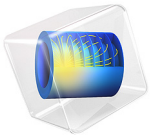


Lithium-Ion Battery with Multiple Intercalating Electrode Materials

Introduction

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 mix 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

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 domains:

- Negative porous electrode: 50 μm
- Separator: 50 μm
- Positive porous electrode: 50 μm

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 intercalate 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 $LiPF_6$ salt in 1:1 EC:DEC (by weight) solvent. The two active materials in the positive electrode are NCA ($Li_yNi_{0.80}Co_{0.15}Al_{0.15}O_2$) and LMO ($Li_yMn_2O_4$ spinel). For the negative electrode, MCMB graphite (Li_xC_6) is used in the model. The material properties of the electrolyte and active materials are taken from the Material Library.

The equilibrium potentials of the positive electrode materials are shown in Figure 1

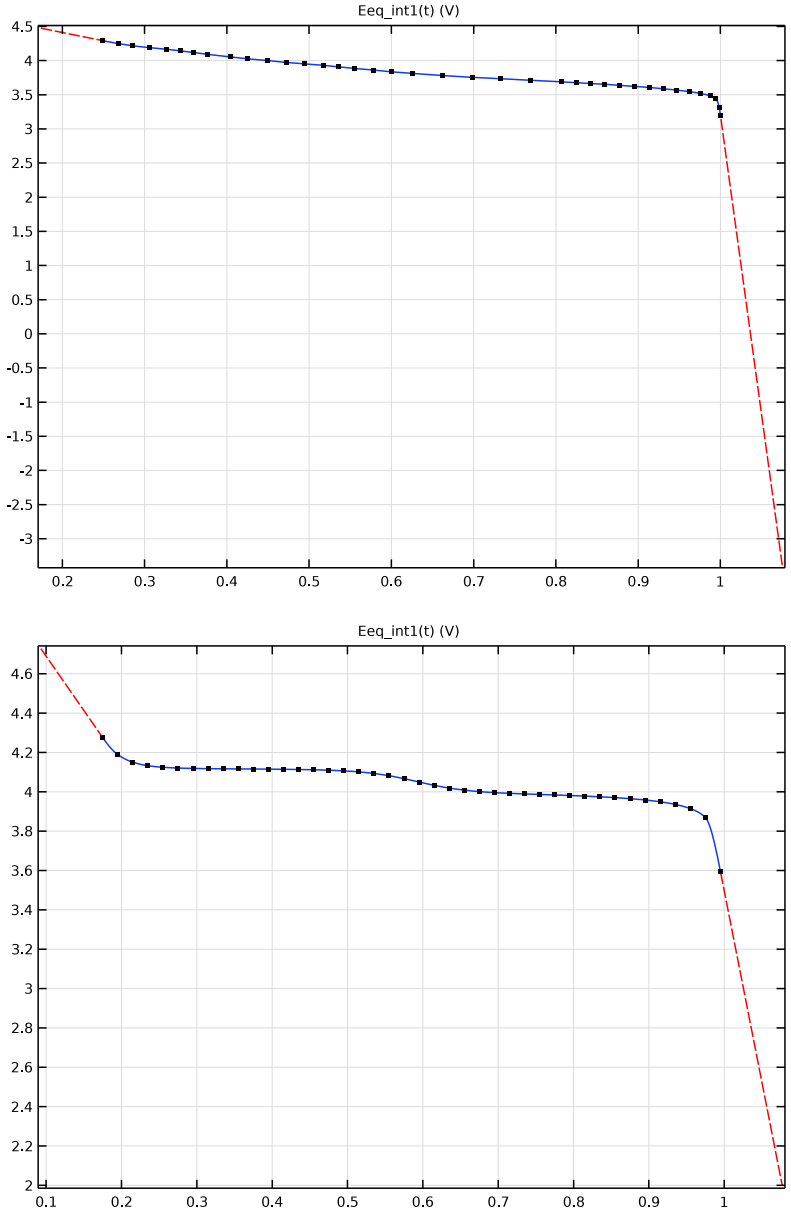


Figure 1: The equilibrium potentials of NCA (top) and LMO (bottom).

The x-axis data in Figure 1 is the state of charge (SOC) in the active material, which is calculated by dividing the surface concentration of lithium with the maximum concentration of lithium in the material.

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 ($11.72\ \mathrm{A/m^2}$).

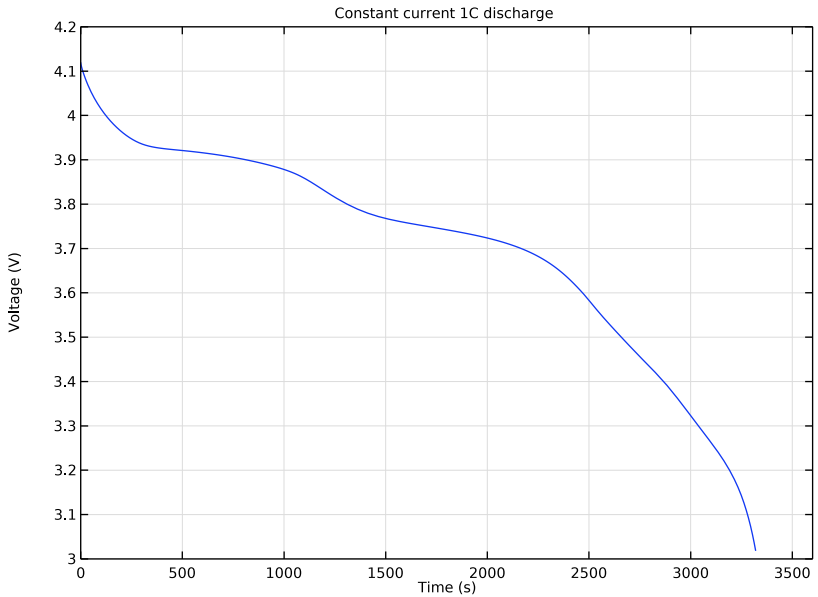


Figure 2: Discharge voltage profile at 1C.

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.

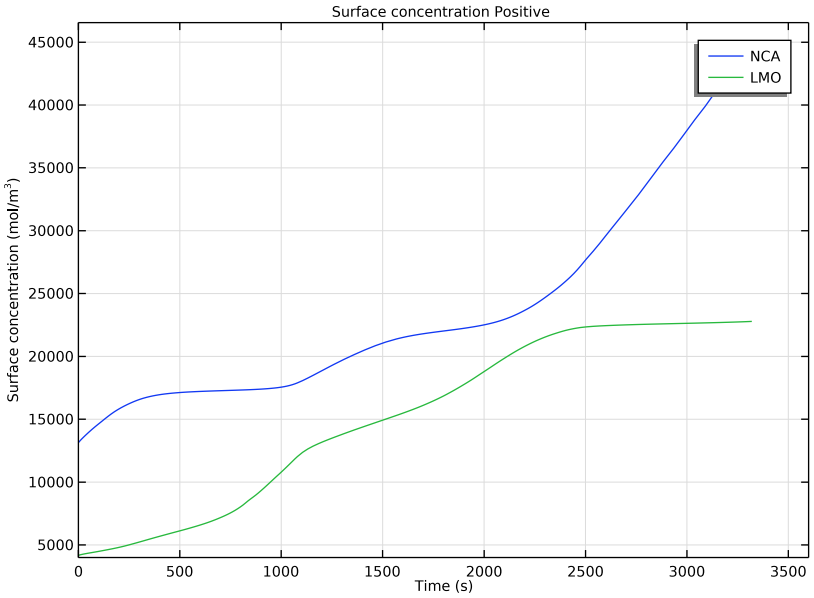


Figure 3: Surface concentration in the active material particles in the positive electrode during 1C discharge.

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.

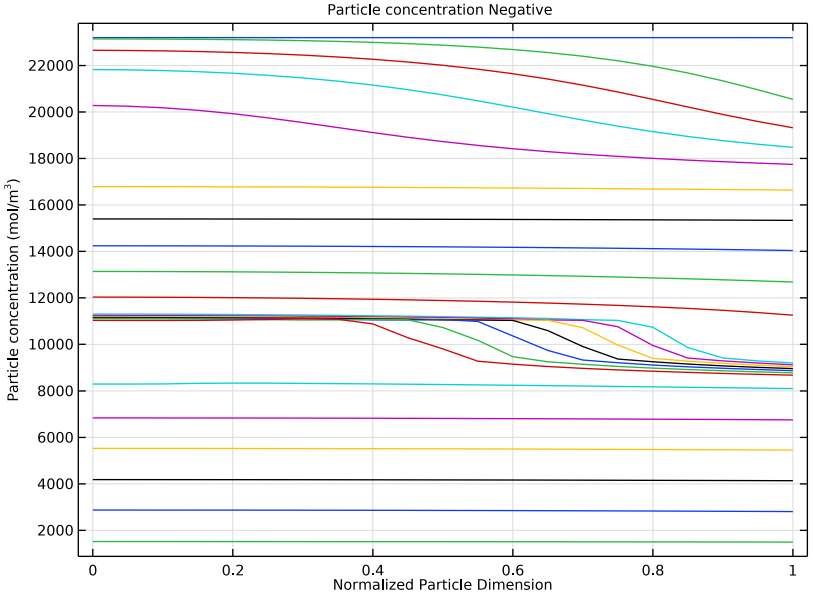


Figure 4: Concentration profiles inside a particle at a particular position in the negative electrode, at various times during 1C discharge.

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.

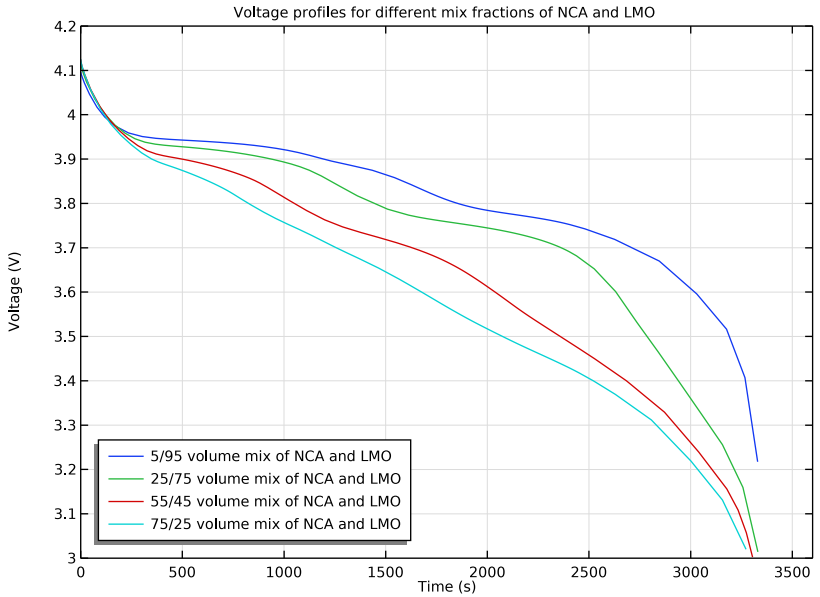


Figure 5: Voltage profiles during 1C discharge for different volume mix fractions of the active materials in the positive electrode.

Reference

1. 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/Batteries,_Lithium-Ion/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 **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

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 `li_battery_multiple_materials_parameters.txt`.

GEOMETRY 1

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

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

All materials are available in the Material Library. Note: In the Materials node, `cEeqref` denotes the maximum lithium concentration in the active material.

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

4 Click **Add to Component** in the window toolbar.

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

6 Click **Add to Component** in the window toolbar.

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

8 Click **Add to Component** in the window toolbar.

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

10 Click **Add to Component** in the window toolbar.

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

MATERIALS

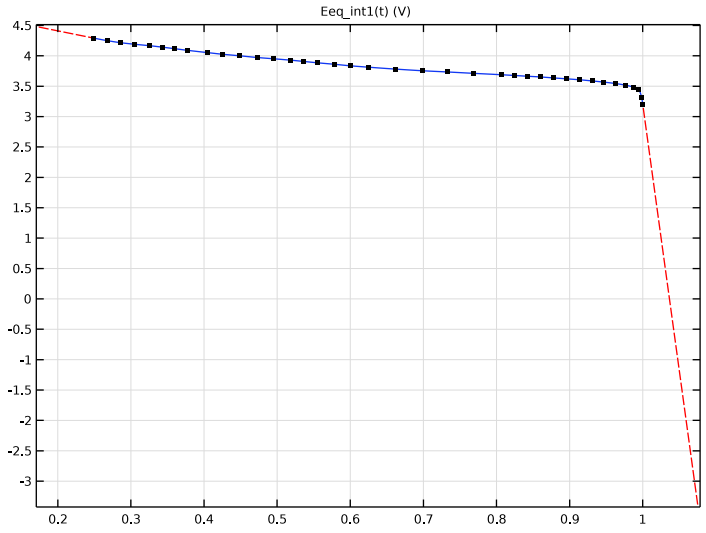
NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3)

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

Interpolation 1 (Eeq_int1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials>NCA, LiNi0.8Co0.15Al0.05O2 (Positive, Li-ion Battery) (mat3)>Equilibrium potential (elpot)** node, then click **Interpolation 1 (Eeq_int1)**.

2 In the **Settings** window for **Interpolation**, click **Plot**.



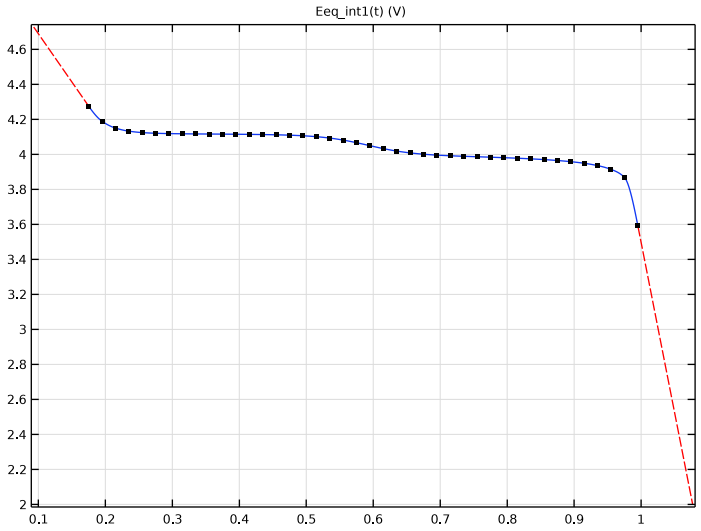
LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4)

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

Interpolation 1 (Eeq_int1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4)>Equilibrium potential (elpot)** node, then click **Interpolation 1 (Eeq_int1)**.

2 In the **Settings** window for **Interpolation**, click **Plot**.



DEFINITIONS

Load the variables for this model from a text file.

Variables 1

1 In the **Home** toolbar, click **Variables** and choose **Local 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 `li_battery_multiple_materials_variables.txt`.

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 diffusivites are simply set to the values available in the Material Library.

Porous Electrode 1

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

2 Select Domain 1 only.

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

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

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

The `liion.epss_neg` variable is calculated automatically by the **Initial Cell Charge Distribution** node in order to balance the capacity of the negative electrode to that of the positive.

6 In the ε_l text field, type `epsl_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 $i_{0,\mathrm{ref}}(T)$ 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 From the **Electrode material** list, choose **NCA, 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_NCA`.

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 `epsl_pos^brugl_pos`.

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

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 **NCA, 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_NCA`.

5 From the **Species concentration transport model** list, choose **Baker-Verbrugge**.

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

4 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_pos_NCA`.

Additional Porous Electrode Material 1

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 ε_s text field, type `epss_pos_LMO`.

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

4 Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_pos_LMO`.

5 From the **Species concentration transport model** list, choose **Baker-Verbrugge**.

6 Locate the **Model Input** section. From the c list, choose **Solid phase concentration, Additional Porous Electrode Material 1 (liion/addm1/pin1)**.

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 $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_pos_LMO`.

5 Locate the **Model Input** section. From the c list, choose **Insertion particle surface concentration, Additional Porous Electrode Material 1 (liion)**.

Separator 1

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

2 Select Domain 2 only.

3 In the **Settings** window for **Separator**, locate the **Porous Matrix Properties** section.

4 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`.

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 From the **Initial battery cell setting** list, choose **Initial cell state-of-charge**.

4 In the $SOC_{\mathrm{cell},0}$ text field, type `SOC_cell0`.

5 In the $Q_{\mathrm{cell},0}$ text field, type `Q_batt`.

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 Select Domain 1 only.

Positive Electrode Selection 1

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

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`.

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**.

DEFINITIONS (COMP1)

Using a boundary integration variable you can access the cell voltage at the end terminal during computation.

Integration 1 (intop1)

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

2 In the **Settings** window for **Integration**, type `EndTerminal` 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.

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`.

Solution 1 (sol1)

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

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** 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**.

5 Right-click **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Stop Condition**.

6 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

7 Click **Add**.

8 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.EndTerminal(comp1.phis)< 3.0`	True (>=1)	√	`Stop expression 1`

9 Locate the **Output at Stop** section. Clear the **Add warning** check box.

10 In the **Model Builder** window, click **Study 1**.

11 In the **Settings** window for **Study**, locate the **Study Settings** section.

12 Clear the **Generate default plots** check box.

13 In the **Study** toolbar, click **Compute**.

RESULTS

Reproduce the plots in the model documentation for 1C discharge, starting with the voltage profile (Figure 2).

Constant current 1C discharge

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. Right-click **1D Plot Group 1** and choose **Rename**.
3. In the **Rename 1D Plot Group** dialog box, type `Constant current 1C discharge` in the **New label** text field.
4. Click **OK**.

Point Graph 1

1. Right-click **Constant current 1C 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 1 (comp1)> Lithium-Ion Battery>phis - Electric potential - V**.

Constant current 1C discharge

1. In the **Model Builder** window, click **Constant current 1C discharge**.
2. In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.
3. Select the **y-axis label** check box.
4. In the associated text field, type `Voltage (V)`.
5. Click to expand the **Title** section. From the **Title type** list, choose **Label**.
6. Locate the **Axis** section. Select the **Manual axis limits** check box.
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 1C 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 1C discharge (Figure 3).

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. Right-click **1D Plot Group 2** and choose **Rename**.

3 In the **Rename 1D Plot Group** dialog box, type `Surface concentration Positive` in the **New label** text field.

4 Click **OK**.

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 (comp1)> Lithium-Ion Battery>Particle intercalation>liion.cs_surface - Insertion particle concentration, surface - mol/m³**.

4 Click to expand the **Legends** section. Select the **Show legends** check box.

5 From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
NCA

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 (comp1)> Lithium-Ion Battery>Particle intercalation>liion.cs_surface_addm1 - Insertion particle surface concentration, Additional Porous Electrode Material 1 - mol/m³**.

3 Locate the **Legends** section. In the table, enter the following settings:

Legends
LMO

Surface concentration Positive

1 In the **Model Builder** window, click **Surface concentration Positive**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **y-axis label** check box.

4 In the associated text field, type `Surface concentration (mol/m<sup>3</sup>)`.

5 Locate the **Title** section. From the **Title type** list, choose **Label**.

6 Locate the **Axis** section. Select the **Manual axis limits** check box.

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 4000.

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 1C 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)**.

Particle concentration Negative

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 Right-click **1D Plot Group 3** and choose **Rename**.

3 In the **Rename 1D Plot Group** dialog box, type `Particle concentration Negative` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

6 From the **Dataset** list, choose **Study 1/Solution 1: xdim Negative (sol1)**.

7 From the **Time selection** list, choose **Interpolated**.

8 In the **Times (s)** text field, type `range(0,200,2000) range(2030,30,2200) range(2300,200,3300)`.

Line Graph 1

1 Right-click **Particle concentration Negative** and choose **Line Graph**.

2 Select Domain 1 only.

The `atxd1()` operator is used to specify the `x` coordinate in the negative electrode of the battery geometry.

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)`.

Particle concentration Negative

1 In the **Model Builder** window, click **Particle concentration Negative**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Normalized Particle Dimension`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `Particle concentration (mol/m<sup>3</sup>)`.

7 Locate the **Title** section. From the **Title type** list, choose **Label**.

8 In the **Particle concentration Negative** 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 **Add Study** in the window toolbar.

5 In the **Model Builder** window, click the root node.

6 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 2: Time Dependent

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

2 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 Right-click **Study 2>Solver Configurations>Solution 3 (sol3)>Time-Dependent Solver 1** and choose **Stop Condition**.

7 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

8 Click **Add**.

9 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
comp1.EndTerminal(comp1.phis)< 3.0	True (>=1)	√	Stop expression 1

10 Locate the **Output at Stop** section. Clear the **Add warning** check box.

11 In the **Model Builder** window, click **Study 2**.

12 In the **Settings** window for **Study**, locate the **Study Settings** section.

13 Clear the **Generate default plots** check box.

14 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 (parametric)

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 Right-click **1D Plot Group 4** and choose **Rename**.

3 In the **Rename 1D Plot Group** dialog box, type `Voltage profiles (parametric)` in the **New label** text field.

4 Click **OK**.

Point Graph 1

1 Right-click **Voltage profiles (parametric)** 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 1 (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** check box.

7 From the **Legends** list, choose **Evaluated**.

8 In the **Legend** text field, type `eval(fr_pos_NCA*100)/eval((1-fr_pos_NCA)*100) volume mix of NCA and LMO`.

Voltage profiles (parametric)

1 In the **Model Builder** window, click **Voltage profiles (parametric)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **y-axis label** check box.

4 In the associated text field, type `Voltage (V)`.

5 Locate the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Voltage profiles for different mix fractions of NCA and LMO`.

7 Locate the **Axis** section. Select the **Manual axis limits** check box.

8 In the **x minimum** text field, type `0`.

9 In the **x maximum** text field, type `3600`.

10 In the **y minimum** text field, type `3.0`.

11 In the **y maximum** text field, type `4.2`.

12 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

13 In the **Voltage profiles (parametric)** toolbar, click  **Plot**.