



Model created in COMSOL Multiphysics 6.4

# Lithium-Ion Battery with Multiple Intercalating Electrode Materials

## *Introduction*

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Lithium-ion batteries can have multiple intercalating materials in both the positive and negative electrodes. For example, the negative electrode can have a mix of different forms of carbon. Similarly, the positive electrode can have a mix of active materials such as transition metal oxides, layered metal oxides, olivines, and so forth. These materials can have different design properties (such as volume fractions, particle sizes), thermodynamic properties (such as equilibrium potentials, maximum lithium concentrations), transport properties (such as solid diffusivities) and kinetic properties (such as intercalation reaction rate constants).

This model example demonstrates the Additional Porous Electrode Material feature in the Lithium-Ion Battery interface. The model describes a lithium-ion battery with two different intercalating materials in the positive electrode, whereas the negative electrode consists of one intercalating material only. The battery performance during discharge for different mixing fractions of the two intercalating materials in the positive electrode is studied. The geometry is in one dimension and the model is isothermal.

## *Model Definition*

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This example models the battery cross section in 1D, which implies that edge effects in the length and height of the battery are neglected. The example uses the following three domains:

- Negative graphite porous electrode (50  $\mu\text{m}$  thick)
- Separator (50  $\mu\text{m}$  thick)
- Positive blended NCA/LMO porous electrode (thickness depending on NCA:LMO ratio; see below)

Two active intercalating materials are considered in the positive electrode and the negative electrode consists of a single intercalating material. The model includes the following processes ([Ref. 1](#)).

- Electronic current conduction in the electrodes
- Ionic charge transport in the pores of the electrodes and separator
- Material transport in the electrolyte, allowing for the introduction of the effects of concentration on ionic conductivity and concentration overpotential, which in this case are obtained from experimental data

- Material transport within the spherical intercalating particles that form the electrodes
- Butler–Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium potential of the intercalating materials in the electrodes.

For the porous electrodes, the effective electrolyte properties are calculated using the Bruggeman relation. Transport in the spherical particles is described using the Baker–Verbrugge diffusion model. This diffusion model considers the gradient of the chemical potential of the intercalating lithium as the driving force for diffusion, as opposed to considering the gradient of lithium concentration for dilute solution treatment (Fick’s Law) of lithium transport in the active material particles. The diffusion equation is expressed in spherical coordinates for the material balance of lithium in the particles. Butler–Volmer electrode kinetics describes the local charge transfer current density in the electrodes. The Butler–Volmer expressions are introduced as source or sink terms in the charge balances and material balances.

### **MATERIAL PROPERTIES**

The electrolyte consists of 1 M  $\text{LiPF}_6$  salt in 1:1 EC:DEC (by weight) solvent. The two active materials in the positive electrode are NCA ( $\text{Li}_y\text{Ni}_{0.80}\text{Co}_{0.15}\text{Al}_{0.15}\text{O}_2$ ) and LMO ( $\text{Li}_y\text{Mn}_2\text{O}_4$  spinel). For the negative electrode, MCMB graphite ( $\text{Li}_x\text{C}_6$ ) is used in the model. The material properties of the electrolyte and active materials are taken from the Battery material library.

The equilibrium potentials of the positive electrode materials are shown in [Figure 1](#)

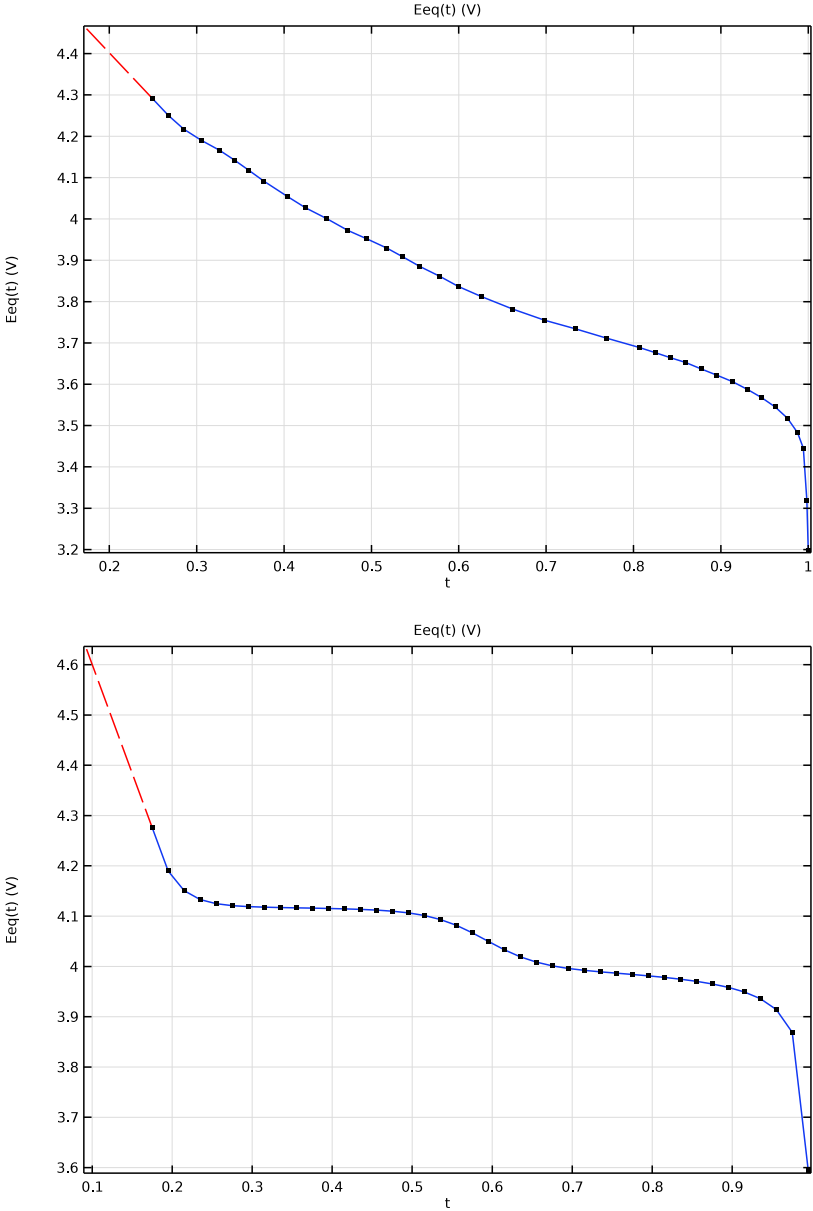


Figure 1: The equilibrium potentials of NCA (top) and LMO (bottom).

The x-axis data in [Figure 1](#) depicts the lithiation level of the active material, which is calculated by dividing the concentration of lithium with the maximum concentration of lithium in the material (the host capacity).

### **ELECTRODE BALANCING**

The thickness of the negative electrode is set to 50  $\mu\text{m}$ , whereas the positive electrode thickness is set to vary with the relative volume fractions of LMO and NMC. The electrode balancing is based on the following criteria:

- In order to avoid lithium plating during fast charging, the host capacity of the negative graphite electrode should be in excess so that an approximate lithiation level of 80% is reached at 100% cell state-of-charge (SOC).
- In order to avoid gassing and other harmful side reactions, the positive electrode potential is limited to about 4.1 V at 100% SOC, corresponding to lithiation levels of 30% and 19% for NCA and LMO, respectively ([Figure 1](#)).

Based on the host capacities ( $c_{s,\text{max}}$ ) and volume fractions ( $\epsilon_s$ ) of the electrode materials, the thickness of the positive electrode may now be computed as

$$L_{\text{pos}} = \frac{0.8\epsilon_{s, \text{Gr}}c_{s, \text{max,Gr}}}{(1 - 0.3)\epsilon_{s, \text{NCA}}c_{s, \text{max,NCA}} + (1 - 0.19)\epsilon_{s, \text{LMO}}c_{s, \text{max,LMO}}} L_{\text{neg}}$$

## Results and Discussion

Figure 2 shows the voltage profile for a 1:2 volume ratio of the two positive electrode materials at a constant current discharge of 1C.

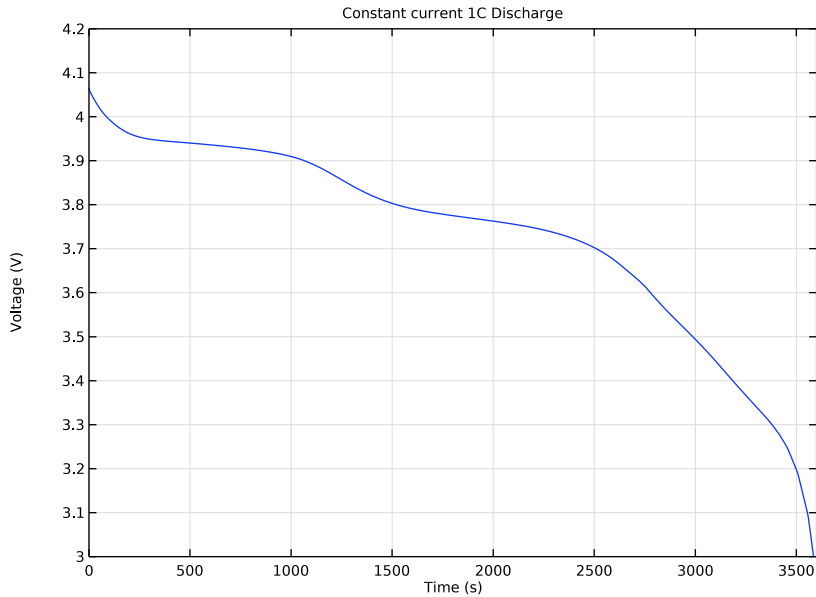


Figure 2: Discharge voltage profile at 1C.

Figure 3 shows the lithium concentration at the surface of the active material particles in the positive electrode (at the positive electrode current collector end) during 1C discharge.

The variation of the surface concentration with time is different in the two active materials. This is because of the different electrochemical properties of the two active materials.

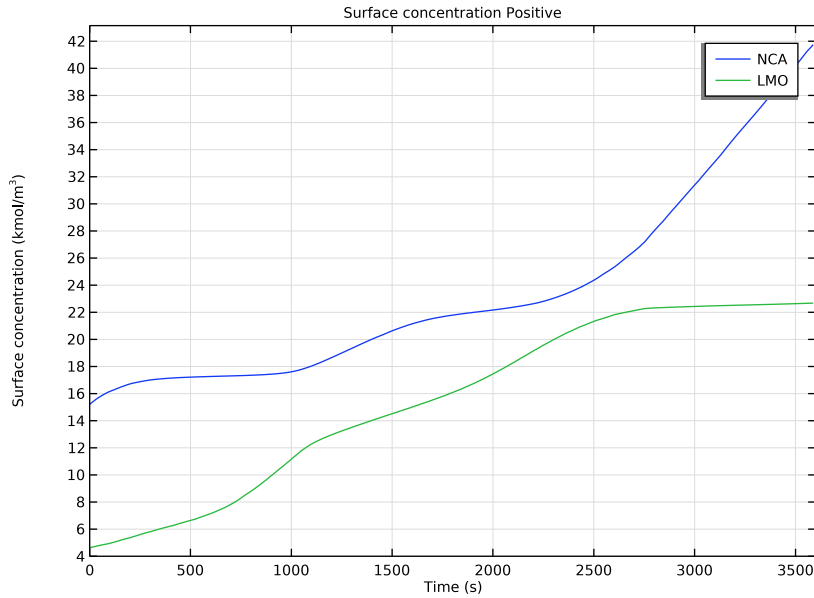
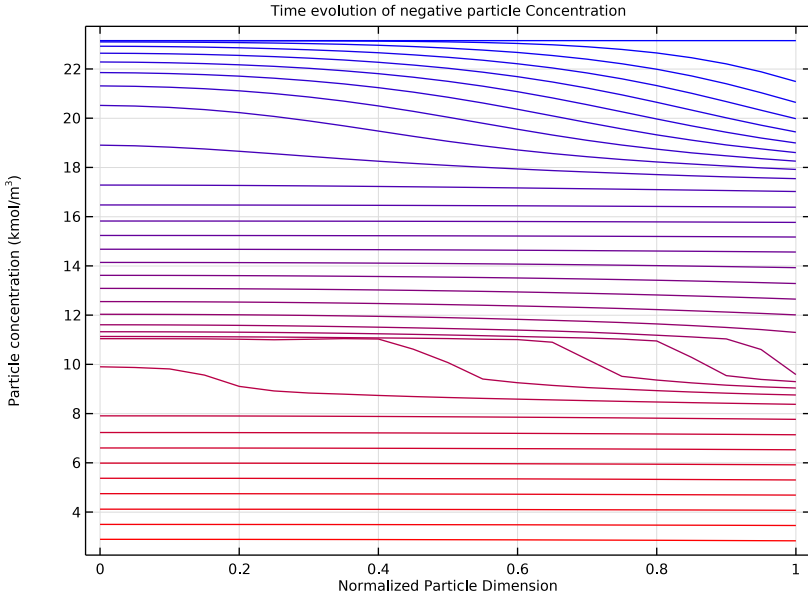


Figure 3: Surface concentration in the active material particles in the positive electrode during 1C discharge.

Figure 4 shows the lithium concentration inside a particle at a particular position in the negative graphite electrode (at the center of the negative electrode) during 1C discharge. The concentration profiles show characteristic ridges, thereby capturing the staging phenomenon seen in multiphase electrodes like graphite. The Baker-Verbrugge diffusion model accounts for the interactions of the lithium-ions within the solid phase through an

activity correction term, and hence provides a realistic representation of the intercalation process.



*Figure 4: Concentration profiles inside a particle at a particular position in the negative electrode, at various times during 1C discharge.*

The voltage profiles during 1C discharge for different volume mix fractions of the active materials in the positive electrode are shown in Figure 5. The shape of the discharge profile has a pronounced dependence on the mix fraction of the active materials in the electrode.

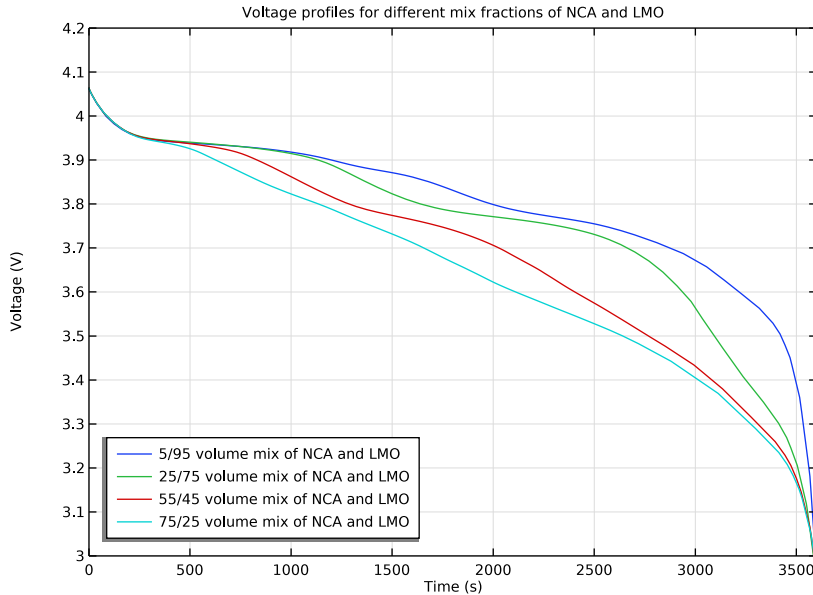


Figure 5: Voltage profiles during 1C discharge for different volume mix fractions of the active materials in the positive electrode.

### Reference


I. P. Albertus, J. Christensen, and J. Newman, “Experiments on and Modeling of Multiple Active Materials in Positive Electrodes for Lithium-Ion Batteries,” *J. Electrochem. Soc.*, vol. 156, no. 7, pp. A606–A618, 2009.

**Application Library path:** Battery\_Design\_Module/Lithium-Ion\_Batteries, \_Performance/li\_battery\_multiple\_materials\_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 .
- 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 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 `li_battery_multiple_materials_parameters.txt`.

## GEOMETRY I

The geometry contains three domains. Create the geometry by specifying the coordinates of the boundaries.

### *Interval I (il)*

- 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:



<b>Lengths (m)</b>
L_neg
L_sep
L_pos

5 Click  **Build Selected**.

## MATERIALS

All materials are available in the Material Library. Note: In the Materials node,  $c_{Eeqref}$  denotes the maximum lithium concentration in the active material.

## 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 1:1 EC:DEC (Liquid, Li-ion Battery)**.
- 4 Click the **Add to Component** button in the window toolbar.
- 5 In the tree, select **Battery > Electrodes > Graphite, LiC6 MCMB (Negative, Li-ion Battery)**.
- 6 Click the **Add to Component** button in the window toolbar.
- 7 In the tree, select **Battery > Electrodes > NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery)**.
- 8 Click the **Add to Component** button in the window toolbar.
- 9 In the tree, select **Battery > Electrodes > LMO, LiMn2O4 Spinel (Positive, Li-ion Battery)**.
- 10 Click the **Add to Component** button in the window toolbar.
- 11 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.

## MATERIALS

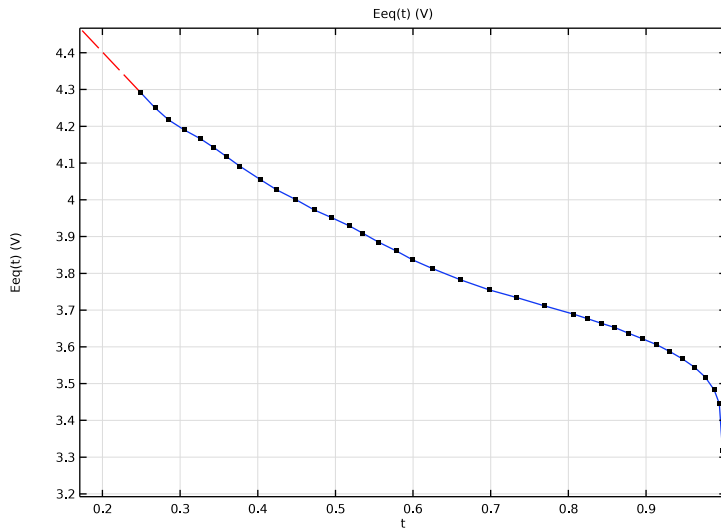
*NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3)*

In the **Model Builder** window, expand the **NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3)** node.

*Interpolation 1 (Eeq, Eeq\_inv)*

- 1 In the **Model Builder** window, expand the **Component 1 (comp1) > Materials > NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3) > Basic (def)** node, then click **Interpolation 1 (Eeq, Eeq\_inv)**.
- 2 In the **Settings** window for **Interpolation**, click to expand the **Plot Parameters** section.
- 3 Clear the **Include right extrapolation** checkbox.

4 Click  **Plot**.



*LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4)*

In the **Model Builder** window, expand the **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4)** node.

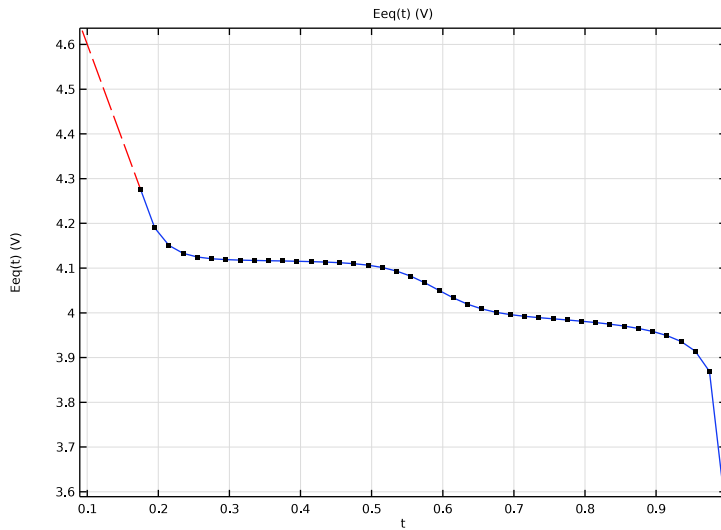
*Interpolation 1 (Eeq, Eeq\_inv)*

1 In the **Model Builder** window, expand the **Component 1 (comp1) > Materials > LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4) > Basic (def)** node, then click **Interpolation 1 (Eeq, Eeq\_inv)**.

2 In the **Settings** window for **Interpolation**, click to expand the **Plot Parameters** section.

3 Clear the **Include right extrapolation** checkbox.

4 Click  **Plot**.



### LITHIUM-ION BATTERY (LIION)

Set up the physics in the insertion electrodes. In this model, the Baker-Verbrugge diffusion model is used in the Particle Intercalation nodes. Note that the Baker-Verbrugge diffusivities are typically different from the Fickian diffusivity values. In this model, the intercalation diffusivities are simply set to the values available in the Material Library.

#### 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  $\epsilon_1$  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 Select Domain 1 only.

- 3 In the **Settings** window for **Porous Electrode**, locate the **Electrode Properties** section.
- 4 In the  $\sigma_s$  text field, type `sigmas_neg`.
- 5 Locate the **Porous Matrix Properties** section. In the  $\epsilon_s$  text field, type `epss_neg`.
- 6 In the  $\epsilon_1$  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. From the **Species concentration transport model** list, choose **Baker–Verbrugge**.
- 5 In the  $r_p$  text field, type `rp_neg`.  
The concentration profiles inside a graphite electrode particle will be analyzed during postprocessing. Hence, it is useful to have a finer resolution along the particle dimension, by setting a linear distribution with 20 elements.
- 6 Click to expand the **Particle Discretization** section. From the **Distribution** list, choose **Linear**.
- 7 In the  $N_{el}$  text field, type 20.

#### *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 Select Domain 3 only.
- 3 In the **Settings** window for **Porous Electrode**, locate the **Electrode Properties** section.
- 4 In the  $\sigma_s$  text field, type `sigmas_pos`.
- 5 Locate the **Porous Matrix Properties** section. In the  $\epsilon_s$  text field, type `epss_pos_NCA`.
- 6 In the  $\epsilon_1$  text field, type `eps1_pos`.

- 7 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the  $f_1$  text field, type  $\text{eps1\_pos}^{\wedge}\text{brug1\_pos}$ .
- 8 From the **Diffusion** list, choose **User defined**. In the  $f_{D1}$  text field, type  $\text{eps1\_pos}^{\wedge}\text{brug1\_pos}$ .

#### *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. From the **Species concentration transport model** list, choose **Baker–Verbrugge**.
- 5 In the  $r_p$  text field, type  $\text{rp\_pos\_NCA}$ .

#### *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  $i_{0,\text{ref}}(T)$  text field, type  $\text{i0ref\_pos\_NCA}$ .

#### *Additional Porous Electrode Material I*

- 1 In the **Physics** toolbar, click **Domains** and choose **Additional Porous Electrode Material**.
- 2 Select Domain 3 only.
- 3 In the **Settings** window for **Additional Porous Electrode Material**, locate the **Volume Fraction** section.
- 4 In the  $\epsilon_s$  text field, type  $\text{epss\_pos\_LMO}$ .

#### *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 **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4)**.
- 4 Locate the **Particle Transport Properties** section. From the **Species concentration transport model** list, choose **Baker–Verbrugge**.

5 In the  $r_p$  text field, type `rp_pos_LMO`.

#### *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 **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4)**.
- 4 Locate the **Electrode Kinetics** section. In the  $i_{0,\text{ref}}(T)$  text field, type `i0ref_pos_LMO`.
- 5 In the **Model Builder** window, click **Lithium-Ion Battery (liion)**.
- 6 In the **Settings** window for **Lithium-Ion Battery**, locate the **Cell Settings** section.
- 7 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, expand the **Lithium-Ion Battery (liion)** node, then 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  $E_{\text{cell}}^{0\%SOC}$  text field, type `E_0_SOC`.
- 4 In the  $E_{\text{cell}}^{100\%SOC}$  text field, type `E_100_SOC`.
- 5 Locate the **Initial Cell Charge Distribution** section. In the  $SOC_0$  text field, type `SOC_cell10`.

#### *Negative Electrode Domain Selection 1*

- 1 In the **Model Builder** window, click **Negative Electrode Domain Selection 1**.
- 2 Select Domain 1 only.


#### *Positive Electrode Domain Selection 1*

- 1 In the **Model Builder** window, click **Positive Electrode Domain Selection 1**.
- 2 Select Domain 3 only.

#### *Electric Ground 1*


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Ground**.
- 2 Select Boundary 1 only.

#### *Load Cycle 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Load Cycle**.
- 2 Select Boundary 4 only.
- 3 In the **Settings** window for **Load Cycle**, locate the **Load Type** section.

- 4 From the list, choose **Galvanostatic**.
- 5 Locate the **Cycling Stop Condition** section. From the list, choose **Minimum voltage**.
- 6 In the  $E_{\min}$  text field, type 3[V].

#### *C Rate 1*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **C Rate**.
- 2 In the **Settings** window for **C Rate**, locate the **C-Rate Multiple** section.
- 3 In the  $C_{\text{set}}$  text field, type -1.


### **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.

### **MESH 1**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
- 2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.
- 3 From the **Element size** list, choose **Fine**.
- 4 Click  **Build All**.

### **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 0 3600.

Store the actual steps taken by the solver to make sure to capture any sudden steep voltage changes.

#### *Solution 1 (sol1)*


- 1 In the **Study** toolbar, click  **Show Default Solver**.

- 2 In the **Model Builder** window, expand the **Solution I (sol1)** node, then click **Time-Dependent Solver I**.
- 3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.
- 4 From the **Times to store** list, choose **Steps taken by solver**.
- 5 In the **Model Builder** window, click **Study I**.
- 6 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 7 Clear the **Generate default plots** checkbox.
- 8 In the **Study** toolbar, click  **Compute**.

## RESULTS

Reproduce the plots in the model documentation for IC discharge, starting with the voltage profile (Figure 2).

### *Constant current IC Discharge*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Constant current IC Discharge in the **Label** text field.

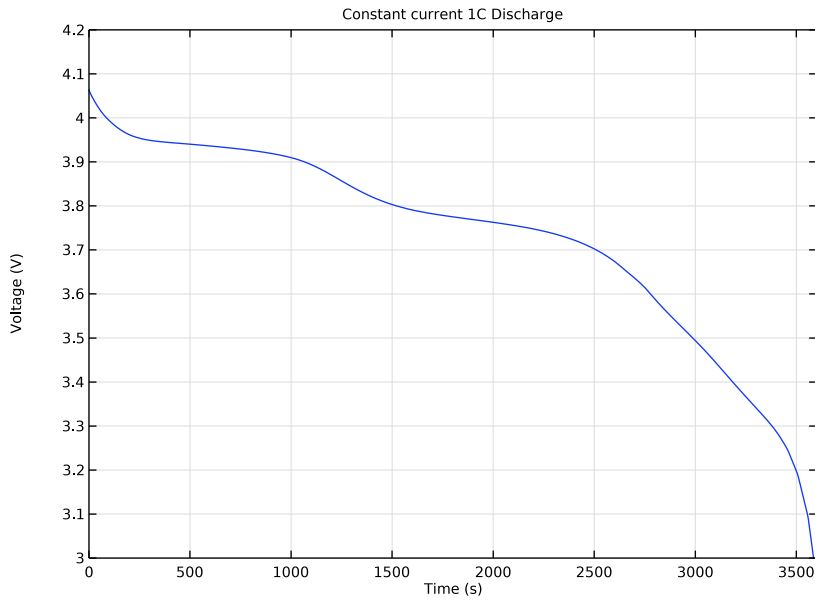
### *Point Graph 1*

- 1 Right-click **Constant current IC Discharge** and choose **Point Graph**.
- 2 Select Boundary 4 only.
- 3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (comp1) > Lithium-Ion Battery > phi\_s - Electric potential - V**.

### *Constant current IC Discharge*


- 1 In the **Model Builder** window, click **Constant current IC Discharge**.
- 2 In the **Settings** window for **ID Plot Group**, click to expand the **Title** section.
- 3 From the **Title type** list, choose **Label**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **y-axis label** checkbox. In the associated text field, type Voltage (V).
- 6 Locate the **Axis** section. Select the **Manual axis limits** checkbox.
- 7 In the **x minimum** text field, type 0.
- 8 In the **x maximum** text field, type 3600.
- 9 In the **y minimum** text field, type 3.0.
- 10 In the **y maximum** text field, type 4.2.

11 In the **Constant current IC Discharge** toolbar, click  **Plot**.



#### *Surface concentration Positive*

The following steps are for plotting the surface concentration in each active material in the positive electrode during IC discharge (Figure 3).

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Surface concentration Positive in the **Label** text field.

#### *Point Graph 1*

- 1 Right-click **Surface concentration Positive** and choose **Point Graph**.
- 2 Select Boundary 4 only.
- 3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp 1) > Lithium-Ion Battery > Particle intercalation > liion.cs\_surface - Insertion particle concentration, surface - mol/m<sup>3</sup>**.
- 4 Locate the **y-Axis Data** section. From the **Unit** list, choose **M**.
- 5 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

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**Legends**

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NCA

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*Point Graph 2*

- 1 Right-click **Point Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp 1) > Lithium-Ion Battery > Particle intercalation > liion.cs\_surface\_addm1 - Insertion particle surface concentration, Additional Porous Electrode Material 1 - mol/m<sup>3</sup>**.
- 3 Locate the **Legends** section. In the table, enter the following settings:

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**Legends**

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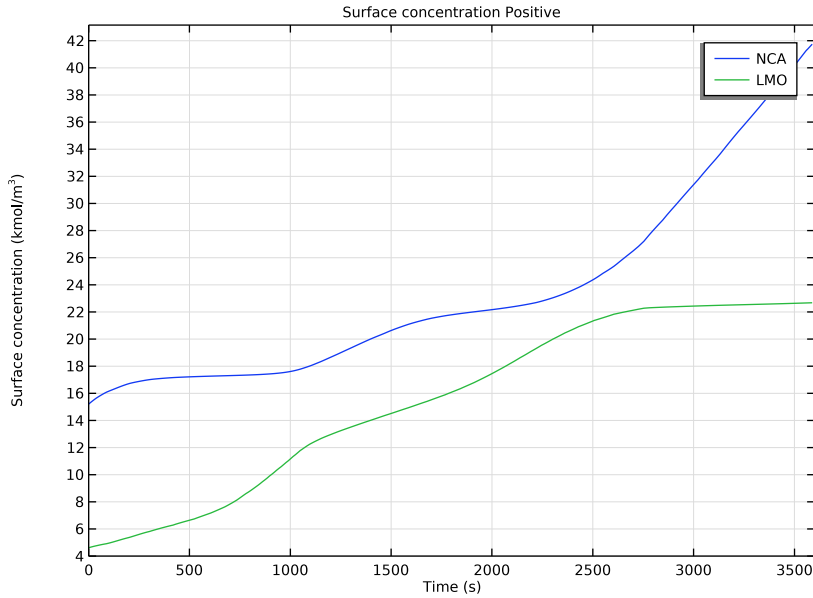
LMO

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*Surface concentration Positive*

- 1 In the **Model Builder** window, click **Surface concentration Positive**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **Label**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **y-axis label** checkbox. In the associated text field, type Surface concentration (kmol/m<sup>3</sup>).
- 6 Locate the **Axis** section. Select the **Manual axis limits** checkbox.
- 7 In the **x minimum** text field, type 0.
- 8 In the **x maximum** text field, type 3600.
- 9 In the **y minimum** text field, type 4.

**10** In the **Surface concentration Positive** toolbar, click  **Plot**.




#### *Study 1/Solution 1 (sol1)*

The following steps are for plotting the concentration profiles inside a particle at a particular position in the negative electrode, at various times during IC discharge (Figure 4). To do this, create a solution dataset that refers to the extra dimension that is set up by the Porous Electrode node corresponding to the negative electrode.

#### *Study 1/Solution 1: xdim Negative*

- 1** In the **Model Builder** window, expand the **Results > Datasets** node.
- 2** Right-click **Results > Datasets > Study 1/Solution 1 (sol1)** and choose **Duplicate**.
- 3** In the **Settings** window for **Solution**, type Study 1/Solution 1: xdim Negative in the **Label** text field.
- 4** Locate the **Solution** section. From the **Component** list, choose **Extra Dimension from Particle Intercalation 1 (liion\_pce1\_pin1\_xdim)**.

#### *Time evolution of negative particle Concentration*

- 1** In the **Results** toolbar, click  **ID Plot Group**.
- 2** In the **Settings** window for **ID Plot Group**, type Time evolution of negative particle Concentration in the **Label** text field.

- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Solution 1: xdim Negative (sol1)**.
- 4 From the **Time selection** list, choose **Interpolated**.
- 5 In the **Times (s)** text field, type range (0, 100, 3300).

#### *Line Graph 1*

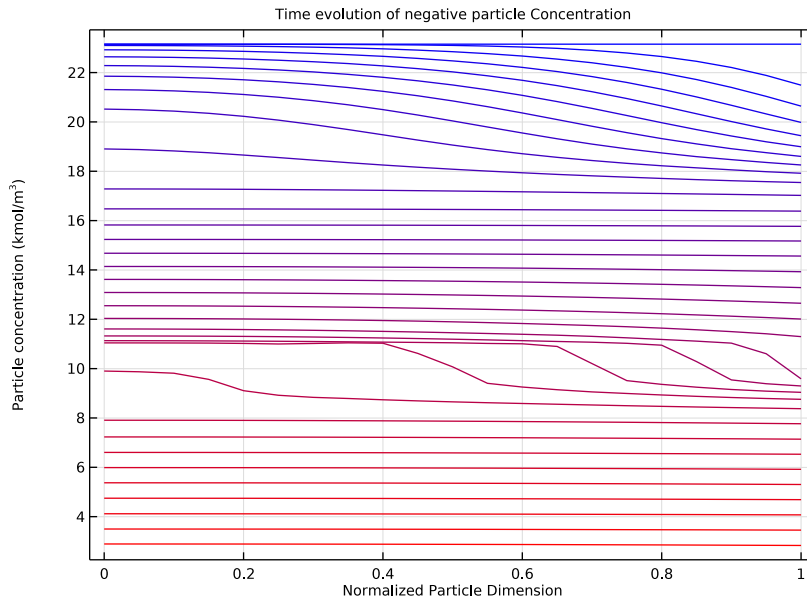
- 1 Right-click **Time evolution of negative particle Concentration** and choose **Line Graph**.
- 2 Select Domain 1 only.
 

The `atxd1()` operator evaluates the concentration at a specified position inside the negative electrode over the length of the particle dimension.
- 3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 4 In the **Expression** text field, type `atxd1(25e-6, liion.cs_pce1)`.
- 5 From the **Unit** list, choose **M**.
- 6 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Gradient**.
- 7 From the **Top color** list, choose **Red**.
- 8 From the **Bottom color** list, choose **Blue**.

#### *Time evolution of negative particle Concentration*

- 1 In the **Model Builder** window, click **Time evolution of negative particle Concentration**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **Label**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **x-axis label** checkbox. In the associated text field, type Normalized Particle Dimension.
- 6 Select the **y-axis label** checkbox. In the associated text field, type Particle concentration (kmol/m<sup>3</sup>).



7 In the **Time evolution of negative particle Concentration** toolbar, click  **Plot**.



## ROOT

Now set up a parametric study for different mix fractions of active materials in the positive electrode.

## ADD STUDY


- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces > Time Dependent with Initialization**.
- 4 Click the **Add Study** button in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

## STUDY 2

*Step 2: Time Dependent*



- 1 In the **Model Builder** window, under **Study 2** 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 0 3600.

### Parametric Sweep

- 1 In the **Study** toolbar, click  **Parametric Sweep**.
- 2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
- 3 Click **+ Add**.
- 4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
fr_pos_NCA (Volume fraction of NCA in NCA/LMO mix)	0.05 0.25 0.55 0.75	


### Solution 3 (sol3)

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 3 (sol3)** node, then click **Time-Dependent Solver 1**.
- 3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.
- 4 From the **Times to store** list, choose **Steps taken by solver**.  
Store only every 3rd time step. This reduces the size of the stored solution and the size of model file.
- 5 In the **Store every Nth step** text field, type 3.
- 6 In the **Model Builder** window, click **Study 2**.
- 7 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 8 Clear the **Generate default plots** checkbox.
- 9 In the **Study** toolbar, click  **Compute**.

## RESULTS

You can plot the voltage profiles from the parametric study (Figure 5) by performing the following steps:

### Voltage profiles for different mix fractions of NCA and LMO

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Voltage profiles for different mix fractions of NCA and LMO in the **Label** text field.

### Point Graph 1

- 1 Right-click **Voltage profiles for different mix fractions of NCA and LMO** and choose **Point Graph**.
- 2 In the **Settings** window for **Point Graph**, locate the **Data** section.

- 3 From the **Dataset** list, choose **Study 2/Parametric Solutions I (sol5)**.
- 4 Select Boundary 4 only.
- 5 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **phis - Electric potential - V**.
- 6 Locate the **Legends** section. Select the **Show legends** checkbox.
- 7 From the **Legends** list, choose **Evaluated**.
- 8 In the **Legend** text field, type  $\text{eval}(\text{fr\_pos\_NCA} * 100) / \text{eval}((1 - \text{fr\_pos\_NCA}) * 100)$   
volume mix of NCA and LMO.

*Voltage profiles for different mix fractions of NCA and LMO*

- 1 In the **Model Builder** window, click  
**Voltage profiles for different mix fractions of NCA and LMO**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.
- 3 Select the **y-axis label** checkbox. In the associated text field, type Voltage (V).
- 4 Locate the **Title** section. From the **Title type** list, choose **Label**.
- 5 Locate the **Axis** section. Select the **Manual axis limits** checkbox.
- 6 In the **x minimum** text field, type 0.
- 7 In the **x maximum** text field, type 3600.
- 8 In the **y minimum** text field, type 3.0.
- 9 In the **y maximum** text field, type 4.2.
- 10 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

II In the **Voltage profiles for different mix fractions of NCA and LMO** toolbar, click  **Plot**.

