Created in COMSOL Multiphysics 5.6

1D Lithium-Ion Battery Model for the Capacity Fade Tutorial

Introduction

This is a template model containing the physics, geometry and mesh of a lithium-ion battery (without any capacity fade reactions or mechanisms added). The Capacity Fade of 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 ($LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$) 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/Batteries,_Lithium-Ion/capacity_fade_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**.

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 `capacity_fade_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 **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 3:7 EC:EMC (Liquid electrolyte, Li-ion Battery)**.

4 Click **Add to Component 1 (comp1)**.

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

6 Click **Add to Component 1 (comp1)**.

7 In the tree, select **Battery>Electrodes>NCA Electrode, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery)**.

8 Click **Add to Component 1 (comp1)**.

9 In the **Home** 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)

Porous Electrode 1

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 **Electrode Properties** section. From the **Electrode material** list, choose **Graphite Electrode, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

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

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

Particle Intercalation 1

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

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

3 From the **Particle material** list, choose **Graphite Electrode, 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** check box.

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 Electrode, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

4 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_neg`.

Separator 1

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 **Porous Matrix Properties** section. In the ε_l text field, type `epsl_sep`.

5 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the f_l text field, type `epsl_sep^brugl_sep`.

6 From the **Diffusion** list, choose **User defined**. In the f_{Dl} text field, type `epsl_sep^brugl_sep`.

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. From the **Electrode material** list, choose **NCA Electrode, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3)**.

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`.

7 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the f_l text field, type `liion.epsl^brugl_pos`.

8 From the **Diffusion** list, choose **User defined**. In the f_{Dl} text field, type `liion.epsl^brugl_pos`.

Particle Intercalation 1

1 In the **Model Builder** window, expand the **Porous Electrode 2** node, then click **Particle Intercalation 1**.

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

3 From the **Particle material** list, choose **NCA Electrode, 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** check box.

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 **NCA Electrode, 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`.

Initial Cell Charge Distribution 1

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

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 `E_min`.

4 In the $Q_{\text{cell,0}}$ text field, type `Q0*1[m^2]`.

5 Locate the **Battery Cell Electrode Balancing** section. In the $f_{\text{cycl,loss}}$ text field, type `0`.

Negative Electrode Selection 1

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

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

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

Positive Electrode Selection 1

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

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

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

Electric Ground 1

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 (COMP1)

Piecewise 1 (pw1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global>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 `capacity_fade_piece_wise.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 `capacity_fade_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,(no_cycles+1)*t_cycling/t_factor)`.