

Capacity Fade of a Lithium-Ion Battery

Introduction

Side reactions and degradation processes may lead to a number of different undesirable effects causing capacity loss in lithium-ion batteries. Typically, aging occurs due to multiple complex phenomena and reactions that are occurring simultaneously at different places in the battery. The degradation rate varies between different stages during a load cycle, depending on potential, local concentration, temperature, and also the direction of the current. Different cell materials age differently, and the combination of different materials may result in further accelerated aging, for instance due to "cross-talk" electrode materials.

This model demonstrates how to model aging in the negative graphite electrode in a lithium ion battery, where a parasitic solid-electrolyte-interface (SEI) forming reaction results in irreversible loss of cyclable lithium. The model also includes the effect of increasing potential losses due to the resistance of the growing SEI film on the electrode particles, as well as the effect of reduced electrolyte volume fraction on the electrolyte charge transport.

Model Definition

BATTERY CHEMISTRY AND AGING REACTION

The battery cell model is created using the Lithium-Ion Battery interface. This model uses the template model 1D Lithium-Ion Battery Model for the Capacity Fade Tutorial, that contains the physics, geometry and mesh of a lithium-ion battery. A more detailed description on how to set up this type of model can be found in the model example 1D Isothermal Lithium-Ion Battery. The template model 1D Lithium-Ion Battery Model for the Capacity Fade Tutorial does not contain any capacity fade reactions or mechanisms. They are included in this model as described below.

In addition to the main graphite-lithium intercalation reaction on the negative electrode, the following parasitic lithium/solvent reduction reaction is also included in the model:

$$S + Li^+ + e^- \rightarrow P_{SEI}$$

where S is the solvent (ethylene carbonate, EC) and P_{SEI} is the product formed in the reaction. The production of P_{SEI} results in loss of cyclable lithium in the battery, and also to an increase of the resistance of the SEI layer (Ref. 1 and Ref. 2) and a reduction of the electrolyte volume fraction in the negative electrode.

The kinetic expression for the SEI forming reaction is based on a paper by Ekström and Lindbergh (Ref. 3). In this paper the SEI formation is assumed to be limited by kinetics

in combination with a diffusion process through the formed SEI film, with the result that the aging slows upon thickening of the film. In addition, when the graphite electrode particles expand, during intercalation into the negative electrode, the aging is however also accelerated due to "cracking" of the SEI film. The graphite expansion rate depends on both the state of charge and the intercalation current. The SEI forming reaction is assumed to be a reduction reaction, resulting in higher reaction rates for lower potentials (that is, the battery state-of charge). The values of the model parameters where fitted, using a lumped zero-dimensional model, to experimental data during cycling and calendar aging for different state-of-charges for a graphite/LFP cell at 45 C. Only the graphite aging effects where assumed in the paper.

In this model example the above 0D model is expanded and applied to a 1D lithium-ion battery model using graphite/NCA electrodes. The kinetics of the parasitic reaction are described by the following kinetics expression for the local current density on the particle surface, $i_{\text{loc. SEI}}(\text{SI unit: A/m}^2)$ in the negative graphite electrode:

$$i_{\text{loc, SEI}} = -(1 + HK) \frac{Ji_{\text{loc, 1C, ref}}}{\exp\left(\frac{\alpha\eta_{\text{SEI}}F}{RT}\right) + \frac{q_{\text{SEI}}fJ}{i_{\text{loc, 1C, ref}}}}$$
(1)

Here

- $i_{\rm loc,1C,ref}$ (A/m²) is the local current density corresponding to a 1C discharge rate.
- *HK*(1) is a dimensionless graphite expansion factor function (depends on the graphite state of charge). *HK* is zero during de-intercalation.
- J(1) dimensionless exchange current density for the parasitic reaction.
- $\alpha(1)$ transfer coefficient of the electrochemical reduction reaction.
- $\eta_{SEI}(V)$ is the overpotential, assuming an equilibrium potential of 0 V versus lithium.
- q_{SEI} (C/m²) is the local accumulated charge due to SEI formation.
- f(1/s) is a lumped nondimensional parameter based on the properties of the SEI film.

The Dissolving-Depositing Species section of the Porous Electrode node is used to solve for an additional degree of freedom to keep track of the formed SEI concentration, c_{SEI} (mol/m³), in the porous electrode according to:

$$\frac{\partial c_{\rm SEI}}{\partial t} = -\frac{v_{\rm SEI} i_{\rm loc, SEI}}{nF}$$

where v_{SEI} is the stoichiometric coefficient of the SEI species in the reaction.

 q_{SEI} above is directly proportional to c_{SEI} according to:

$$q_{\rm SEI} = \frac{Fc_{\rm SEI}}{A_v} \tag{2}$$

where A_v (1/m) is the electrode surface area.

FILM RESISTANCE CALCULATION

The thickness of the SEI layer, δ_{film} , is then calculated from the SEI concentration as:

$$\delta_{\text{film}} = \frac{c_{\text{SEI}} M_P}{A_v \rho_P} + \delta_{\text{film},0}$$

where M_P (0.16 kg/mol) is the molar weight and ρ_P (1600 kg/m³) is the density of the product formed by the side reaction. The initial film thickness at t=0, $\delta_{\text{film},0}$, is assumed to be 1 nm.

The resistance of the SEI layer, $R_{\rm film}$ ($\Omega \cdot m^2$), used in the negative electrode, is then calculated from:

$$R_{\rm film} = \frac{\delta_{\rm film}}{\kappa}$$

LOAD CYCLE, EVENTS, AND APPLIED CURRENT

The switching between the different stages of the load cycle is modeled by the event-based Charge-Discharge Cycling boundary feature.

The battery is cycled in the following sequence of operation modes:

- I Constant current charge at 1 C until the cell voltage exceeds 4.1 V
- 2 Constant voltage charge at 4.1 V until the charge current drops below C/20 (0.81 A)
- 3 Constant current discharge at 1 C until the cell voltage drops below 2.5 V

TIME ACCELERATING FACTOR

Typically a battery needs many cycles to show any prominent capacity loss, and the incremental cycle-to-cycle differences in cycling behavior can therefore usually be assumed to be very small.

By assuming that every simulated charge-discharge-cycle in the model represents an average aging behavior for a larger number of cycles τ , and by further assuming that, over one complete charge-discharge cycle, all lithium captured in the SEI layer can be seen as

stemming from the negative electrode, the capacity loss can be accelerated by rewriting the stoichiometry of the SEI forming reaction by adding the reaction formula

$$(\tau - 1)S + (\tau - 1)Li(s) \rightarrow (\tau - 1)P_{SEI}$$

to

$$S + Li^+ + e^- \rightarrow P_{SEI}$$

resulting in

$$\tau S + Li^+ + e^- + (\tau - 1)Li(s) \rightarrow \tau P_{SEI}$$

 τ can here be seen as a time accelerating factor, representing how many real cycles each simulated battery cycle should represent. In the model, τ is set to 250.

POSTPROCESSING (PLOTTING)

The capacity fade model defines filter variables in the definitions, which are used to determine the onset of discharge cycle (dch_start_filter), charge cycle (ch_start_filter), first cycle (first_cycle_filter), and last cycle (last_cycle_filter) for the load cycle applied during the charge-discharge of the battery. These variables are used while plotting the results after solving the model. See the postprocessing in the Modeling Instructions below.

Results and Discussion



Figure 1 shows the cell voltage during discharge for different cycle numbers.

Figure 1: Cell voltage during discharge.

Figure 2 and Figure 3 show the relative capacity versus time and cycle number, respectively. Both the capacity based on the total amount of cyclable lithium and the nominal 1C discharge capacity (based on the time spent during the 1C discharge part of the load cycle) decrease continuously, but with a higher capacity fade rate during the first cycles. Both capacities decay similarly, about 20% during the 2000 cycles of the study, indicating that the main contributor to the 1 C discharge capacity fade is the loss of lithium, and not a significantly increased internal resistance due to film formation or worsened ion transport in the negative electrode.



Figure 2: Capacity versus total accumulated cycling time.



Figure 3: Capacity versus cycle number.

Figure 4 depicts the change in electrolyte volume fraction. Due to a, on average, higher SEI forming rate close to the separator, the reduction in the electrolyte volume fraction is more pronounced there. A similar trend is seen in Figure 5, which depicts the change in the potential drop over the SEI film. Due to a higher amount of formed SEI close to the separator, the increase in potential drop is higher there.



Figure 4: Electrolyte volume fraction versus cycle number.



Figure 5: SEI film potential drop versus cycle number.

Finally, the local states of charge in the electrodes at the boundaries facing the separator are shown in Figure 6.



Figure 6: Local state-of-charge on the separator-electrode boundaries.

References

1. P. Ramadass, B. Haran, P. Gomadam, R. White, and B. Popov, "Development of first principles capacity fade model for li-ion cells," *J. Electrochemical Society*, vol. 151, no. 2, pp. A196–A203, 2004.

2. G. Ning, R. White, and B. Popov, "A generalized cycle life model of rechargeable Liion batteries", *Electrochimica Acta*, vol 51, pp. 2012–2022, 2006.

3. H. Ekström and G. Lindbergh "A model for predicting capacity fade due to SEI formation in a commercial Graphite/LiFePO₄ cell", *J. Electrochemical Society*, vol 162, pp. A1003–A1007, 2015.

Application Library path: Battery_Design_Module/Batteries,_Lithium-Ion/ capacity_fade

Modeling Instructions

Start this tutorial by opening a seed file that contains a 1D battery model, without any capacity fade reactions or mechanisms added.

APPLICATION LIBRARIES

- I From the File menu, choose Application Libraries.
- 2 In the Application Libraries window, select Battery Design Module>Batteries, Lithium-Ion> capacity_fade_seed in the tree.
- 3 Click 🔮 Open.

LITHIUM-ION BATTERY (LIION)

Run this model in Constant Current-Constant Voltage (CCCV) mode using the Charge-Discharge cycling boundary node.

Charge-Discharge Cycling 1

- I In the Model Builder window, expand the Component I (compl) node.
- 2 Right-click Component I (compl)>Lithium-Ion Battery (liion) and choose Electrode> Charge-Discharge Cycling.
- **3** Select Boundary 4 only.
- 4 In the Settings window for Charge-Discharge Cycling, locate the Discharge Settings section.
- **5** In the I_{dch} text field, type -i_1C.
- **6** In the V_{\min} text field, type E_min.
- 7 Locate the Charge Settings section. In the I_{ch} text field, type i_1C.
- 8 In the V_{max} text field, type E_max.
- 9 Select the Include constant voltage charging check box.
- **IO** In the I_{upper} text field, type I_min_ch.

II Locate the Start Mode section. From the Start with list, choose Charge first.

Porous Electrode 1

Now use the Dissolving-Depositing species functionality to define the SEI layer thickness on the negative electrode.

- I In the Model Builder window, click Porous Electrode I.
- 2 In the Settings window for Porous Electrode, click to expand the Dissolving-Depositing Species section.
- 3 Click + Add.

4 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
sei	rho_sei	M_sei

You can control if the volume change induced by a dissolving of depositing species should affect the electrolyte and/or electrode volume fractions. In this case we will assume the formed SEI reduces the electrolyte volume fraction only.

5 Clear the Add volume change to electrode volume fraction check box.

Also add a film resistance that depends on the deposited film thickness.

- 6 Click to expand the Film Resistance section. From the Film resistance list, choose Thickness and conductivity.
- 7 In the s₀ text field, type dfilm_0.
- 8 From the Δs list, choose Total film thickness change (liion/pcel).
- **9** In the σ_{film} text field, type kappa_film.

Porous Electrode Reaction 2

Add a second porous electrode reaction on the negative electrode to account for the parasitic lithium/solvent SEI forming reduction reaction, and set the stoichiometric coefficient for the degradation reaction.

- I In the Physics toolbar, click Attributes and choose Porous Electrode Reaction.
- **2** In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.
- 3 From the E_{eq} list, choose User defined. Locate the Electrode Kinetics section. From the i_{loc,expr} list, choose User defined. In the associated text field, type I_SEI*(cycle_no> 0). The I_SEI variable was already defined in the seed file. You find the definition on the Component I>Definitions>Variables I node.
- 4 Locate the **Stoichiometric Coefficients** section. In the $v_{Li\theta}$ text field, type (t_factor-1). The t_factor parameter is used to speed up the capacity fade per simulated cycle. You can read more about how the parameter is defined in the model documentation above.
- **5** In the **Stoichiometric coefficients for dissolving-depositing species:** table, enter the following settings:

Species	Stoichiometric coefficient (I)
sei	t_factor

6 Click to expand the **Heat of Reaction** section. From the list, choose **User defined**. This is just a cosmetic setting to avoid the Materials node reporting missing material properties. The Heat of Reaction settings are not used in the model.

DEFINITIONS (COMPI)

Also add a domain integration operator with the default name intop1. It will be used during postprocessing to integrate the amount of cyclable lithium in the battery in order to calculate the remaining capacity.

Integration 1 (intop1)

- I In the Definitions toolbar, click 🖉 Nonlocal Couplings and choose Integration.
- 2 In the Settings window for Integration, locate the Source Selection section.
- 3 From the Selection list, choose Negative Electrode.

STUDY I

The physics part of the model is now complete. Tweak the solver settings before computing.

Solution 1 (soll) In the Study toolbar, click **Show Default Solver**.

Step 1: Current Distribution Initialization

Disable the aging reaction in the initialization study step.

I In the Model Builder window, under Study I click

Step 1: Current Distribution Initialization.

- **2** In the Settings window for Current Distribution Initialization, locate the **Physics and Variables Selection** section.
- **3** Select the Modify model configuration for study step check box.
- 4 In the tree, select Component I (comp1)>Lithium-Ion Battery (liion)>Porous Electrode I> Porous Electrode Reaction 2.
- **5** Right-click and choose **Disable**.

Solution 1 (soll)

Add a stop condition that makes use of a cycle number variable comp1.cycle_no defined at the **Component I>Definitions>Variables I** node. This variable in turn is based on an internal variable defined by the Charge-Discharge Cycling node.

I In the Model Builder window, expand the Solution I (soll) node.

- 2 Right-click Study I>Solver Configurations>Solution I (soll)>Time-Dependent Solver I and choose Stop Condition.
- 3 In the Settings window for Stop Condition, locate the Stop Expressions section.
- 4 Click + Add.
- **5** In the table, enter the following settings:

Stop expression	Stop if	Active	Description
<pre>comp1.cycle_no> (no_cycles)</pre>	True (>=1)	\checkmark	Stop expression 1

6 Locate the Output at Stop section. From the Add solution list, choose Steps before and after stop.

By enabling storing the solution before and after events, the solution data for the first and last time step of the constant charge current, constant voltage and constant discharge current stages will be stored.

- 7 Clear the Add warning check box.
- 8 In the Model Builder window, click Study I.
- 9 In the Settings window for Study, locate the Study Settings section.
- **10** Clear the **Generate default plots** check box. For this model we are not interested in the default plots.
- II In the **Study** toolbar, click **Compute**. The model should solve in about a minute or so.

RESULTS

Using the variables E_cell> and I_cell, defined at the **Component I>Definitions> Variables I** node, you can create a plot of the first load cycle as follows:

Load cycle

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Load cycle in the Label text field.
- 3 Click to expand the Title section. From the Title type list, choose None.
- 4 Locate the Plot Settings section. Select the Two y-axes check box.

Global I

- I Right-click Load cycle and choose Global.
- 2 In the Settings window for Global, locate the y-Axis Data section.

3 In the table, enter the following settings:

Expression	Unit	Description
I_cell	A	Cell current

Filter I

- I Right-click Global I and choose Filter.
- 2 In the Settings window for Filter, locate the Point Selection section.
- **3** In the **Logical expression for inclusion** text field, type first_cycle_filter.

Global 2

- I In the Model Builder window, under Results>Load cycle right-click Global I and choose Duplicate.
- 2 In the Settings window for Global, locate the y-Axis section.
- **3** Select the **Plot on secondary y-axis** check box.
- 4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
E_cell	V	Cell potential

5 In the Load cycle toolbar, click 🗿 Plot.



Discharge curve comparison

The following creates a comparison plot of the constant current discharge curves (Figure 1).

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Discharge curve comparison in the Label text field.
- **3** Locate the **Title** section. From the **Title type** list, choose **Manual**.
- 4 In the Title text area, type Color Legend: Number of cycles.
- 5 Locate the Plot Settings section.
- 6 Select the y-axis label check box. In the associated text field, type Cell potential (V).

Global I

- I Right-click Discharge curve comparison and choose Global.
- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
E_cell	V	Discharge voltage

- 4 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- **5** In the **Expression** text field, type (t-liion.cdc1.t_dch_start).

The Charge-Discharge Cycling node stores the latest time for switching to discharge mode in the liion.cdc1.t_dch_start variable. The above expression hence defines the time elapsed since the discharge started within each cycle.

Filter I

I Right-click Global I and choose Filter.

The seed model contained a number of definitions for filter variables, defined under the **Component I>Definitions>Variables I** node. These variables have either the value 1 or 0, depending on the charging state of the battery. In the postprocessing part of this tutorial we will use these filter variables extensively to filter out different time ranges of the solution data.

- 2 In the Settings window for Filter, locate the Point Selection section.
- 3 In the Logical expression for inclusion text field, type dch_filter.
- 4 Locate the Line Segment Selection section. Clear the Decreasing x check box.

Color Expression 1

- I In the Model Builder window, right-click Global I and choose Color Expression.
- 2 In the Settings window for Color Expression, locate the Expression section.
- 3 In the **Expression** text field, type cycle_no.
- **4** In the **Discharge curve comparison** toolbar, click **O** Plot.

SEI layer potential drop at IC

The following creates a plot of the potential drop over the SEI layer, using the liion.deltaphi variable defined by the Film Resistance section of the Porous Electrode 1 node (Figure 5).

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type SEI layer potential drop at 1C 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 check box. In the associated text field, type Potential drop over SEI layer (V).

Point Graph I

- I Right-click SEI layer potential drop at IC and choose Point Graph.
- **2** Select Boundary 1 only.
- 3 In the Settings window for Point Graph, locate the y-Axis Data section.
- 4 In the Expression text field, type -liion.deltaphi.
- 5 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- **6** In the **Expression** text field, type cycle_no.
- 7 Select the **Description** check box. In the associated text field, type Cycle number.
- 8 Click to expand the Legends section. Select the Show legends check box.
- 9 From the Legends list, choose Manual.

IO In the table, enter the following settings:

Legends

At negative electrode-current collector

Filter I

I Right-click Point Graph I and choose Filter.

- 2 In the Settings window for Filter, locate the Point Selection section.
- 3 In the Logical expression for inclusion text field, type dch_start_filter.

Point Graph 2

- I In the Model Builder window, under Results>SEI layer potential drop at IC right-click Point Graph I and choose Duplicate.
- 2 In the Settings window for Point Graph, locate the Selection section.
- 3 Click Clear Selection.
- 4 Select Boundary 2 only.
- **5** Locate the **Legends** section. In the table, enter the following settings:

Legends

At negative electrode-separator

6 In the SEI layer potential drop at IC toolbar, click 🗿 Plot.

Electrolyte volume fraction

I In the Model Builder window, right-click SEI layer potential drop at IC and choose Duplicate.

The electrolyte volume fraction will decrease as a result of the formed SEI. Plot the volume fraction (Figure 4) as follows:

- 2 In the Settings window for ID Plot Group, type Electrolyte volume fraction in the Label text field.
- **3** Locate the **Plot Settings** section. In the **y-axis label** text field, type **Electrolyte volume** fraction (1).

Point Graph 1

- I In the Model Builder window, expand the Electrolyte volume fraction node, then click Point Graph I.
- 2 In the Settings window for Point Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type liion.epsl.

Point Graph 2

- I In the Model Builder window, click Point Graph 2.
- 2 In the Settings window for Point Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type down(liion.epsl).

The down() operator indicates in this case that the value on the electrode side of the point should be used, not the default mean of the values on each side.

4 In the **Electrolyte volume fraction** toolbar, click **O Plot**.

Capacity vs. time

Now plot the capacity versus time (Figure 2). We will compute the remaining capacity in two ways: 1) based on the integral of charge used for forming the SEI layer and 2) based on the time elapsed during the 1C discharge.

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- **2** In the **Settings** window for **ID Plot Group**, type **Capacity vs.** time in the **Label** text field.
- 3 Locate the Title section. From the Title type list, choose None.
- 4 Locate the Plot Settings section.
- **5** Select the **x-axis label** check box. In the associated text field, type Time (days) (d).
- 6 Select the y-axis label check box. In the associated text field, type Relative capacity (1).

Global I

- I Right-click Capacity vs. time and choose Global.
- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
(QO-comp1.intop1(Q_SEI))/(QO)	1	

- 4 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 5 In the Expression text field, type t*t_factor.
- 6 Select the **Description** check box.
- 7 From the **Unit** list, choose **d**.
- 8 In the Description text field, type Time (days).
- 9 Click to expand the Legends section. From the Legends list, choose Manual.

IO In the table, enter the following settings:

Legends

Based on cyclable lithium

Filter I

- I Right-click Global I and choose Filter.
- 2 In the Settings window for Filter, locate the Point Selection section.

3 In the Logical expression for inclusion text field, type ch_start_filter.

Global 2

- I In the Model Builder window, under Results>Capacity vs. time right-click Global I and choose Duplicate.
- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
(t-liion.cdc1.t_dch_start)/1[h]	1	

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

Legends			
Nominal	1C	discharge	capacity

Capacity vs. time

- I In the Model Builder window, click Capacity vs. time.
- 2 In the Capacity vs. time toolbar, click **O** Plot.

Capacity vs. cycle number

You may also plot the capacity fade versus the cycle number (Figure 3) as follows:

- I Right-click Capacity vs. time and choose Duplicate.
- 2 In the Settings window for ID Plot Group, type Capacity vs. cycle number in the Label text field.
- 3 Locate the Plot Settings section. In the x-axis label text field, type Cycle number (1).

Global I

- I In the Model Builder window, expand the Capacity vs. cycle number node, then click Global I.
- 2 In the Settings window for Global, locate the x-Axis Data section.
- 3 In the **Expression** text field, type cycle_no.

Global 2

- I In the Model Builder window, click Global 2.
- 2 In the Settings window for Global, locate the x-Axis Data section.
- 3 In the **Expression** text field, type cycle_no.
- **4** In the **Capacity vs. cycle number** toolbar, click **OM Plot**.

Local state-of-charge at separator-electrode interface

Now plot the local state of charge in electrodes during the first and last cycles (Figure 6).

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Local state-of-charge at separator-electrode interface 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** check box. In the associated text field, type **SOC** (1).

Point Graph 1

- I Right-click Local state-of-charge at separator-electrode interface and choose Point Graph.
- **2** Select Boundary 2 only.
- 3 In the Settings window for Point Graph, locate the y-Axis Data section.
- **4** In the **Expression** text field, type liion.socloc_surface.
- 5 Click to expand the Title section. Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 6 In the **Expression** text field, type t-liion.cdc1.t_ch_start.
- 7 Locate the Legends section. Select the Show legends check box.
- 8 From the Legends list, choose Manual.
- **9** In the table, enter the following settings:

Legends

Negative Electrode - First Cycle

Filter I

- I Right-click Point Graph I and choose Filter.
- 2 In the Settings window for Filter, locate the Point Selection section.
- 3 In the Logical expression for inclusion text field, type first_cycle_filter.

Point Graph 2

- I In the Model Builder window, under Results>Local state-of-charge at separatorelectrode interface right-click Point Graph I and choose Duplicate.
- 2 In the Settings window for Point Graph, locate the Selection section.
- 3 Click Clear Selection.
- 4 Select Boundary 3 only.

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

Legends

Positive Electrode - First Cycle

Point Graph 3

- I Right-click Point Graph I and choose Duplicate.
- 2 In the Settings window for Point Graph, locate the Legends section.
- **3** In the table, enter the following settings:

Legends

Negative Electrode - Last Cycle

Filter I

- I In the Model Builder window, expand the Point Graph 3 node, then click Filter I.
- 2 In the Settings window for Filter, locate the Point Selection section.
- 3 In the Logical expression for inclusion text field, type last_cycle_filter.

Point Graph 4

- I In the Model Builder window, under Results>Local state-of-charge at separatorelectrode interface right-click Point Graph 2 and choose Duplicate.
- 2 In the Settings window for Point Graph, locate the Legends section.
- **3** In the table, enter the following settings:

Legends

Positive Electrode - Last Cycle

Filter I

- I In the Model Builder window, expand the Point Graph 4 node, then click Filter I.
- 2 In the Settings window for Filter, locate the Point Selection section.
- **3** In the **Logical expression for inclusion** text field, type last_cycle_filter.
- **4** In the Local state-of-charge at separator-electrode interface toolbar, click **O** Plot.