Model created in COMSOL Multiphysics 6.4

1D Lithium-Ion Battery Drive-Cycle Monitoring

Introduction

This application shows how a battery cell subjected to a hybrid electric vehicle drive cycle can be investigated using the Lithium-Ion Battery interface in COMSOL. The model is based on the Lithium-Ion Battery Base Model in 1D.

In Figure 1, an example of an electric vehicle with three critical components of a simplified battery management system is displayed. When the vehicle runs according to a specific drive cycle, the temperature and voltage of the battery will vary and be monitored. This tells the monitoring unit, usually with the help of some type of algorithm, the state of charge (SOC) of the battery, and decides, for instance, whether the battery is empty or full. In those two cases, the control unit will stop the discharge and charge, respectively. Monitored elevated temperature can also trigger the control unit.

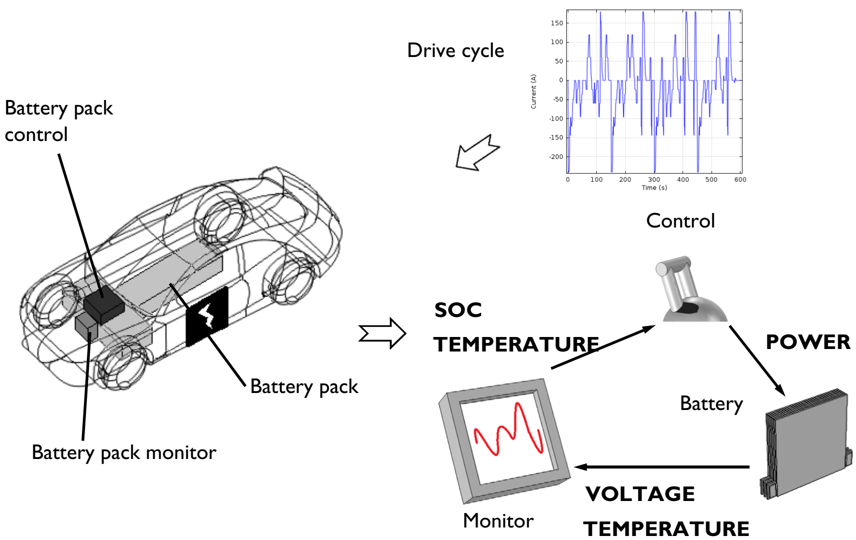


Figure 1: Electric vehicle with key components within the battery management system visualized. As the flowchart to the right shows, the battery voltage and temperature are monitored and act as inputs to the control unit.

What the Lithium-Ion Battery interface can do here is to predict the battery behavior or make comparisons between computed and monitored properties. So the simulations will in fact act as either a premonitoring step of the battery or a tool to understand the battery behavior during the cycle better. The latter is possible, since the model setup includes the physical properties and can therefore calculate some properties that are difficult to measure, for instance:

- The internal resistance and polarization in each part of the battery cell
- The individual degrees of lithiation of each electrode material
- The individual electrode potentials

At the same time, the model setup opens up the possibility to vary battery design parameters. For instance, materials and thickness of electrodes can easily be changed to evaluate their effect on the overall performance.

Model Definition

The model is set up in 1D for a graphite/NMC battery cell. A more detailed description of the model can be found in Lithium-Ion Battery Base Model in 1D.

Drive cycle data containing C-rate versus time is imported and used as current load in the model. The drive cycle contains C-rates up to 20C and represents that of a typical hybrid electric vehicle. Figure 2 shows the drive cycle.

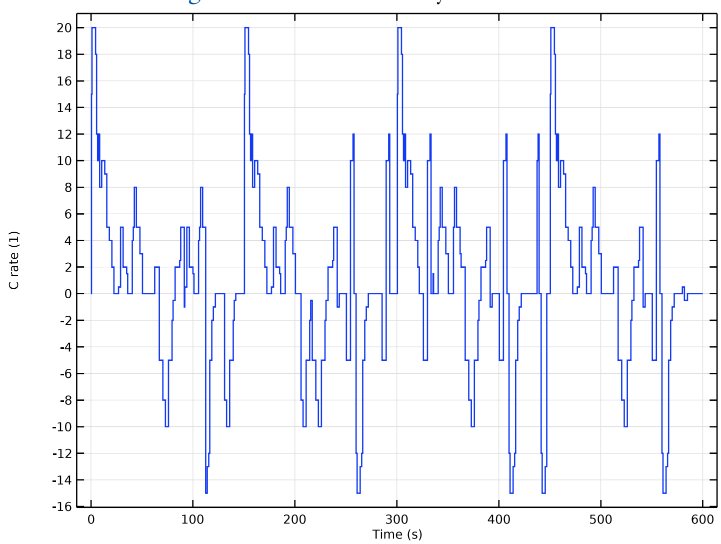


Figure 2: Drive cycle, defined as C-rate versus time.

The Modeling Instructions shows how to open up the base model and apply the load cycle to the battery model. First a shorter 60 s simulation is performed, and the preliminary analysis of the results indicate too low potentials in the negative electrode (an indication of lithium plating susceptibility). The battery is then made more power optimized by using thinner electrodes, and the simulation is then recomputed for 600 s. The results of the final simulation is discussed in the next section.

Results and Discussion

Figure 3 shows the cell voltage, and the corresponding open circuit voltage and the current levels (on the secondary *y*-axis) versus time. The cell voltage varies between 3.3 V and 4.1 V, while the open-circuit voltage (OCV), the voltage the cell would relax to if left at open circuit for a longer time, varies considerably less.

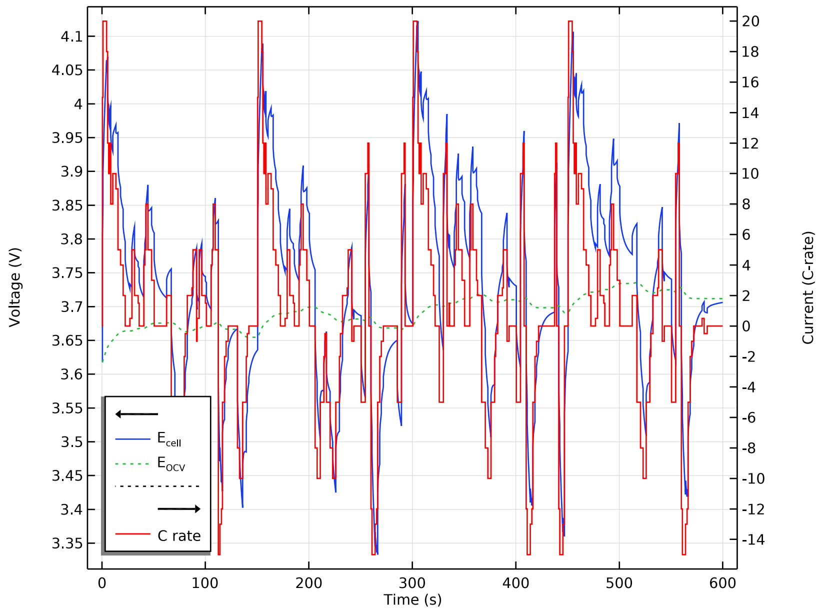


Figure 3: Cell voltage and open-circuit cell voltage, together with charge/discharge current C-rate.

Figure 4 shows the total polarization, computed as the difference between the cell OCV and the cell voltage under load, and the current load. The two curves exhibit a dynamically changing nonlinear relationship with respect to each other. This stems from the contributions from several different phenomena to the total cell polarization of the cell. The models Lithium-Ion Battery Rate Capability and Power Losses in a Lithium-Ion Battery further look into the origin of these potential losses.

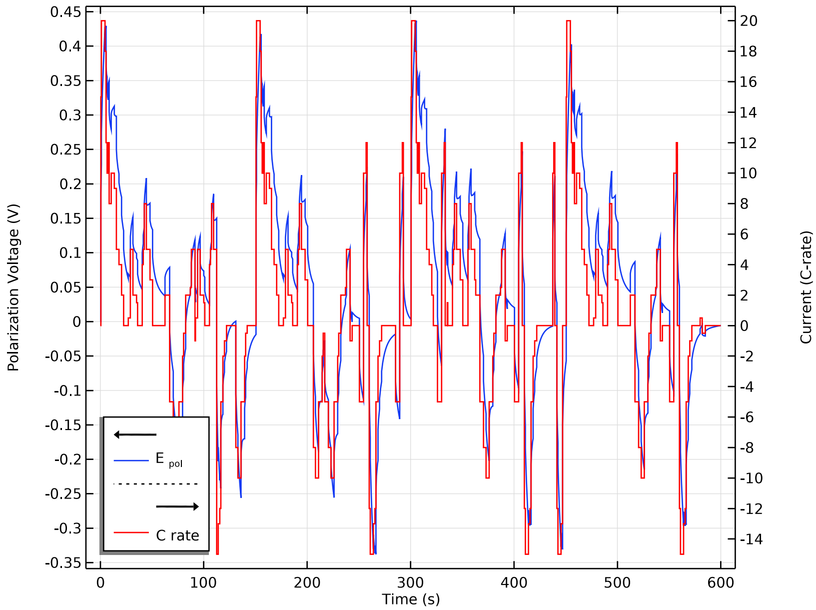


Figure 4: Total polarization and load.

The SOC and the corresponding degrees of lithiation in each electrode are shown in Figure 5.

Figure 5: SOC of cell and electrodes at load during drive cycle.

The load cycle is not charge-neutral, resulting in an increase of the cell SOC from 25% to about 40% at the end of the simulation.

The degree of lithiation levels will impact the corresponding electrode potentials, in combination with the different contributions to the cell polarization. Figure 6 shows the potential in the positive electrode at two locations during the simulation: At the boundary between the separator and the electrode, and at the boundary between the electrode and the current collector. Analyzing these potentials is important since too high positive electrode potentials may result in, for instance, decomposition of the electrode host material. Generally the potentials vary more at the electrode-separator boundary compared to the electrode-current collector boundary. This is a result from the nonhomogeneous current distribution in the cell.

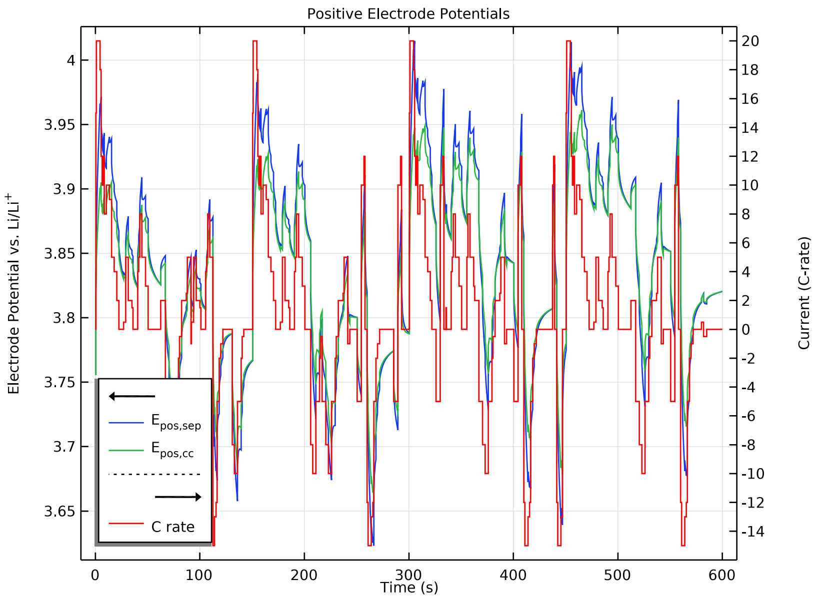


Figure 6: Positive electrode potentials.

Similarly, Figure 7 shows the corresponding negative electrode potentials. At the separator, the negative electrode potential drops below 0 V vs. Li/Li^+ during some of the 20C charge pulses. This will result in lithium plating, which in turn may accelerate battery aging and capacity loss. A conclusion from this work is hence that for a battery with this configuration, the BMS system would have to, in some way, protect the battery from excessively large (>10C) charging currents.

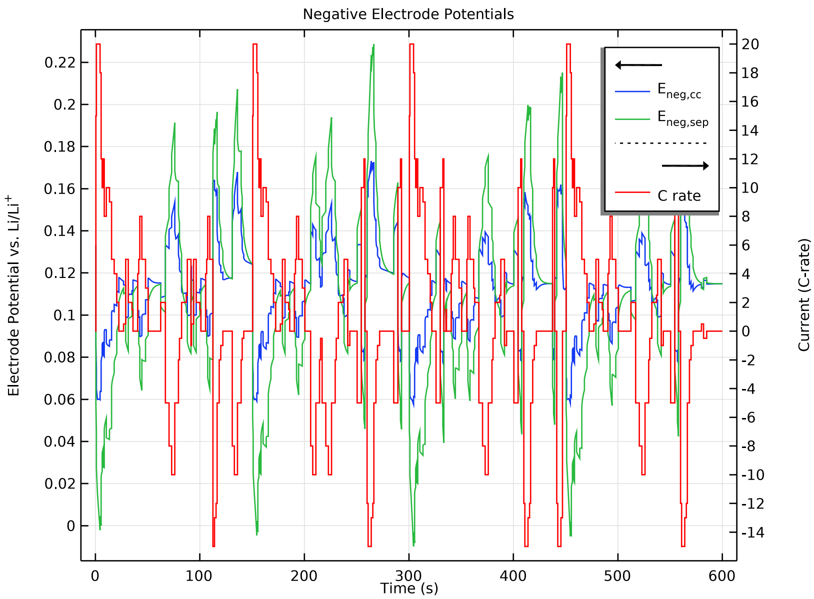


Figure 7: Negative electrode potentials.

Notes About the COMSOL Implementation

To reduce the computation time for the model, the Particle Intercalation node option **Fast assembly in particle dimension** is enabled. Enabling this option applies an alternative method for assembling the diffusion equation in the particle dimension. This alternative method typically decreases computation time for 1D models. For this model, the reduction in computation time is about 20%. Regardless of whether **Fast assembly in particle dimension** is selected or not, the same diffusion equations are solved for.

Application Library path: `Battery_Design_Module/Lithium-Ion_Batteries, _Performance/lib_drive_cycle`

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

2 In the **Application Libraries** window, select **Battery Design Module > Lithium-Ion Batteries, Performance > lib_base_model_1d** in the tree.

3 Click **Open**.

In this tutorial, we will run the battery model you just loaded versus a specified drive cycle. First for 60 s, then for 600 s.

LITHIUM-ION BATTERY (LIION)

Load Cycle 1

1 In the **Model Builder** window, expand the **Component 1 (comp1) > Lithium-Ion Battery (liion)** node, then click **Load Cycle 1**.

2 In the **Settings** window for **Load Cycle**, locate the **Continuation Conditions** section.

3 Select the **Use elapsed time only** checkbox.

C Rate 1

1 In the **Model Builder** window, expand the **Load Cycle 1** node, then click **C Rate 1**.

2 In the **Settings** window for **C Rate**, locate the **C-Rate Multiple** section.

3 From the **Input type** list, choose **Step sequence**.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `lib_drive_cycle_data.txt`.

Porous Electrode - Negative

In the **Particle Intercalation** nodes of the **Porous Electrode** features, it is useful to enable fast assembly in the particle dimension option. This option enables an alternative method for assembling of the diffusion equation in the particle dimension, that typically decreases computation time for 1D models (for this model by about 20%). Note that the same diffusion equations are solved for regardless of assembly method.

Particle Intercalation 1

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

2 In the **Settings** window for **Particle Intercalation**, click to expand the **Particle Discretization** section.

3 Select the **Fast assembly in particle dimension** checkbox.

Particle Intercalation 1

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

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

3 Select the **Fast assembly in particle dimension** checkbox.

GLOBAL DEFINITIONS

Parameters 1

Modify the parameter for the initial state of charge of the battery. This will impact the initial solid concentration levels (degrees of lithiation) defined in the **Particle Intercalation** child nodes to the **Porous Electrode** nodes.

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
`soc_init`	`0.25`	0.25	`Initial SOC`

STUDY 1

Step 2: Time Dependent

The model is now ready for solving. First set the solver to run a simulation 60 s of cycling time only.

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 2: Time Dependent**.

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

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

4 In the **Output times** text field, type `range(0,1,60)`.

The problem is now ready for solving.

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

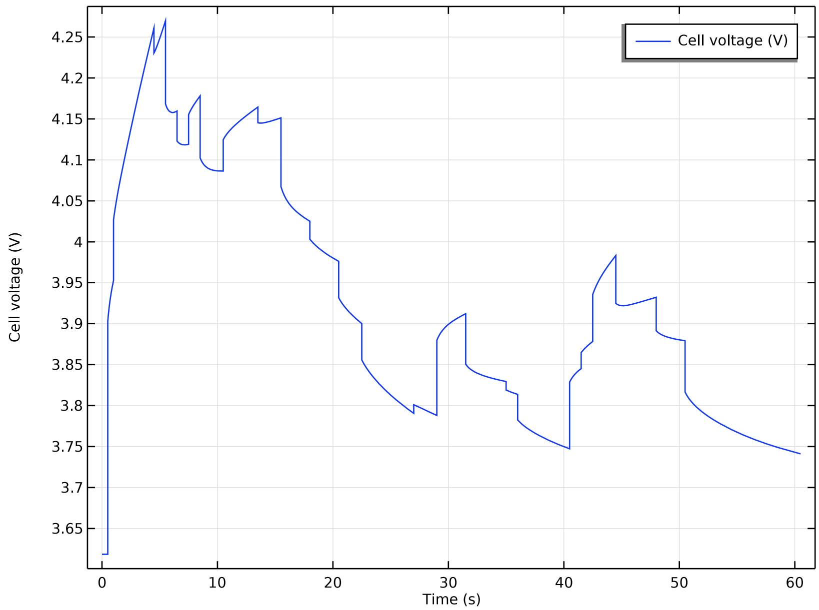
RESULTS

Probe Plot Group 1

A probe plot of the battery voltage versus time is plotted automatically during the simulation:

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 1**.

2 In the **Probe Plot Group 1** toolbar, click **Plot**.



Create a plot of the cell voltage and corresponding current load as follows:

Cell Voltage and Load

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Cell Voltage and Load` in the **Label** text field.

Global 1

1 Right-click **Cell Voltage and Load** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **E_cell - Cell voltage - V**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
E_cell	V	Cell voltage

4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **E_ocv_cell - Open-circuit cell voltage - V**.

5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

6 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
E_{cell}
E_{OCV}

Global 2

1 In the **Model Builder** window, right-click **Cell Voltage and Load** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **Load Cycle 1** > **liion.lc1.C_app - C rate - 1**.

3 Locate the **Coloring and Style** section. From the **Color** list, choose **Red**.

Cell Voltage and Load

1 In the **Model Builder** window, click **Cell Voltage and Load**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

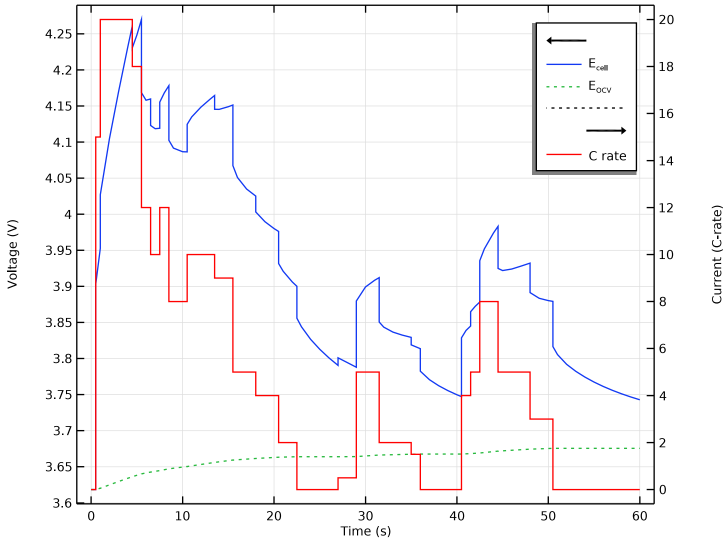
4 Locate the **Plot Settings** section. Select the **Two y-axes** checkbox.

5 Select the **y-axis label** checkbox. In the associated text field, type `Voltage (V)`.

6 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Current (C-rate)`.

7 In the table, select the **Plot on secondary y-axis** checkbox for **Global 2**.

8 In the **Cell Voltage and Load** toolbar, click **Plot**.



Duplicate this plot and modify it slightly to create a plot of the total polarization.

Total Polarization and Load

1 Right-click **Cell Voltage and Load** and choose **Duplicate**.

2 In the **Model Builder** window, click **Cell Voltage and Load 1**.

3 In the **Settings** window for **1D Plot Group**, type `Total Polarization and Load` in the **Label** text field.

4 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Polarization Voltage (V)`.

Global 1

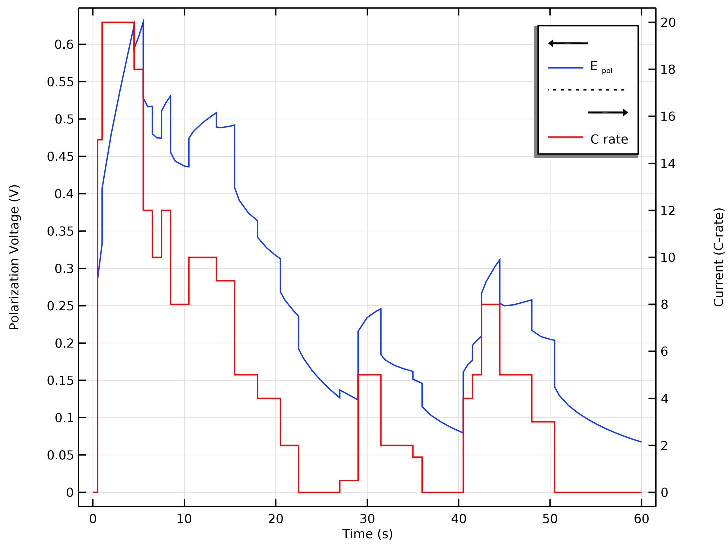
1 In the **Model Builder** window, click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **E_pol_tot - Total battery cell polarization - V**.

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

Legends
`E <sub>pol</sub>`

4 In the **Total Polarization and Load** toolbar, click **Plot**.



State of charge and average lithiation levels

Create also a plot of the state of charge and the corresponding lithiation levels of the electrodes.

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `State of charge and average lithiation levels` in the **Label** text field.

3 Locate the **Title** section. 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 `SOC or SOL (1)`.

Global 1

1 Right-click **State of charge and average lithiation levels** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **soc_cell - Battery cell state of charge - 1**.

3 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **sol_pos - Degree of lithiation, positive - 1**.

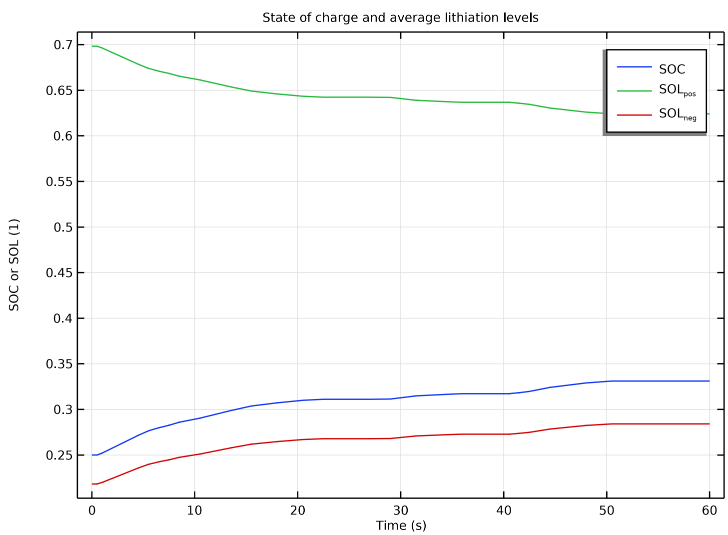
4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **sol_neg - Degree of lithiation, negative - 1**.

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

6 In the table, enter the following settings:

Legends
SOC
SOL_{pos}
SOL_{neg}

7 In the **State of charge and average lithiation levels** toolbar, click **Plot**.



Positive Electrode Potentials

Now plot the electrode potentials in the positive electrode as follows:

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Positive Electrode Potentials` in the **Label** text field.

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

4 Locate the **Plot Settings** section. Select the **Two y-axes** checkbox.

5 Select the **y-axis label** checkbox. In the associated text field, type Electrode Potential vs. Li/Li⁺.

6 Select the **Secondary y-axis label** checkbox. In the associated text field, type Current (C-rate).

7 Locate the **Legend** section. From the **Position** list, choose **Upper right**.

Point Graph 1

1 Right-click **Positive Electrode Potentials** and choose **Point Graph**.

2 Select Boundaries 3 and 4 only.

3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type phis-phil.

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:

Legends
E_{pos,sep}
E_{pos,cc}

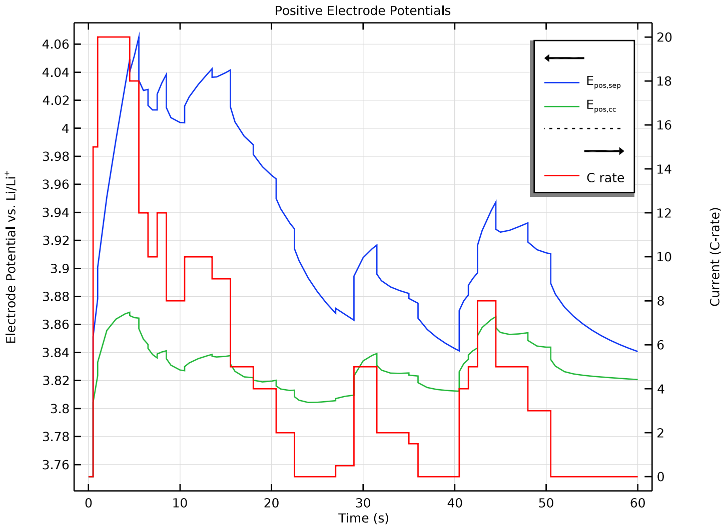
Global 2

In the **Model Builder** window, under **Results** > **Total Polarization and Load** right-click **Global 2** and choose **Copy**.

Global 2

1 In the **Model Builder** window, right-click **Positive Electrode Potentials** and choose **Paste Global**.

2 In the **Positive Electrode Potentials** toolbar, click **Plot**.



The potentials versus Li/Li+ are generally varying more at the electrode-separator boundary compared to the electrode-current collector boundary. This is due to an uneven current distribution in the cell.

Negative Electrode Potentials

1 Right-click **Positive Electrode Potentials** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Negative Electrode Potentials` in the **Label** text field.

Point Graph 1

1 In the **Model Builder** window, expand the **Negative Electrode Potentials** node, then click **Point Graph 1**.

2 In the **Settings** window for **Point Graph**, locate the **Selection** section.

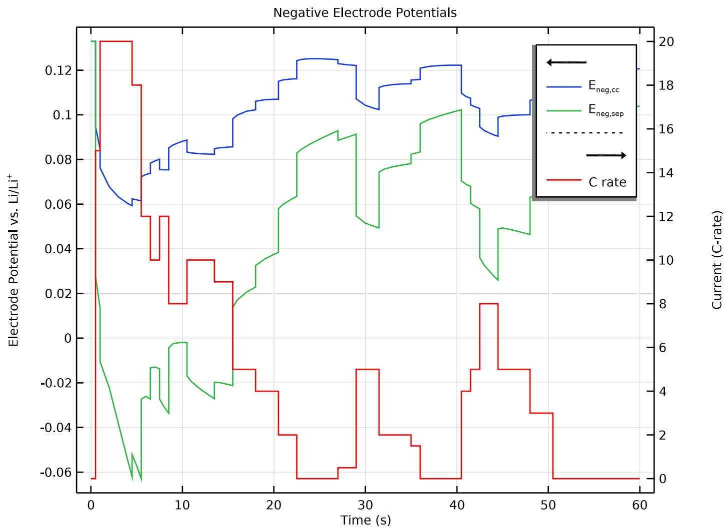
3 Click **Clear Selection**.

4 Select Boundaries 1 and 2 only.

5 Click to expand the **Legends** section. In the table, enter the following settings:

Legends
E_{neg,cc}
E_{neg,sep}

6 In the **Negative Electrode Potentials** toolbar, click **Plot**.



GLOBAL DEFINITIONS

Parameters 1

The negative potential reaching levels below 0 V versus Li/Li+ at the separator-electrode boundary is problematic since this may result in lithium plating in the cell. Making the electrodes thinner will make the battery more power optimized. Reduce the positive electrode thickness. The negative electrode thickness is automatically reduced based on the correlation defined in the **Parameters 1** node.

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
L_pos	25[um]	2.5E-5 m	Positive electrode thickness

STUDY 1

Step 2: Time Dependent

Now increase the solver time to 600 s and recompute.

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(0,1,600)`.

4 In the **Study** toolbar, click **= Compute**.

You may now compare the plots with the corresponding figures of the Results and Discussion section above.

RESULTS

Cell Voltage and Load

1 In the **Model Builder** window, under **Results** click **Cell Voltage and Load**.

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

3 From the **Position** list, choose **Lower left**.

4 In the **Cell Voltage and Load** toolbar, click **Plot**.

Total Polarization and Load

1 In the **Model Builder** window, click **Total Polarization and Load**.

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

3 From the **Position** list, choose **Lower left**.

4 In the **Total Polarization and Load** toolbar, click **Plot**.

State of charge and average lithiation levels

1 In the **Model Builder** window, click **State of charge and average lithiation levels**.

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

3 From the **Position** list, choose **Middle left**.

4 In the **State of charge and average lithiation levels** toolbar, click **Plot**.

Positive Electrode Potentials

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

2 In the **Positive Electrode Potentials** toolbar, click **Plot**.

Negative Electrode Potentials

1 In the **Model Builder** window, click **Negative Electrode Potentials**.

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

3 From the **Position** list, choose **Upper right**.

4 In the **Negative Electrode Potentials** toolbar, click **Plot**.

Plating potentials (below 0 V) in the negative electrode are seen during the largest charge pulses. A more power-optimized battery (for instance using thinner electrodes) would be required in order to avoid plating entirely.