Created in COMSOL Multiphysics 6.3

SEI Formation in 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 during a load cycle, depending on potential, local concentration, temperature, and the direction of the current. Different cell materials age differently, and the combination of different materials may result in further acceleration of aging, for instance due to "cross-talk" between electrode materials.

This model demonstrates how to model aging in the negative graphite electrode in a lithium ion battery, where a parasitic solid-electrolyte-interphase (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 SEI Formation Tutorial, which contains the physics, geometry, and mesh of a lithium-ion battery. A more detailed description of 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 SEI Formation Tutorial does not contain any SEI forming 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:

$$\mathrm{S} + \mathrm{Li}^{+} + \mathrm{e}^{-} \rightarrow \mathrm{P}_{\mathrm{SEI}}$$

where S is the solvent (ethylene carbonate, EC) and $\mathrm{P}_{\mathrm{SEI}}$ is the product formed in the reaction. The production of $\mathrm{P}_{\mathrm{SEI}}$ results in loss of cyclable lithium in the battery, increase in the resistance of the SEI layer (Ref. 1 and Ref. 2), and in 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 Li intercalation into the negative electrode, the aging is 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, lower battery state-of charge). The values of the model parameters were fitted, using a lumped zero-dimensional model, to experimental data obtained during cycling and calendar aging, for different state of charges, for a graphite/LFP cell, at 45°C. Only graphite aging effects were considered in the paper.

In this model example, the 0D model of the paper 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, $i_{\mathrm{loc,\,SEI}}$(SI unit: A/m^2), in the negative graphite electrode:

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

Here

- $i_{\mathrm{loc,1C,ref}}$ (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) is the dimensionless exchange current density for the parasitic reaction.
- α (1) is the 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

$$\frac{dc_{\mathrm{SEI}}}{dt} = -\frac{\upsilon_{\mathrm{SEI}}i_{\mathrm{loc,\,SEI}}}{nF}$$

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

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

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

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 (0.16 kg/mol) is the molar weight and ρ_P (1600 kg/m^3) is the density of the product formed by the side reaction. The initial film thickness at $t = 0$, $\delta_{\mathrm{film},0}$, is assumed to be 1 nm.

The resistance of the SEI layer, R_{film} ($\Omega\cdot\mathrm{m}^2$), 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 1C until the cell voltage exceeds 4.1 V
2. Constant voltage charge at 4.1 V until the charge current drops below C/20
3. Constant current discharge at 1C until the cell voltage drops below 2.5 V

TIME ACCELERATING FACTOR

Typically, a battery will need to be cycled many times to show any capacity loss. 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

$$(\tau - 1)\mathrm{S} + (\tau - 1)\mathrm{Li(s)} \rightarrow (\tau - 1)\mathrm{P}_{\mathrm{SEI}}$$

to

$$\mathrm{S} + \mathrm{Li}^{+} + \mathrm{e}^{-} \rightarrow \mathrm{P}_{\mathrm{SEI}}$$

resulting in

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

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 100.

POSTPROCESSING (PLOTTING)

This model defines filter variables in the definitions, which are used to determine the onset of the 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.

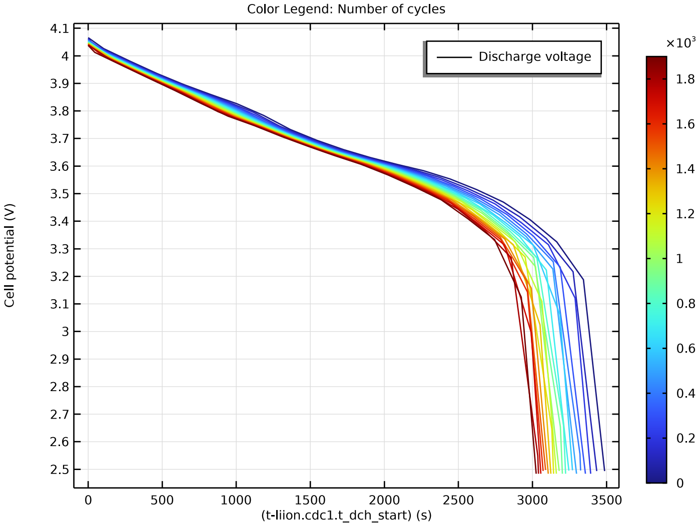


Figure 1: Cell voltage during discharge.

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 1C 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.

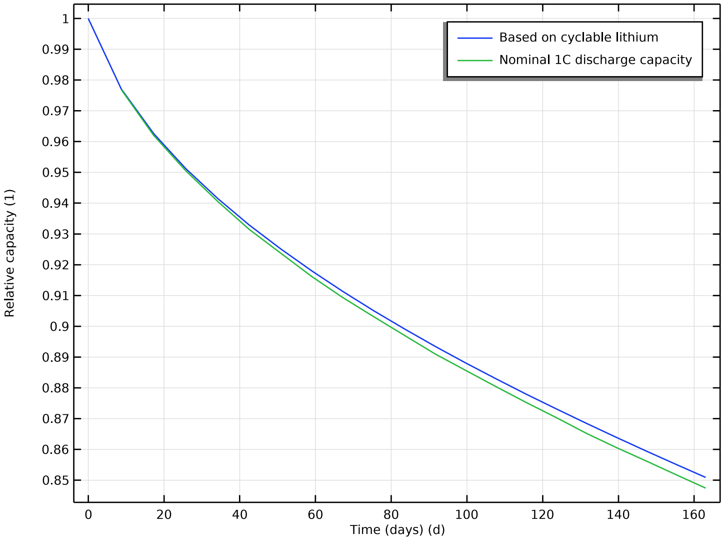


Figure 2: Capacity versus total accumulated cycling time.

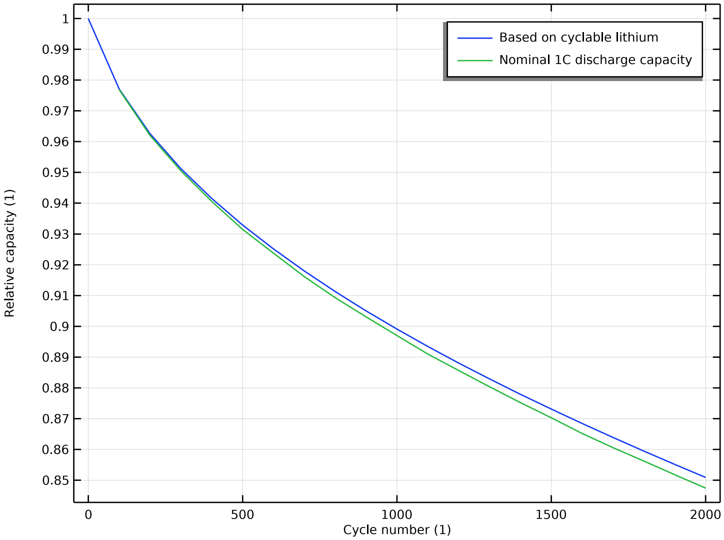


Figure 3: Capacity versus cycle number.

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.

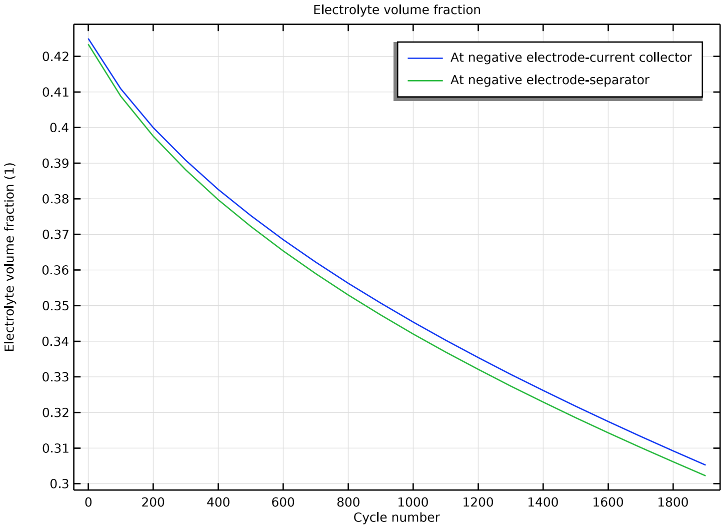


Figure 4: Electrolyte volume fraction versus cycle number.

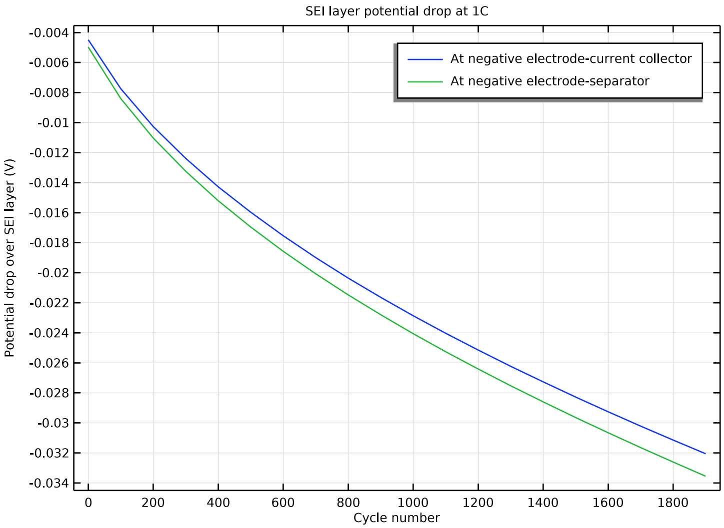


Figure 5: SEI film potential drop versus cycle number.

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

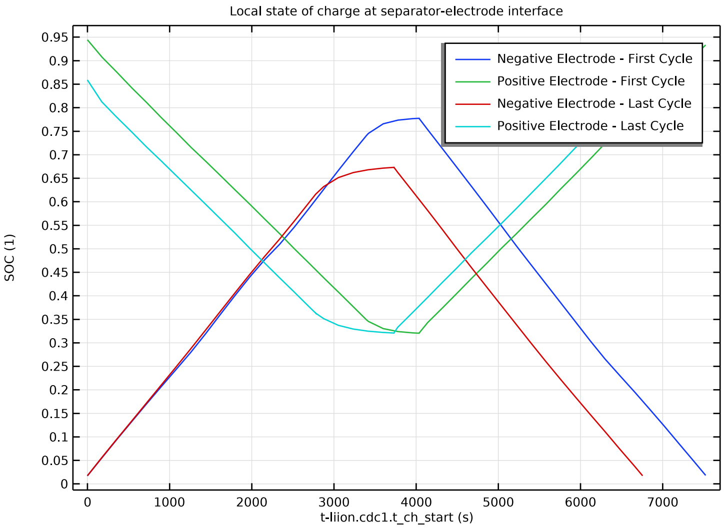


Figure 6: Local state-of-charge on the separator-electrode boundaries.

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. Electrochem. Soc.*, 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," *Electrochim. 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. Electrochem. Soc.,* vol. 162, pp. A1003–A1007, 2015.

Application Library path: `Battery_Design_Module/Lithium-Ion_Batteries,` `_Aging_and_Abuse/sei_formation`

Modeling Instructions

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

APPLICATION LIBRARIES

1. From the **File** menu, choose **Application Libraries**.
2. In the **Application Libraries** window, select **Battery Design Module** > **Lithium-Ion Batteries, Aging and Abuse** > **sei_formation_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

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 Phase** > **Charge-Discharge Cycling**.
3. Select Boundary 4 only.
4. In the **Settings** window for **Charge-Discharge Cycling**, locate the **Discharge Settings** section.
5. From the list, choose **C-rate multiple**.
6. In the $C_{\text{rate,dch}}$ text field, type `-C_rate`.
7. In the V_{min} text field, type `E_min`.
8. Locate the **Charge Settings** section. From the list, choose **C-rate multiple**.
9. In the $C_{\text{rate,ch}}$ text field, type `C_rate`.
10. In the V_{max} text field, type `E_max`.
11. Select the **Include constant voltage charging** checkbox.
12. In the I_{upper} text field, type `I_upper`.
13. Locate the **Start Mode** section. From the **Start with** list, choose **Charge first**.

    Run the model at this stage, before adding any aging reactions, in order to check that the battery model cycles correctly.

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(0,180,10000)`.
4. In the **Model Builder** window, click **Study 1**.
5. In the **Settings** window for **Study**, locate the **Study Settings** section.
6. Clear the **Generate default plots** checkbox. For this model we are not interested in the default plots.
7. In the **Home** toolbar, click = **Compute**. The model should solve in a few seconds.

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 **Results** toolbar, click ∿ **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** checkbox.

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**.

   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`.

Global 2

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

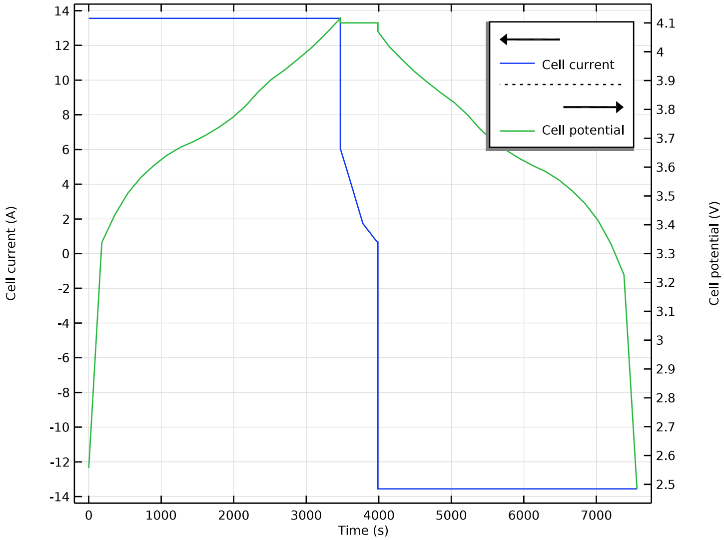
2 In the **Settings** window for **Global**, locate the **y-Axis** section.

3 Select the **Plot on secondary y-axis** checkbox.

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**.



LITHIUM-ION BATTERY (LIION)

Now return to the battery model and add the needed features for defining the SEI formation reaction. Use the Dissolving-Depositing species functionality to define the SEI layer thickness on the negative electrode.

Porous Electrode 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Lithium-Ion Battery (liion)** 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** checkbox.

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`.

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.

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 $i_{\mathrm{loc,expr}}$ list, choose **User defined**. In the associated text field, type `I_SEI`. 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 $\nu_{\mathrm{Li}\theta}$ 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 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

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.

Step 1: Current Distribution Initialization

Disable the aging reaction in the initialization study step.

1 In the **Model Builder** window, under **Study 1** 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** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Lithium-Ion Battery (liion)** > **Porous Electrode 1** > **Porous Electrode Reaction 2**.

5 Right-click and choose **Disable**.

Step 2: Time Dependent

1 In the **Model Builder** window, 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(0,180,t_cycling)`.

Solution 1 (sol1)

1 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** node.

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.

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

3 Right-click **Time-Dependent Solver 1** and choose **Stop Condition**.

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

5 Click + **Add**.

6 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.cycle_no>(no_cycles-0.5)`	True (>=1)	√	`Stop expression 1`

7 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.

8 Clear the **Add information** checkbox.

9 In the **Model Builder** window, click **Fully Coupled 1**.

10 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.

Change the nonlinear method to use a constant damping factor and a minimal jacobian update scheme. This makes the solver less robust, but faster.

11 From the **Nonlinear method** list, choose **Constant (Newton)**.

12 In the **Damping factor** text field, type `0.8`.

13 In the **Study** toolbar, click = **Compute**. The model should solve in about a minute or so.

RESULTS

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

Discharge curve comparison

1 In the **Results** toolbar, click ∿ **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 **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** checkbox. In the associated text field, type `Cell potential (V)`.

Global 1

1 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 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 `dch_filter`.

4 Locate the **Line Segment Selection** section. Clear the **Decreasing x** checkbox.

Color Expression 1

1 In the **Model Builder** window, right-click **Global 1** 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 **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 **Results** toolbar, click ∿ **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.
5. Select the **y-axis label** checkbox. 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** checkbox. In the associated text field, type `Cycle number`.
8. Click to expand the **Legends** section. Select the **Show legends** checkbox.
9. From the **Legends** list, choose **Manual**.
10. 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, 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 cyclable charge between 0% and 100% SOC and 2) based on the time elapsed during the 1C discharge.

1 In the **Results** toolbar, click **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.
5. Select the **x-axis label** checkbox. In the associated text field, type `Time (days) (d)`.
6. Select the **y-axis label** checkbox. In the associated text field, type `Relative capacity (1)`.

Global 1

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

   An internal state-of-health (SOH) variable, based on the cyclable lithium, is computed automatically by the **SOC and Initial Charge Distribution** node.
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** > **liion.SOH_cell - Cell state of health - 1**.
3. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
4. In the **Expression** text field, type `t*t_factor`.
5. Select the **Description** checkbox.
6. From the **Unit** list, choose **d**.
7. In the **Description** text field, type `Time (days)`.
8. Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
9. 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**.

   To compute a state-of-health variable based on the 1C discharge capacity, we divide the 1C discharge time for each cycle by the discharge time for the first cycle (which can be deduced by inspecting the **Discharge curve comparison** plot).

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)/3570[s]`	1	

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

Legends
`Nominal 1C discharge capacity`

Filter 1

1. In the **Model Builder** window, expand the **Global 2** 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 `ch_start_filter_cycled_once`.

Capacity vs. time

1. In the **Model Builder** window, under **Results** 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**.

Filter 1

1. In the **Model Builder** window, expand the **Global 2** 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 `ch_start_filter_cycled_once`.

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 **Results** toolbar, click **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.
5. Select the **y-axis label** checkbox. 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** checkbox.
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**.