **Porous Electrode 1**.

2 In the **Settings** window for **Porous Electrode**, locate the **Porous Matrix Properties** section.

3 In the ε_s text field, type `liion.epss_neg`.

4 In the ε_l text field, type `1-liion.epss_neg`.

Porous Electrode 2

1 In the **Model Builder** window, click **Porous Electrode 2**.

2 In the **Settings** window for **Porous Electrode**, locate the **Porous Matrix Properties** section.

3 In the ε_s text field, type `liion.epss_pos`.

4 In the ε_l text field, type `1-liion.epss_pos`.

Electric Ground 1

Finish by setting the boundary conditions. Ground is set as reference at the leftmost boundary, the negative electrode current collector. A current is applied at the rightmost boundary, the positive electrode current collector. Set for instance the 1C discharge rate with the 1C current available with the Initial Cell Charge Distribution feature.

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

2 Select Boundary 1 only.

Electrode Current 1

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

2 Select Boundary 4 only.

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

4 In the $I_{\mathrm{s,total}}$ text field, type `-liion.I_1C`.