Created in COMSOL Multiphysics 6.1

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.

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.

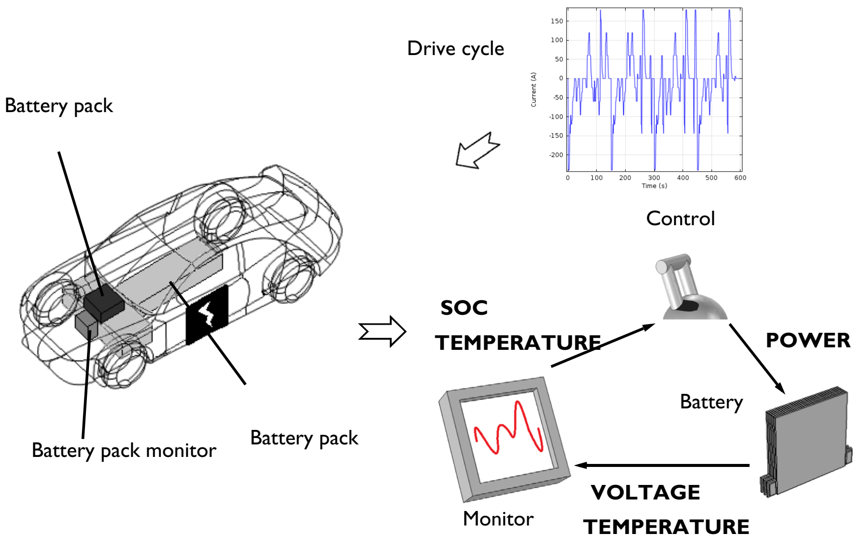


Figure 1: Electric vehicle with key components within the battery management system visualized. As the flowchart to the right shows, the battery voltage and temperature are monitored and act as inputs to the control unit.

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 pre-monitoring 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:

- internal resistance and polarization in each part of the battery cell,

- more accurate cell SOC, and
- SOC of each electrode material.

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

In this example, the advanced monitoring possibilities of the Lithium-Ion Battery interface are highlighted.

Model Definition

The model is set up for a graphite/LMO battery cell. The materials are available from the Battery Material Library and mainly default settings are selected. The model domains consist of:

- Negative porous electrode: Graphite (MCMB Li_xC_6) active material and electronic conductor.
- Separator.
- Positive porous electrode: LMO ($LiMn_2O_4$) active material, electronic conductor, and filler.
- Electrolyte: 1.0 M $LiPF_6$ in EC:DEC (1:1 by weight).

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

The Lithium-Ion Battery interface accounts for:

- electronic conduction in the electrodes,
- ionic charge transport in the electrodes and electrolyte/separator,
- material transport in the electrolyte, allowing for the introduction of the effects of concentration on ionic conductivity and concentration overpotential, and
- material transport within the spherical particles that form the electrodes, and
- Butler-Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium potential.

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 can be that of a typical hybrid electric vehicle. In Figure 2, the cycle is displayed with the C-rate recalculated to current (1C equals 12 A).

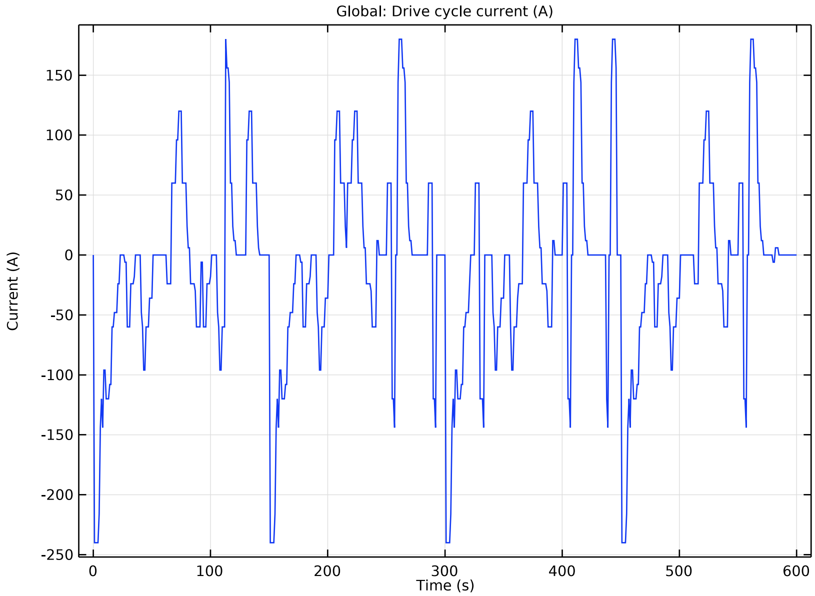


Figure 2: Drive cycle used in the model.

The initial cell voltage is set to 3.9 V, using the Initial Cell Charge Distribution feature.

More battery parameters and additional variable definitions used here are found in the Lithium-Ion Battery Seed application.

Results and Discussion

In Figure 3 the cell voltage and electrode potentials are shown. The cell voltage varies between 3.6 V and 4.25 V, while the open-circuit voltage varies considerably less. Of the two electrodes, the positive electrode potential varies slightly more than the negative electrode during the cycle, approximately 0.3 V. For prolonged lifetime and better safety, the battery should operate only within a specific voltage span. Since the upper and lower voltage limits for this battery cell chemistry are 4.2 V and 3.3 V, respectively, the battery design seems to fulfill this requirement.

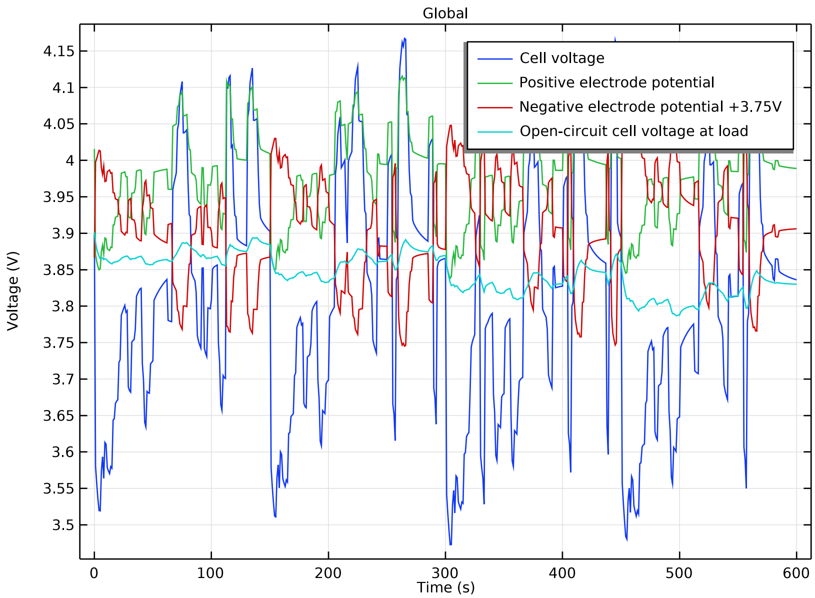


Figure 3: Cell voltage and open-circuit cell voltage, together with electrode potential during drive cycle.

The polarization gives an indication of the internal resistance and, normally, a large polarization reduce the battery lifetime and causes increased heat generation. The polarization during the pulse is displayed in Figure 4. Note that the sign of the polarization quickly changes when the current load shifts between charge and discharge.

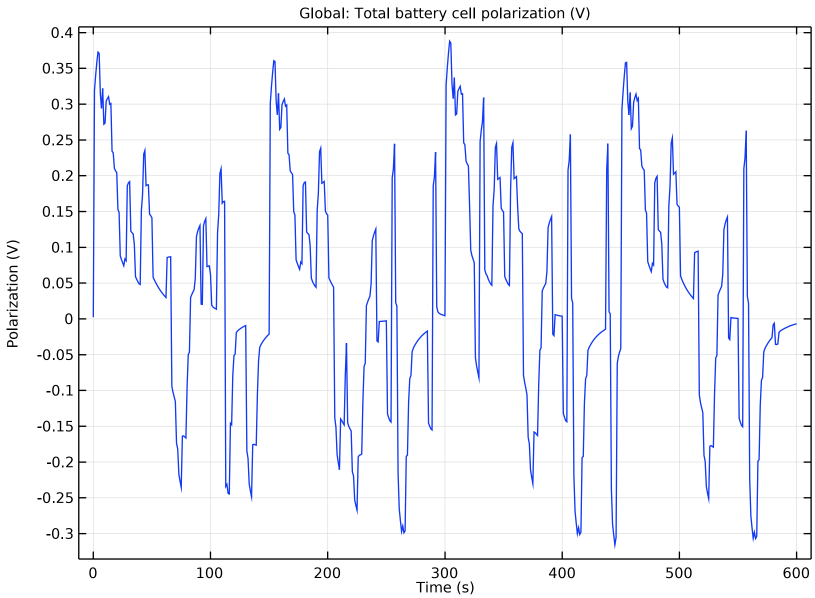


Figure 4: Total polarization during drive cycle.

The SOC is monitored in Figure 5. It shows that the cell and materials seem to be far from exhausted. The cell SOC is well within 0-100 %, the positive electrode is within 65-80 %

(SOC window 17.5-100 %), and the negative electrode within 14-29 % (SOC window 0-98%). This causes less strain on the battery and improves the stability of the system.

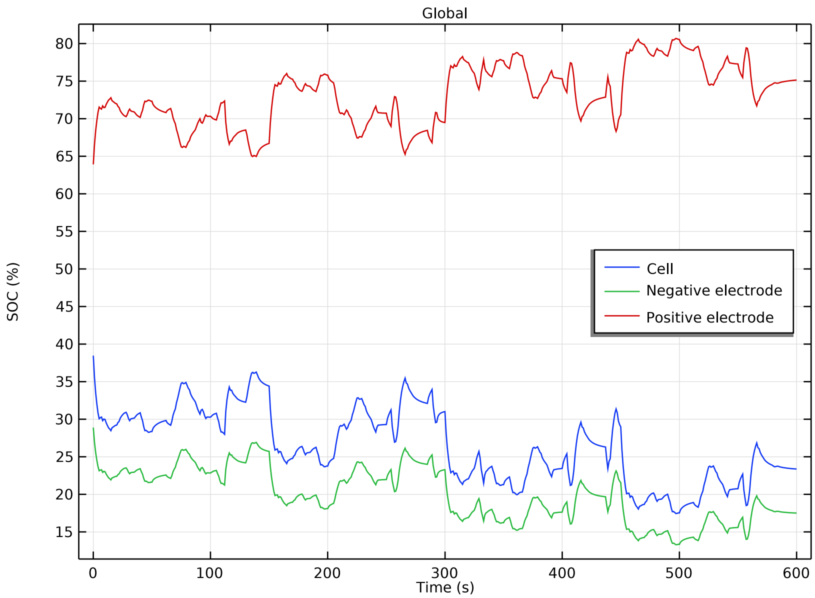


Figure 5: SOC of cell and electrodes at load during drive cycle.

Considering the results, this type of battery design seems suitable for the drive cycle.

For further reading on polarization and rate-capability, see Lithium-Ion Battery Rate Capability and Lithium-Ion Battery Internal Resistance.

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/li_battery_drive_cycle`

Modeling Instructions

APPLICATION LIBRARIES

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

2 In the **Application Libraries** window, select **Battery Design Module>Batteries, Lithium-Ion>li_battery_seed** 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 100 s, then for 600 s.

GLOBAL DEFINITIONS

A hybrid electric vehicle drive cycle, C-rates vs. time, is imported from a text file.

Interpolation 1 (int1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global>Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

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

6 Click **Import**.

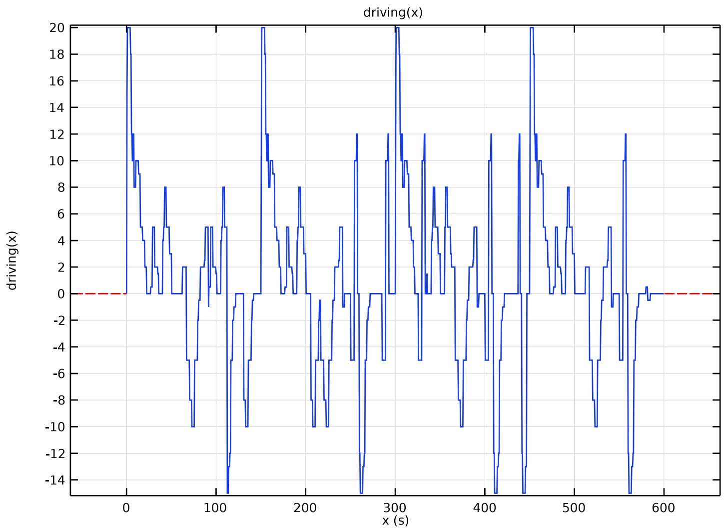
7 Find the **Functions** subsection. In the table, enter the following settings:

Function name	Position in file
driving	1

8 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
Column 1	s

9 Click **Plot**.



DEFINITIONS (COMP1)

Load the variables from a text file. Additionally, use the imported C-rate to create a current variable.

Variables 1

1. In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.
2. Right-click **Component 1 (comp1)>Definitions** and choose **Variables**.
3. In the **Settings** window for **Variables**, locate the **Variables** section.
4. Click **Load from File**.
5. Browse to the model's Application Libraries folder and double-click the file `li_battery_management_variables.txt`.
6. In the table, enter the following settings:

Name	Expression	Unit	Description
`I_drive`	`-liion.I_1C*driving(t)`	A	`Drive cycle current`

(The internally defined `liion.I_1C` variable used above defines the constant current required to completely charge or discharge the battery in 1 hour. The variable is defined by the **Initial Cell Charge Distribution** node.)

LITHIUM-ION BATTERY (LIION)

Electrode Current 1

1. In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **Electrode Current 1**.
2. In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.
3. In the $I_{\mathrm{s,total}}$ text field, type `I_drive`.

Porous Electrode 1

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. Note that the same diffusion equations are solved for regardless of assembly method. Additionally, specify the reference exchange current density for the electrode kinetics in the **Porous Electrode Reaction** nodes.

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**, click to expand the **Particle Discretization** section.
3. 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 **Electrode Kinetics** section.
3. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_neg`.

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 **Particle Discretization** section.
3. 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 **Electrode Kinetics** section.

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_pos`.

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(0,1,100)`.

Solution 1 (sol1)

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

Set the **Steps taken by solver** to **Intermediate** to ensure that sudden transients in the drive cycle are resolved by the time-dependent solver. Also, enable the nonlinear controller to improve handling of sudden load 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**, click to expand the **Time Stepping** section.

4 From the **Steps taken by solver** list, choose **Intermediate**.

5 Select the **Nonlinear controller** check box.

The problem is now ready for solving.

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

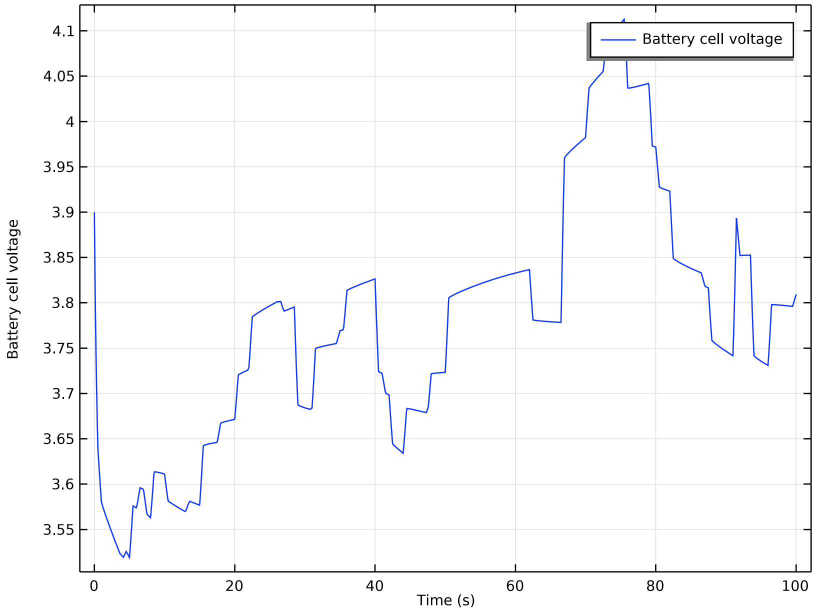
RESULTS

Probe Plot Group 6

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 6**.

2 In the **Probe Plot Group 6** toolbar, click **Plot**.



STUDY 1

Step 2: Time Dependent

Increase the solver time to 600 s.

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 **Home** toolbar, click **Compute**.

RESULTS

Create Figure 2 to illustrate the current during the drive cycle.

Current

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

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

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** check box. In the associated text field, type `Current (A)`.

Global 1

1. Right-click **Current** 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>I_drive - Drive cycle current - A**.
3. Click to expand the **Legends** section. Clear the **Show legends** check box.
4. In the **Current** toolbar, click **Plot**.

Cell and Electrode Voltages

Create Figure 3 to display the electrode potentials and the cell voltage. For comparison, include the open-circuit cell voltage (at load, concentration gradient in the electrode particles accounted for).

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Cell and Electrode Voltages` in the **Label** text field.
3. Locate the **Plot Settings** section.
4. Select the **y-axis label** check box. In the associated text field, type `Voltage (V)`.

Global 1

1. Right-click **Cell and Electrode Voltages** 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>Ecell - Battery cell voltage - V**.
3. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>Epos - Positive electrode potential - V**.
4. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>Eneg - Negative electrode potential - V**.
5. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>EOCVcell_load - Open-circuit cell voltage, at load - V**.
6. Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`Eneg+3.75[V]`	V	

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

8 In the table, enter the following settings:

Legends
Cell voltage
Positive electrode potential
Negative electrode potential +3.75V
Open-circuit cell voltage at load

9 In the **Cell and Electrode Voltages** toolbar, click **Plot**.

Polarization

Create Figure 4 to plot the total polarization during the drive cycle.

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

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

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** check box. In the associated text field, type `Polarization (V)`.

Global 1

1 Right-click **Polarization** 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>Total_polarization - Total battery cell polarization - V**.

3 Locate the **Legends** section. Clear the **Show legends** check box.

4 In the **Polarization** toolbar, click **Plot**.

SOC

In order to investigate if the cell and electrodes are cycled within their allowed SOC windows, Figure 5 is created. Plot the respective SOCs at load.

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

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

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** check box. In the associated text field, type `SOC (%)`.

Global 1

1 Right-click **SOC** 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>SOCcell_load - State-of-charge of cell, at load**.

3 Click **Add 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.soc_surface_pce1 - Average surface SOC, Porous Electrode 1**.

4 Click **Add 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.soc_surface_pce2 - Average surface SOC, Porous Electrode 2**.

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

Expression	Unit	Description
SOCcell_load*100	1	
liion.soc_surface_pce1*100	1	
liion.soc_surface_pce2*100	1	

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

7 In the table, enter the following settings:

Legends
Cell
Negative electrode
Positive electrode

SOC

1 Click the **Zoom Extents** button in the **Graphics** toolbar.

2 In the **Model Builder** window, click **SOC**.

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

4 From the **Position** list, choose **Middle right**.

5 In the **SOC** toolbar, click **Plot**.