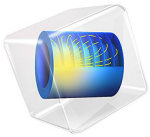


Capacity Fade of a Lithium-Ion Battery

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, and the degradation rate varies between different certain 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 example 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 an 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 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 both on 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, $i_{\text{loc, SEI}}$(SI unit: A/m^2) in the negative graphite electrode:

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

Here

- $i_{\text{loc,1C,ref}}$ (A/m^2) 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.
- α (1) transfer coefficient of the electrochemical reduction reaction.
- η_{SEI} (V) is the overpotential, assuming an equilibrium potential of 0 V versus lithium.
- q_{SEI} (C/m^2) 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/m^3), in the porous electrode according to:

$$\frac{\partial c_{\text{SEI}}}{\partial t} = -\frac{\upsilon_{\text{SEI}} i_{\text{loc, SEI}}}{nF}$$

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

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

$$q_{\mathrm{SEI}} = \frac{F c_{\mathrm{SEI}}}{A_v} \tag{2}$$

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:

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

where M_P (0.1 kg/mol) is the molar weight and ρ_P (2100 kg/m^3) is the density of the product formed by the side reaction. The initial film thickness at t=0, $\delta_{film,0}$, is assumed to be 1 nm.

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

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

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:

1. 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 0.1 A
3. Constant current discharge at 1 C until the cell voltage drops below 3.1 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 every simulated charge-discharge-cycle in the model to represent an average aging behavior for a larger number of cycles τ, and further assuming that over one complete charge-discharge cycle, all lithium captured in the SEI layer can been 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.

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

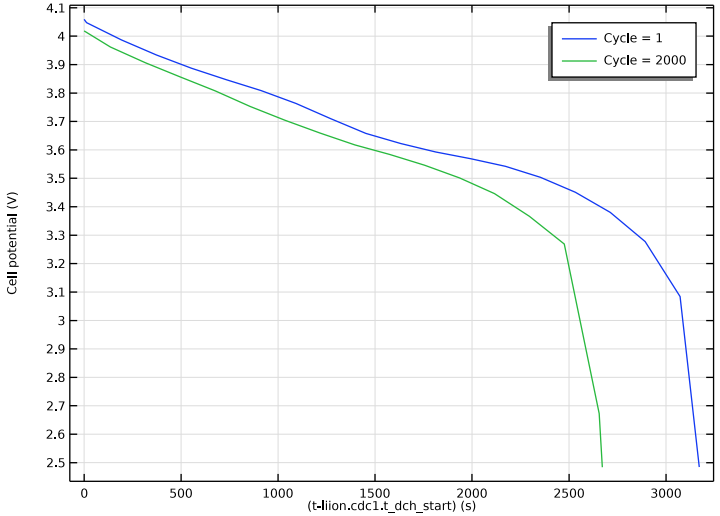


Figure 1: Cell voltage during discharge.

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.

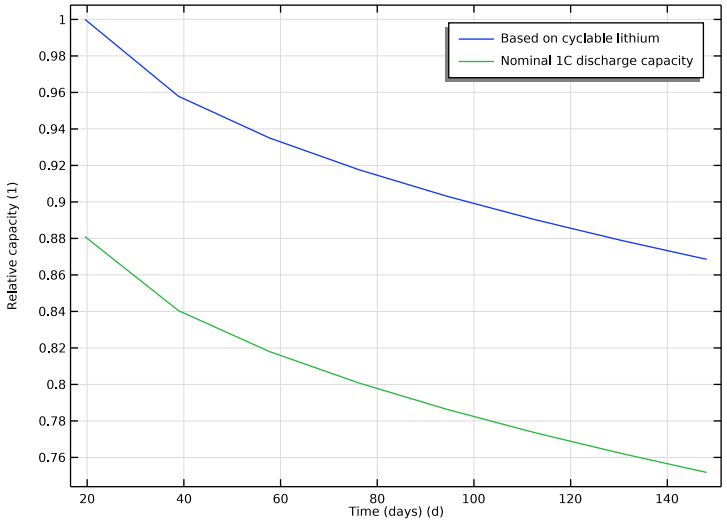


Figure 2: Capacity versus total accumulated cycling time.

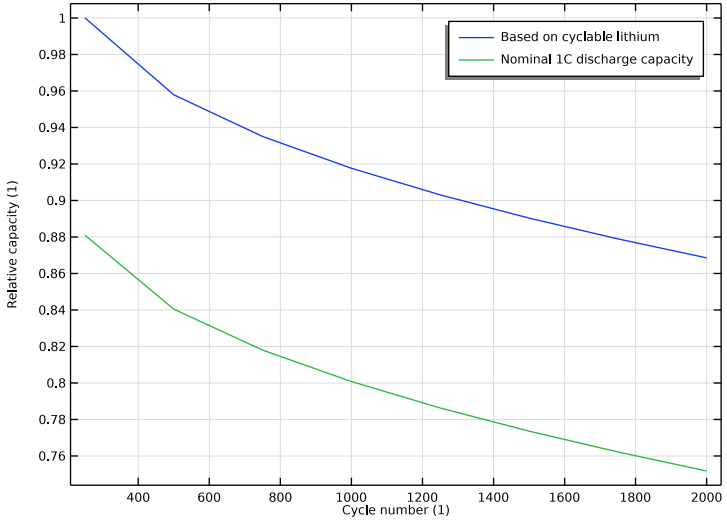


Figure 3: Capacity versus cycle number.

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.

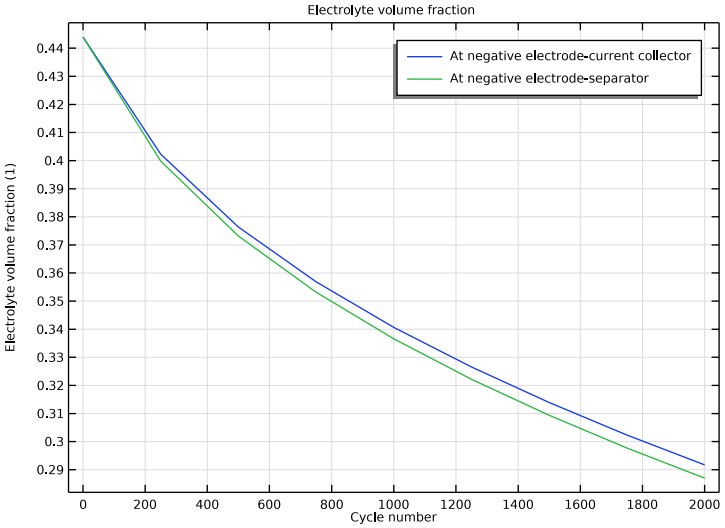


Figure 4: Electrolyte volume fraction versus cycle number.

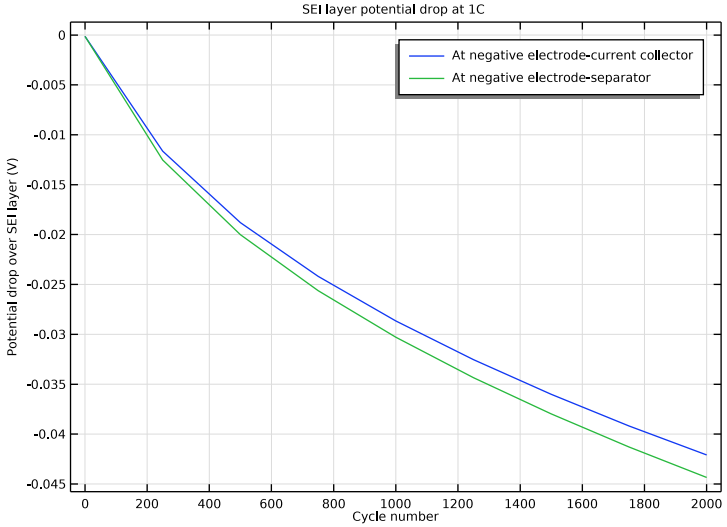


Figure 5: SEI film potential drop versus cycle number.

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

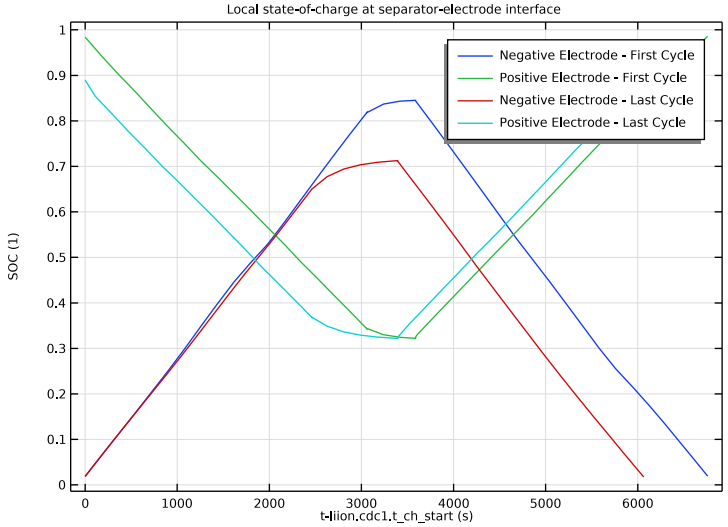


Figure 6: Local state-of-charge on the separator-electrode boundaries.

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 Li-ion 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/$LiFePO_4$ 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.

From the **File** menu, choose **Open**.

Browse to the model's Application Libraries folder and double-click the file `capacity_fade_seed.mph`.

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

1. In the **Model Builder** window, expand the **Component 1 (comp1)** node.
2. Right-click **Component 1 (comp1)>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.
10. In the I_{upper} text field, type `I_min_ch`.
11. 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.

1. In the **Model Builder** window, click **Porous Electrode 1**.
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 s_0 text field, type `dfilm_0`.

8 From the Δs list, choose **Total film thickness change (liion/pce1)**.

9 In the σ_{film} text field, type `kappa_film`.

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.

Porous Electrode Reaction 2

1 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 1>Definitions>Variables 1** node.

4 Locate the **Stoichiometric Coefficients** section. In the $\nu_{Li\theta}$ 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 (1)
sei	t_factor

6 Click to expand the **Heat of Reaction** section. From the dE_{eq}/dT 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 (COMP1)

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)

1 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 1

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

Solution 1 (sol1)

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

Step 1: Current Distribution Initialization

Disable the aging reaction in the initialization study step.

1 In the **Model Builder** window, 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 **Physics and variables selection** tree, select **Component 1 (comp1)>Lithium-Ion Battery (liion)>Porous Electrode 1>Porous Electrode Reaction 2**.
5 Click **Disable**.

Solution 1 (sol1)

Add a stop condition that makes use of a cycle number variable `comp1.cycle_no` defined at the **Component 1>Definitions>Variables 1** node. This variable in turn is based on an internal variable defined by the Charge-Discharge Cycling node.

1 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.
2 Right-click **Time-Dependent Solver 1** 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
comp1.cycle_no> (no_cycles)	True (>=1)	√	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 1**.

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.

11 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 1>Definitions> Variables 1** node, you can create a plot of the first load cycle as follows:

Load 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 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 1

1 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 1

1 Right-click **Global 1** 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

1 In the **Model Builder** window, under **Results>Load cycle** right-click **Global 1** and choose **Duplicate**.

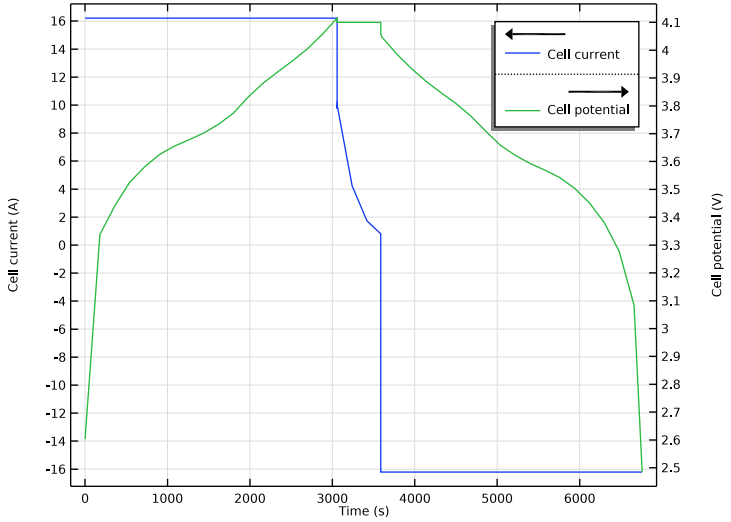
2 In the **Settings** window for **Global**, locate the **y-Axis** section.

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).

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

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

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

4 Locate the **Plot Settings** section. Select the **y-axis label** check box.

5 In the associated text field, type `Cell potential (V)`.

First cycle

1 Right-click **Discharge curve comparison** and choose **Global**.

2 In the **Settings** window for **Global**, type `First cycle` in the **Label** text field.

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

Expression	Unit	Description
`E_cell`	`V`	`Cycle = 1`

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 1

1 Right-click **First cycle** and choose **Filter**.

The seed model contained a number of definitions for filter variables, defined under the **Component 1>Definitions>Variables 1** 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 `first_cycle_filter* dch_filter`.

Last cycle

1 In the **Model Builder** window, right-click **First cycle** and choose **Duplicate**.

2 In the **Settings** window for **Global**, type `Last cycle` in the **Label** text field.

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

Expression	Unit	Description
`E_cell`	`V`	`Cycle = 2000`

Filter 1

1 In the **Model Builder** window, expand the **Last cycle** node, then click **Filter 1**.

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* dch_filter`.

4 In the **Discharge curve comparison** toolbar, click **Plot**.

SEI layer potential drop at 1C

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).

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

2 In the **Settings** window for **1D 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. Select the **y-axis label** check box.

5 In the associated text field, type `Potential drop over SEI layer (V)`.

Point Graph 1

1 Right-click **SEI layer potential drop at 1C** 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.

8 In the associated text field, type `Cycle number`.

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

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

11 In the table, enter the following settings:

Legends
`At negative electrode-current collector`

Filter 1

1 Right-click **Point Graph 1** 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

1 In the **Model Builder** window, under **Results>SEI layer potential drop at 1C** right-click **Point Graph 1** 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 1C** toolbar, click  **Plot**.

Electrolyte volume fraction

1 In the **Model Builder** window, right-click **SEI layer potential drop at 1C** 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 **1D 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

1 In the **Model Builder** window, expand the **Electrolyte volume fraction** node, then click **Point Graph 1**.

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

1 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, i.e. not the default mean of the values on each side.

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

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

2 In the **Settings** window for **1D 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. Select the **x-axis label** check box.

5 In the associated text field, type `Time (days) (d)`.

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

7 In the associated text field, type `Relative capacity (1)`.

Global 1

1 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
`(Q0-comp1.intop1(Q_SEI))/(Q0)`	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**.

10 In the table, enter the following settings:

Legends
`Based on cyclable lithium`

Filter 1

1 Right-click **Global 1** 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

1 In the **Model Builder** window, under **Results>Capacity vs. time** right-click **Global 1** 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

1 In the **Model Builder** window, click **Capacity vs. time**.

2 In the **Capacity vs. time** toolbar, click **Plot**.

Capacity vs. cycle number

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

1 Right-click **Capacity vs. time** and choose **Duplicate**.

2 In the **Settings** window for **1D 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 1

1 In the **Model Builder** window, expand the **Capacity vs. cycle number** node, then click **Global 1**.

2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `cycle_no`.

Global 2

1 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 **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).

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

2 In the **Settings** window for **1D 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. Select the **y-axis label** check box.

5 In the associated text field, type `SOC (1)`.

Point Graph 1

1 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 1

1 Right-click **Point Graph 1** 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

1 In the **Model Builder** window, under **Results>Local state-of-charge at separator-electrode interface** right-click **Point Graph 1** 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

1 Right-click **Point Graph 1** 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 1

1 In the **Model Builder** window, expand the **Point Graph 3** node, then click **Filter 1**.

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

1 In the **Model Builder** window, under **Results>Local state-of-charge at separator-electrode 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 1

1 In the **Model Builder** window, expand the **Point Graph 4** node, then click **Filter 1**.

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  **Plot**.