



Model created in COMSOL Multiphysics 6.4

# Lithium Plating and Stripping

## *Introduction*

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Lithium plating on the negative electrode in preference to lithium intercalation is known to reduce capacity and to be a safety concern for lithium-ion batteries. Harsh charge conditions such as high currents (fast charging) and/or low temperatures can lead to lithium plating. The plated lithium is partially reversible in a process called stripping during battery discharge.

This example shows how to model the lithium plating/stripping reaction in the negative graphite electrode in a lithium-ion battery. The resulting capacity loss is predicted for different C-rates and temperatures. The example demonstrates how the Porous Electrode node can incorporate the electrochemical plating/stripping reaction.

## *Model Definition*

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### **GENERAL**

The model is set up in 1D for a graphite/NMC battery cell using a 1.0 M LiPF<sub>6</sub> in EC:EMC (3:7 by weight) electrolyte. Properties for these materials are taken from the Battery material library.

The model consists of the following three domains:

- Negative porous electrode: Graphite (MCMB Li<sub>x</sub>C<sub>6</sub>) active material (~112 μm).
- Separator (30 μm).
- Positive porous electrode: NMC 811 active material (70 μm).

The Arrhenius equation is used to model the temperature variation of the intercalation exchange current densities. In addition, temperature-dependent electrolyte properties are defined automatically by adding the electrolyte from the material library.

The Lithium-Ion Battery interface is used, accounting for:

- Electronic conduction in the electrodes
- Ionic charge transport in the electrodes and electrolyte/separator
- Material transport in the electrolyte, allowing for including the effects of concentration on ionic conductivity and concentration overpotentials
- Material transport within the solid spherical particles in the electrodes

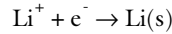
- Butler–Volmer electrode intercalation kinetics using experimentally measured equilibrium potentials
- An additional electrochemical reaction, in this case lithium plating/stripping (detailed description below).

More information on the general description can be found in the [1D Isothermal Lithium-Ion Battery](#) example. The lithium plating/stripping formulations are based on the investigations in [Ref. 1–Ref. 3](#) and the details are presented below.

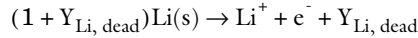
### LITHIUM PLATING/STRIPPING REACTION

The lithium plating/stripping is defined as an additional reaction to the main graphite-lithium intercalation reaction on the negative electrode. This is done using an additional **Porous Electrode Reaction** in the **Porous Electrode** node for the negative electrode.

The plating is considered to be a pure electrochemical reaction:



The reverse reaction, stripping, is considered to only partially dissolve the plated lithium electrochemically. The remaining plated lithium is regarded to be irreversibly lost (a loss in lithium inventory) and is often referred to as “dead lithium” ([Ref. 1](#)). The stoichiometric coefficient of the dead lithium fraction,  $Y_{\text{Li, dead}}$ , is set to 0.1 in this example, can be incorporated into the stripping reaction expression in the following way:



The electrochemical reaction current,  $i_{\text{Li}}$ , is defined by concentration-dependent Butler–Volmer kinetics:

$$i_{\text{Li}} = i_{0, \text{ref}} \left( \frac{c_1}{c_{1, \text{ref}}} \right)^{0.5} \left( F_a \exp\left( \frac{F\eta_{\text{Li}}}{2RT} \right) - \exp\left( -\frac{F\eta_{\text{Li}}}{2RT} \right) \right) \quad (1)$$

where the pre-exponential factor for the anodic term  $F_a$  is defined as:

$$F_a = \frac{c_{\text{Li(s)}}}{c_{\text{Li(s), cov}}} \quad \text{if} \quad \frac{c_{\text{Li(s)}}}{c_{\text{Li(s), cov}}} \leq 1 \quad (2)$$

$$F_a = 1 \quad \text{if} \quad \frac{c_{\text{Li(s)}}}{c_{\text{Li(s), cov}}} > 1$$

In the expressions above

- $i_{0,\text{ref}}$  is the reference exchange current density defined at 1 M lithium ion concentration.
- $c_l$  is the lithium ion concentration in the electrolyte.
- $c_{l,\text{ref}}$  is the reference lithium ion concentration, equal to 1 M.
- $c_{\text{Li}(s),\text{cov}}$  is the concentration of a monolayer fully covered with plated lithium on the negative active material. The monolayer thickness is set to 0.1 nm.
- $c_{\text{Li}(s)}$  is the plated lithium concentration.
- $\eta_{\text{Li}}$  is the lithium plating/stripping overpotential in which the equilibrium potential,  $E_{\text{eq,Li}}$ , is 0 V versus lithium:

$$\eta_{\text{Li}} = \phi_s - \phi_l - E_{\text{eq,Li}} = \phi_s - \phi_l \quad (3)$$

The plated and dead lithium concentrations,  $c_{\text{Li}(s)}$  and  $c_{\text{Li, Dead}}$ , are computed using the in-built **Dissolving–Depositing Species** feature in the main Porous Electrode node. The dissolving–deposited concentrations are computed by integrating the reaction source/sink terms using the following two equations:

$$\frac{dc_{\text{Li}(s)}}{dt} = \frac{-v_{\text{Li}(s)} a_v i_{\text{plate}}}{nF} \quad (4)$$

$$\frac{dc_{\text{Li, dead}}}{dt} = \frac{-v_{\text{Li, Dead}} a_v i_{\text{plate}}}{nF} \quad (5)$$

where  $a_v$  is the specific surface area ( $\text{m}^2/\text{m}^3$ ) of the active material particles.

The stoichiometric coefficients,  $v_{\text{Li}(s)}$  and  $v_{\text{Li, Dead}}$ , follow the reaction expression above and are set as follows:

- For plating,  $i_{\text{plate}} < 0$ :

$$v_{\text{Li}(s)} = 1 \quad (6)$$

$$v_{\text{Li, dead}} = 0 \quad (7)$$

- For stripping,  $i_{\text{plate}} > 0$ :

$$v_{\text{Li}(s)} = 1 + Y_{\text{Li, dead}} \quad (8)$$

$$v_{\text{Li, dead}} = -Y_{\text{Li, dead}} \quad (9)$$

## CHARGE-DISCHARGE CYCLE

To evaluate the plating/stripping reaction, a full charge-discharge cycle is simulated. The upper and lower cutoff voltages are set to 4.2 V and 2.7 V, respectively. The cycle consists of a constant current charge period up to the upper cutoff voltage followed by a constant voltage charge period at the upper cutoff voltage and a constant current discharge period to the lower cutoff voltage. The battery is set to be completely discharged initially.

### *Results and Discussion*

To investigate the impact of current, the charge-discharge cycle is simulated for three different constant current rates (C-rates) at 298 K. The influence of temperature is studied by simulating the cycle for 1C current at three different temperatures.

The cell voltages as functions of SOC are displayed in [Figure 1](#) and [Figure 2](#) for the C-rate and temperature studies, respectively. Large variations with cycling conditions are shown.

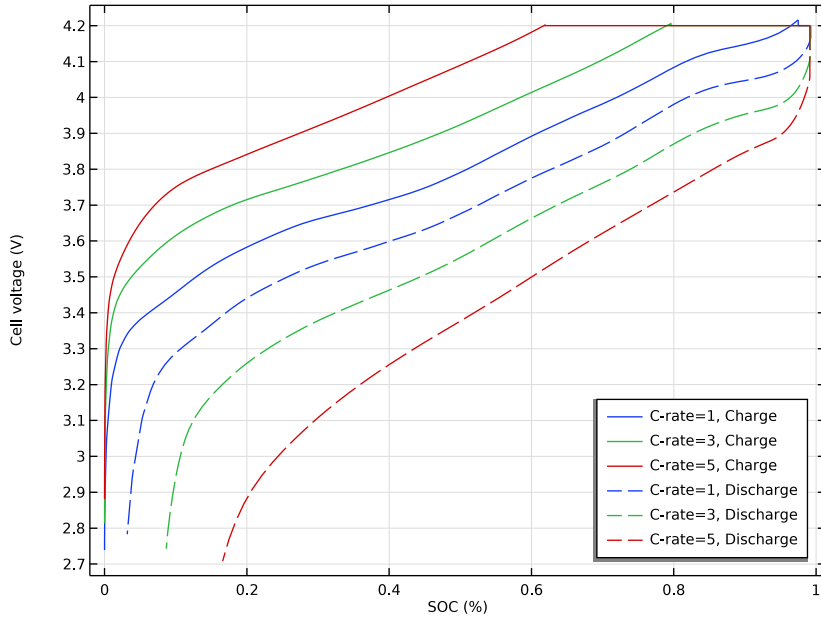


Figure 1: Cell voltage versus SOC for 1C, 3C, and 5C charge-discharge cycles at 298 K.

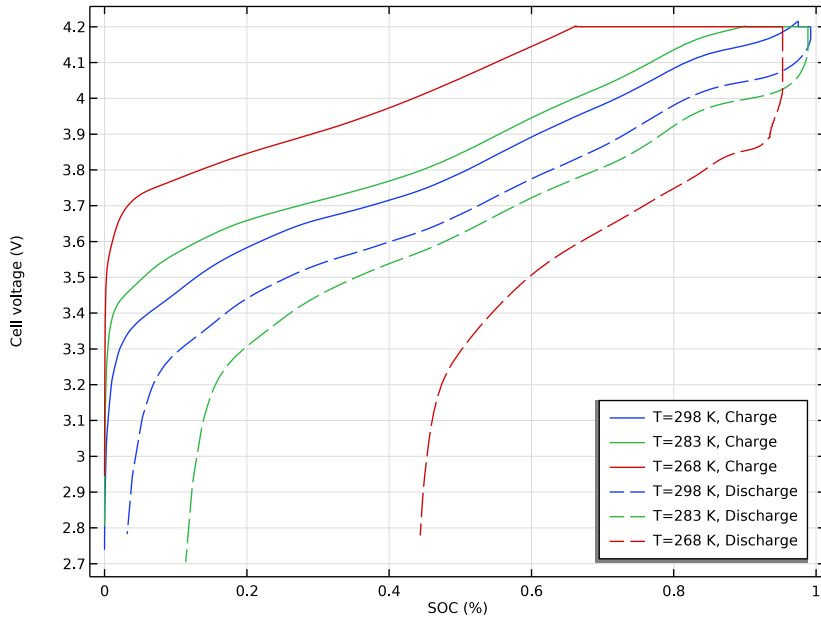


Figure 2: Cell voltage versus SOC at 298 K, 283 K, and 268 K for 1C charge-discharge cycle.

The susceptibility to plating can be seen in the electrode potential at the negative electrode. A potential equal to or lower than 0 V is indicative of lithium plating. In Figure 3 and Figure 4, the electrode potential at the electrode-separator and current collector-electrode boundaries are shown during charge. The former boundary is most

susceptible to lithium plating in all results. The lowest cell temperature case has a potential below 0 V for a long period during charge.

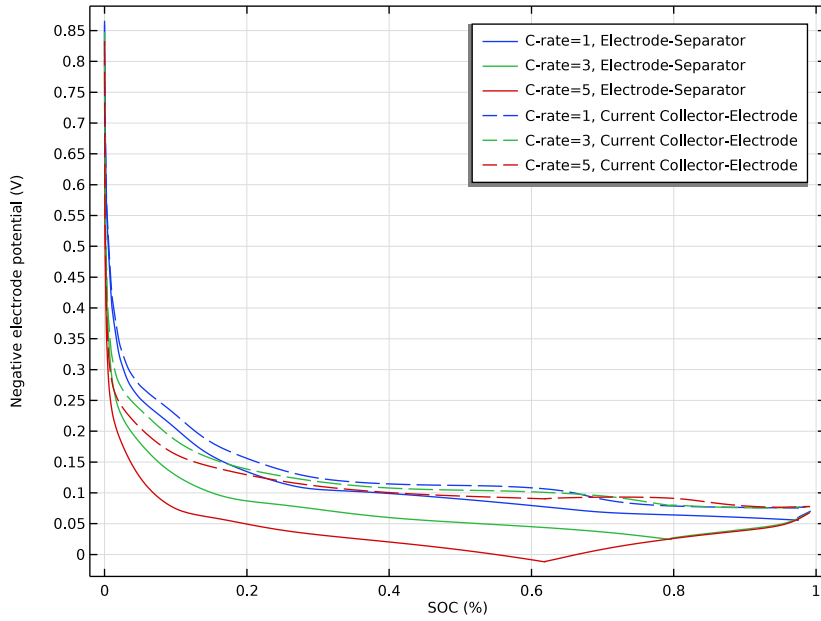


Figure 3: Negative electrode potential at the electrode-separator and current collector-electrode boundaries for 1C, 3C, and 5C charge-discharge cycles at 298 K.

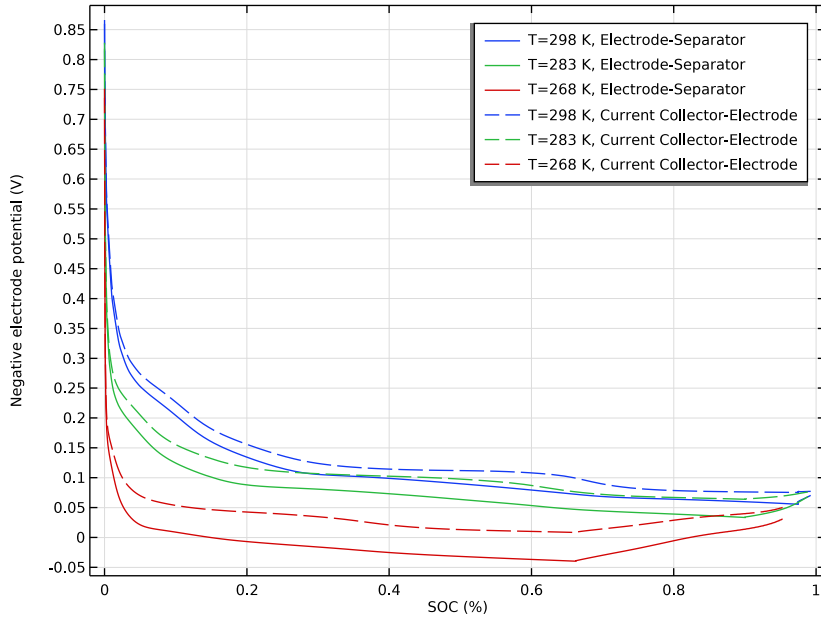


Figure 4: Negative electrode potential at the electrode–separator and current collector–electrode boundaries at 298 K, 283 K, and 268 K for 1C charge–discharge cycle.

The total lithium film thickness, that is, plated and dead lithium, at the electrode–separator interface is displayed in Figure 5 and Figure 6 over the cycle. Increased C-rate increases the plating to some extent. Lowered temperature increases the plating to the greatest

extent. Most of the plating is reversible during the cycle. The irreversible part is due to the formation of dead lithium and reduces the lithium inventory.

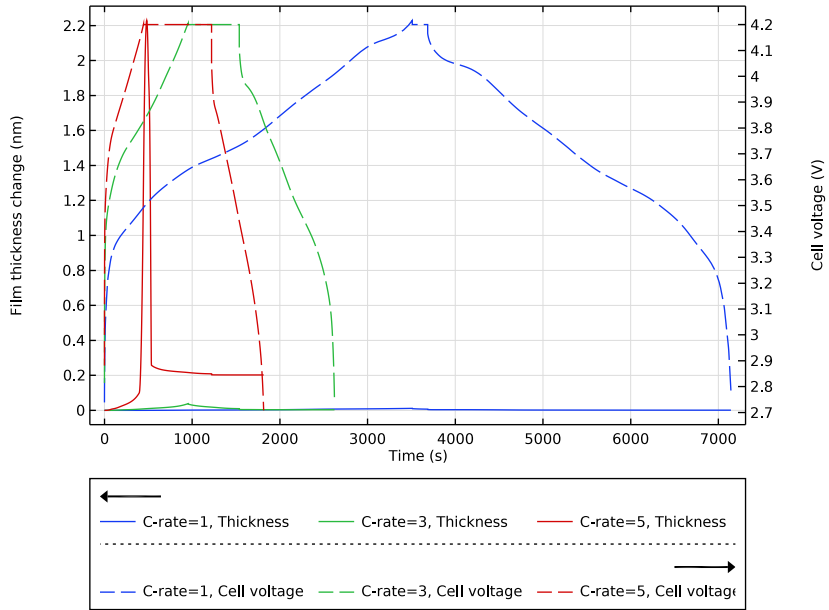


Figure 5: Total lithium film thickness variation at the electrode-separator boundary for 1C, 3C, and 5C at 298 K.

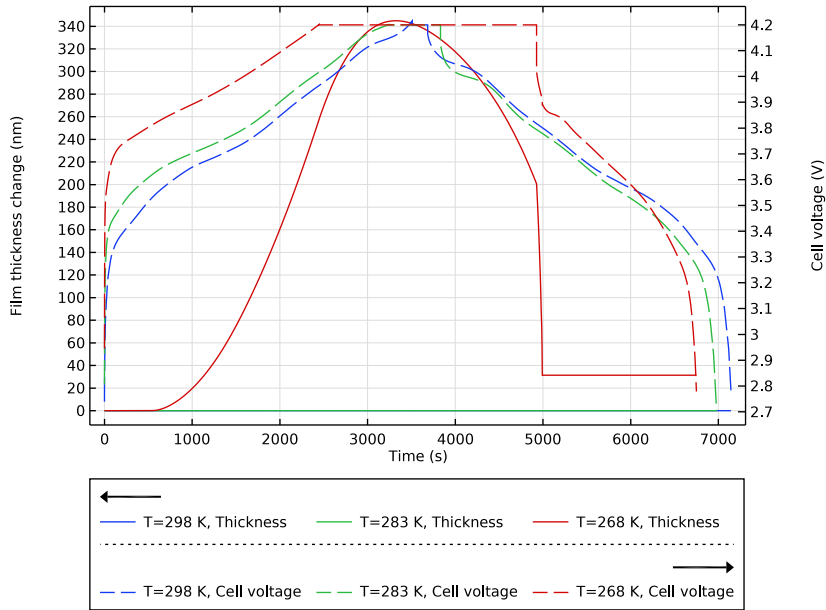


Figure 6: Total lithium film thickness variation at the electrode-separator boundary for 298 K, 283 K, and 268 K at 1C constant current rate.

In the two last figures (Figure 7 and Figure 8), the amount of dead lithium in terms of lithium inventory loss in the cell during cycling is shown. The loss is substantial at the lowest temperature, in all other cases most of the lithium is reversible.

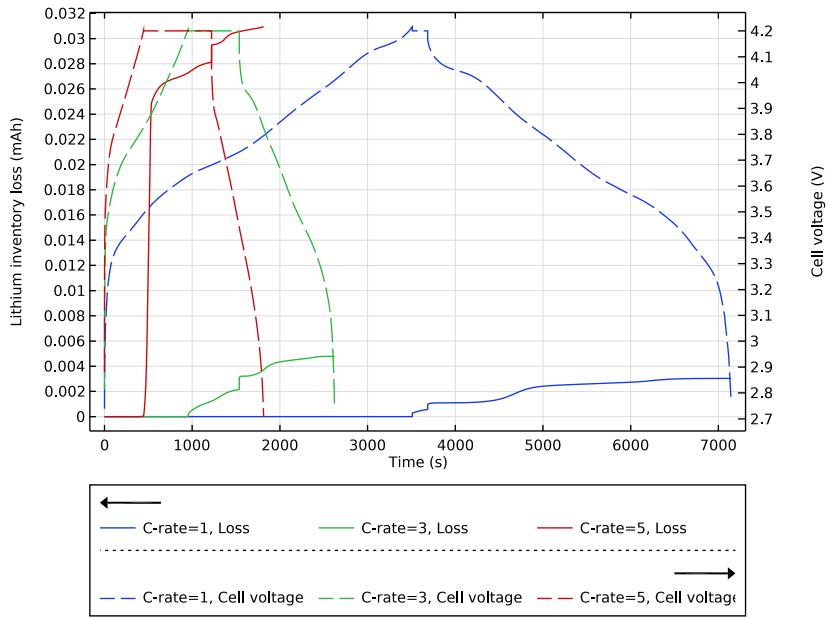


Figure 7: Lithium inventory loss for 1C, 3C, and 5C cycles at 298 K.

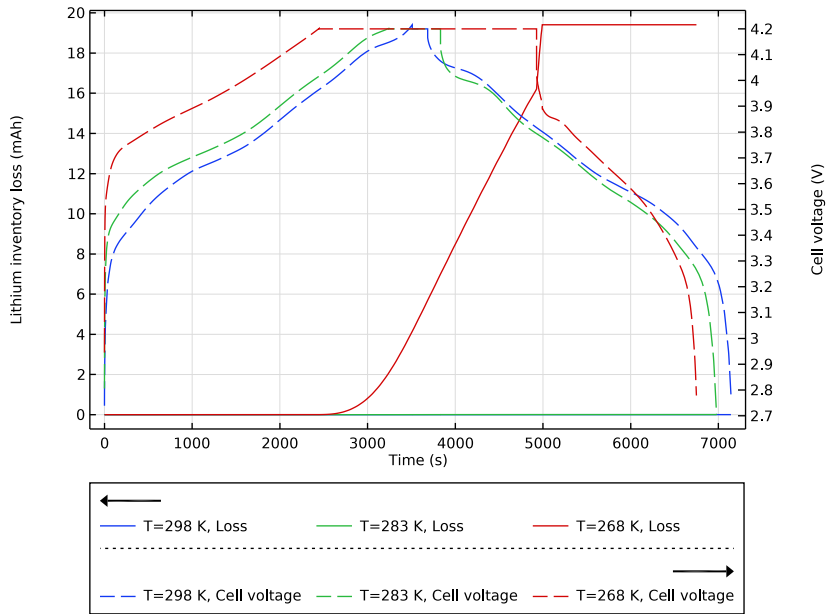


Figure 8: Lithium inventory loss for 298 K, 283 K, and 268 K cycles at 1C constant current rate.

## References

1. S.E.J. O’Kane, I.D. Campbell, M.W.J. Marzook, G.J. Offer, and M. Marinescu, “Physical Origin of the Differential Voltage Minimum Associated with Lithium Plating in Li-Ion Batteries,” *J. Elec. Soc.*, vol. 167, pp. 090540, 2020.
2. X.-G. Yang, S. Ge, T. Liu, Y. Leng, and C.-Y. Wang, “A look into the voltage plateau signal for detection and quantification of lithium plating in lithium-ion cells,” *J. Power Sources*, vol. 395, pp. 251–261, 2018.
3. S.E.J. O’Kane, W. Ai, G. Madabattula, D. Alonso-Alvarez, R. Timms, V. Sulzer, J.S. Edge, B. Wu, G.J. Offer, and M. Marinescu, “Lithium-ion battery degradation: how to model it,” *Phys. Chem. Chem. Phys.*, vol. 24, pp. 7909–7922, 2022.

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**Application Library path:** Battery\_Design\_Module/Lithium-Ion\_Batteries, \_Aging\_and\_Abuse/li\_plating


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## Modeling Instructions




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

### NEW


In the **New** window, click  **Model Wizard**.

### MODEL WIZARD


- 1 In the **Model Wizard** window, click  **ID**.
- 2 In the **Select Physics** tree, select **Electrochemistry > Batteries > Lithium-Ion Battery (liion)**.
- 3 Click **Add**.
- 4 Click  **Study**.
- 5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces > Time Dependent with Initialization**.
- 6 Click  **Done**.

### GLOBAL DEFINITIONS

#### Model Parameters

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters I**.
- 2 In the **Settings** window for **Parameters**, type Model Parameters in the **Label** text field.  
Load the parameters from a text file.
- 3 Locate the **Parameters** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `li_plating_parameters.txt`.

### ADD MATERIAL

- 1 In the **Materials** toolbar, click  **Add Material** to open the **Add Material** window.  
Add some data for the electrolyte and the electrodes from the material library.
- 2 Go to the **Add Material** window.
- 3 In the tree, select **Battery > Electrolytes > LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery)**.
- 4 Right-click and choose **Add to Component I (comp1)**.
- 5 In the tree, select **Battery > Electrodes > Graphite, LixC6 MCMB (Negative, Li-ion Battery)**.
- 6 Right-click and choose **Add to Component I (comp1)**.
- 7 In the tree, select **Battery > Electrodes > NMC 811, LiNi0.8Mn0.1Co0.1O2 (Positive, Li-ion Battery)**.

8 Right-click and choose **Add to Component 1 (comp1)**.

9 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.

## GEOMETRY 1

Draw the model geometry by defining the individual thicknesses of the negative electrode, the separator, and the positive electrode.

### *Interval 1 (i1)*

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 From the **Specify** list, choose **Interval lengths**.

4 In the table, enter the following settings:

<b>Lengths (m)</b>
L_neg
L_sep
L_pos

5 Click  **Build Selected**.

## MATERIALS

### *LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)*

Now assign the previously added materials to the different domains of the geometry. Create selections at the same time to facilitate choosing the same domains later on.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** click **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.

2 Select Domain 2 only.

3 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

4 Click  **Create Selection**.



5 In the **Create Selection** dialog, type Separator in the **Selection name** text field.

6 Click **OK**.


### *Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)*

1 In the **Model Builder** window, click **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

- 3 Click  **Clear Selection**.
- 4 Select Domain 1 only.
- 5 Click  **Create Selection**.
- 6 In the **Create Selection** dialog, type Negative Electrode in the **Selection name** text field.
- 7 Click **OK**.

*NMC 811, LiNi0.8Mn0.1Co0.1O2 (Positive, Li-ion Battery) (mat3)*

- 1 In the **Model Builder** window, click **NMC 811, LiNi0.8Mn0.1Co0.1O2 (Positive, Li-ion Battery) (mat3)**.
- 2 Select Domain 3 only.
- 3 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 4 Click  **Create Selection**.
- 5 In the **Create Selection** dialog, type Positive Electrode in the **Selection name** text field.
- 6 Click **OK**.

#### DEFINITIONS

Add some variables for the electrodes.

*Variables Positive Electrode*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type Variables Positive Electrode in the **Label** text field.
- 3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Positive Electrode**.
- 5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
Arrreh	$\exp((Ea\_pos/R\_const) * (1/(T\_ref\_pos) - 1/(T)))$		Arrhenius kinetics correction


*Variables Negative Electrode*

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

- 2 In the **Settings** window for **Variables**, type Variables Negative Electrode in the **Label** text field.
- 3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Negative Electrode**.
- 4 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
Arreh	$\exp((E_{a\_neg}/R\_const) * (1/(T\_ref\_neg) - 1/(T)))$		Arrhenius kinetics correction

#### *Integration - Negative*

- 1 In the **Definitions** toolbar, click  **Nonlocal Couplings** and choose **Integration**.
- 2 In the **Settings** window for **Integration**, type Integration - Negative in the **Label** text field.
- 3 Locate the **Source Selection** section. From the **Selection** list, choose **Negative Electrode**.
- 4 In the **Operator name** text field, type negative.

### **LITHIUM-ION BATTERY (LIION)**

Now start defining the physics. Use the **SOC and Initial Charge Distribution** node to calculate the initial charge distribution in the cell.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lithium-Ion Battery (liion)**.
- 2 In the **Settings** window for **Lithium-Ion Battery**, locate the **Cross-Sectional Area** section.
- 3 In the  $A_c$  text field, type  $A_{cell}$ .
- 4 Locate the **Cell Settings** section. Select the **Define cell state of charge (SOC) and initial charge inventory** checkbox.

#### *SOC and Initial Charge Distribution 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Lithium-Ion Battery (liion)** click **SOC and Initial Charge Distribution 1**.
- 2 In the **Settings** window for **SOC and Initial Charge Distribution**, locate the **State-of-Charge Definition** section.
- 3 From the list, choose **User defined**. In the  $E_{cell}^{0\%SOC}$  text field, type  $V_{low}$ .
- 4 In the  $E_{cell}^{100\%SOC}$  text field, type  $V_{high}$ .
- 5 Locate the **Initial Cell Charge Distribution** section. In the  $SOC_0$  text field, type  $SOC_{cell\_init}$ .

6 In the  $f_{\text{loss,neg}}$  text field, type Li\_loss.

#### *Negative Electrode Domain Selection 1*

- 1 In the **Model Builder** window, click **Negative Electrode Domain Selection 1**.
- 2 In the **Settings** window for **Negative Electrode Domain Selection**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Negative Electrode**.



#### *Positive Electrode Domain Selection 1*

- 1 In the **Model Builder** window, click **Positive Electrode Domain Selection 1**.
- 2 In the **Settings** window for **Positive Electrode Domain Selection**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Positive Electrode**.

#### *Separator 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Lithium-Ion Battery (liion)** click **Separator 1**.
- 2 In the **Settings** window for **Separator**, locate the **Porous Matrix Properties** section.
- 3 In the  $\epsilon_1$  text field, type eps1\_sep.

#### *Porous Electrode - Negative*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.  
In the negative electrode, add lithium metal and dead lithium as dissolving-depositing species. Allow only volume changes due to lithium plating/stripping affect the electrolyte volume fraction.
- 2 In the **Settings** window for **Porous Electrode**, type Porous Electrode - Negative in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **Negative Electrode**.
- 4 Locate the **Electrolyte Properties** section. From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.
- 5 Locate the **Electrode Properties** section. In the  $\sigma_s$  text field, type sigmas\_neg.
- 6 Locate the **Porous Matrix Properties** section. In the  $\epsilon_s$  text field, type eps\_s\_neg.
- 7 In the  $\epsilon_1$  text field, type eps1\_neg.
- 8 Locate the **Effective Transport Parameter Correction** section. From the **Electric conductivity** list, choose **No correction**.
- 9 Click to expand the **Dissolving-Depositing Species** section. Click  **Add**.

10 Click **+** **Add**.

11 In the table, enter the following settings:

Species	Density (kg/m <sup>3</sup> )	Molar mass (kg/mol)
LiMetal	rhoLi	MLi
LiDead	rhoLi	MLi

12 Clear the **Add volume change to electrode volume fraction** checkbox.

#### *Particle Intercalation I*

- 1 In the **Model Builder** window, click **Particle Intercalation I**.
- 2 In the **Settings** window for **Particle Intercalation**, locate the **Particle Transport Properties** section.
- 3 In the  $r_p$  text field, type `rp_neg`.

#### *Porous Electrode Reaction - Intercalation*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Lithium-Ion Battery (liion) > Porous Electrode - Negative** click **Porous Electrode Reaction I**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, type Porous Electrode Reaction - Intercalation in the **Label** text field.
- 3 Locate the **Electrode Kinetics** section. In the  $i_{0,\text{ref}}(T)$  text field, type `Arreh*`  
`i0_ref_neg`.


#### *Porous Electrode Reaction - Lithium Plating and Stripping*

- 1 In the **Model Builder** window, right-click **Porous Electrode Reaction - Intercalation** and choose **Duplicate**.  
Define the lithium plating/stripping reaction in an additional porous electrode reaction node. A fraction,  $Y_{\text{dead}}$ , will form dead lithium during stripping.
- 2 In the **Settings** window for **Porous Electrode Reaction**, type Porous Electrode Reaction - Lithium Plating and Stripping in the **Label** text field.
- 3 Locate the **Equilibrium Potential** section. From the  $E_{\text{eq}}$  list, choose **User defined**. Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Concentration dependent kinetics**.
- 4 In the  $i_0$  text field, type `i0_ref_LiMetal*(c1/1[M])^0.5`.
- 5 In the  $C_R$  text field, type `min(liion.c_pce1_LiMetal/(cLicov*liion.Av_pce1_per2),1)`.
- 6 Locate the **Stoichiometric Coefficients** section. In the  $v_{\text{Li}\theta}$  text field, type 0.

7 In the **Stoichiometric coefficients for dissolving–depositing species:** table, enter the following settings:

Species	Stoichiometric coefficient (I)
LiMetal	if(liion.iloc_per2<0,1,1+Ydead)
LiDead	if(liion.iloc_per2>0,-Ydead,0)

#### *Porous Electrode - Positive*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.
- 2 In the **Settings** window for **Porous Electrode**, type Porous Electrode - Positive in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **Positive Electrode**.
- 4 Locate the **Electrolyte Properties** section. From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.
- 5 Locate the **Electrode Properties** section. In the  $\sigma_s$  text field, type sigmas\_pos.
- 6 Locate the **Porous Matrix Properties** section. In the  $\epsilon_s$  text field, type eps\_s\_pos.
- 7 In the  $\epsilon_l$  text field, type eps\_l\_pos.



#### *Particle Intercalation I*

- 1 In the **Model Builder** window, expand the **Porous Electrode - Positive** node, then click **Particle Intercalation I**.
- 2 In the **Settings** window for **Particle Intercalation**, locate the **Particle Transport Properties** section.
- 3 In the  $r_p$  text field, type rp\_pos.

#### *Porous Electrode Reaction I*

- 1 In the **Model Builder** window, click **Porous Electrode Reaction I**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Electrode Kinetics** section.
- 3 In the  $i_{0,\text{ref}}(T)$  text field, type Arreh\*i0\_ref\_pos.



#### *Electric Ground I*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Ground**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Electric Ground**, locate the **Boundary Selection** section.
- 4 Click  **Create Selection**.
- 5 In the **Create Selection** dialog, type Negative CC in the **Selection name** text field.

6 Click **OK**.

Use the Charge-Discharge node to set up the load cycle (constant charge - constant voltage - constant discharge) between the cut-off limits.

#### *Charge-Discharge Cycling I*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Charge-Discharge Cycling**.
- 2 Select Boundary 4 only.
- 3 In the **Settings** window for **Charge-Discharge Cycling**, locate the **Boundary Selection** section.
- 4 Click  **Create Selection**.
- 5 In the **Create Selection** dialog, type Positive CC in the **Selection name** text field.
- 6 Click **OK**.
- 7 In the **Settings** window for **Charge-Discharge Cycling**, locate the **Discharge Settings** section.
- 8 From the list, choose **C-rate multiple**.
- 9 In the  $C_{rate,dch}$  text field, type -C\_rate.
- 10 In the  $V_{min}$  text field, type Vlow.
- 11 Locate the **Charge Settings** section. From the list, choose **C-rate multiple**.
- 12 In the  $C_{rate,ch}$  text field, type C\_rate.
- 13 In the  $V_{max}$  text field, type Vhigh.
- 14 Select the **Include constant voltage charging** checkbox.
- 15 In the  $I_{upper}$  text field, type I\_taper.
- 16 Locate the **Start Mode** section. From the **Start with** list, choose **Charge first**.

## **GLOBAL DEFINITIONS**

#### *Default Model Inputs*

- 1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.
- 2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.
- 3 In the tree, select **General > Temperature (K) - minput.T**.
- 4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type T.

## **MESH I**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
- 2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extremely fine**.

4 Click  **Build All**.


### STUDY - C - RATE

Use a parametric sweep to study the impact of the C-rate.


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

2 In the **Settings** window for **Study**, type Study - C-Rate in the **Label** text field.

#### Parametric Sweep

1 In the **Study** toolbar, click  **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click  **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
C_rate (C-rate)	1 3 5	

#### 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, 100/C\_rate, 3600\*6/C\_rate).

4 In the **Model Builder** window, click **Study - C-Rate**.

5 In the **Settings** window for **Study**, locate the **Study Settings** section.

6 Clear the **Generate default plots** checkbox.

#### Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.

4 From the **Times to store** list, choose **Steps taken by solver**.

5 Right-click **Study - C-Rate > Solver Configurations > Solution 1 (sol1) > Time-Dependent Solver 1** and choose **Stop Condition**.

Define a stop condition that terminates the simulation at the lower cut-off limit at discharge.

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

7 Click  **Add**.

8 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
comp1.liion.cdc1.phi s0<(Vlow*(t>3600/ C_rate))	True (>=1)	√	Stop expression 1


9 Locate the **Output at Stop** section. Clear the **Add information** checkbox.

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

## RESULTS

Start creating the model figures.

### *Cell Voltage, C-rate*

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

2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study - C-Rate/Parametric Solutions 1 (sol3)**.

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

5 In the **Label** text field, type **Cell Voltage, C-rate**.

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** checkbox. In the associated text field, type **SOC (%)**.

8 Select the **y-axis label** checkbox. In the associated text field, type **Cell voltage (V)**.

9 Locate the **Legend** section. Select the **Show legends** checkbox.

10 From the **Position** list, choose **Lower right**.

### *Global I*

1 Right-click **Cell Voltage, C-rate** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1) > Lithium-Ion Battery > Charge-Discharge Cycling 1 > liion.cdc1.phis0 - Cell potential - V**.

3 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1) > Lithium-Ion Battery > liion.SOC\_cell - Cell state of charge - I**.

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

5 In the table, enter the following settings:

Legends
C-rate=1, Charge
C-rate=3, Charge
C-rate=5, Charge

#### Filter 1


- 1 Right-click **Global 1** and choose **Filter**.
- 2 In the **Settings** window for **Filter**, locate the **Line Segment Selection** section.
- 3 Clear the **Decreasing x** checkbox.

#### Global 2


- 1 In the **Model Builder** window, under **Results > Cell Voltage, C-rate** right-click **Global 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Global**, click to expand the **Coloring and Style** section.
- 3 Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 4 From the **Color** list, choose **Cycle (reset)**.
- 5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.
- 6 In the table, enter the following settings:

Legends
C-rate=1, Discharge
C-rate=3, Discharge
C-rate=5, Discharge

#### 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 **Line Segment Selection** section.
- 3 Clear the **Increasing x** checkbox.
- 4 Select the **Decreasing x** checkbox.
- 5 In the **Cell Voltage, C-rate** toolbar, click  **Plot**.

#### Lithium Plating Current, C-rate

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Lithium Plating Current, C-rate in the **Label** text field.

- 3 Locate the **Data** section. From the **Dataset** list, choose **Study - C-Rate/ Parametric Solutions I (sol3)**.
- 4 Locate the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Plot Settings** section.
- 6 Select the **y-axis label** checkbox. In the associated text field, type **Plating/stripping current (A)**.
- 7 Locate the **Legend** section. Select the **Show legends** checkbox.

*Global 1*

- 1 Right-click **Lithium Plating Current, C-rate** 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
<code>negative(liion.iv_per2)*A_cell</code>	A	

- 4 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
- 5 In the table, enter the following settings:

Legends
C-rate=1, Current
C-rate=3, Current
C-rate=5, Current

*Global 2*

- 1 Right-click **Global 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Global**, click to expand the **Coloring and Style** section.
- 3 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1) > Lithium-Ion Battery > Charge-Discharge Cycling 1 > liion.cdcl.phis0 - Cell potential - V**.
- 4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 5 From the **Color** list, choose **Cycle (reset)**.

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

---

**Legends**

---

C-rate=1, Cell voltage

---

C-rate=3, Cell voltage

---


C-rate=5, Cell voltage

---

*Lithium Plating Current, C-rate*

- 1 In the **Model Builder** window, click **Lithium Plating Current, C-rate**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.
- 3 Select the **Two y-axes** checkbox.
- 4 Select the **Secondary y-axis label** checkbox. In the associated text field, type Cell voltage (V).
- 5 In the table, select the **Plot on secondary y-axis** checkbox for **Global 2**.
- 6 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.
- 7 From the **Position** list, choose **Bottom**.

*Plating Susceptibility, C-rate*

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Plating Susceptibility, C-rate in the **Label** text field.
- 3 Locate the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Data** section. From the **Dataset** list, choose **Study - C-Rate/ Parametric Solutions 1 (sol3)**.
- 5 Locate the **Plot Settings** section.
- 6 Select the **x-axis label** checkbox. In the associated text field, type SOC (%).
- 7 Select the **y-axis label** checkbox. In the associated text field, type Negative electrode potential (V).

*Point Graph 1*

- 1 Right-click **Plating Susceptibility, C-rate** 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 phi<sub>s</sub>-phi<sub>l</sub>.


- 5 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1) > Lithium-Ion Battery > liion.SOC\_cell - Cell state of charge - 1**.
- 6 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 7 From the **Legends** list, choose **Manual**.
- 8 In the table, enter the following settings:

Legends
C-rate=1, Electrode-Separator
C-rate=3, Electrode-Separator
C-rate=5, Electrode-Separator


#### *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 `liion.cdc1.Icell>0`.

#### *Point Graph 2*

- 1 In the **Model Builder** window, under **Results > Plating Susceptibility, C-rate** right-click **Point Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Point Graph**, locate the **Selection** section.
- 3 Click to select the  **Activate Selection** toggle button.
- 4 In the list box, select **2**.
- 5 Click  **Remove from Selection**.
- 6 Select **Boundary 1** only.
- 7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 8 From the **Color** list, choose **Cycle (reset)**.
- 9 Locate the **Legends** section. In the table, enter the following settings:

Legends
C-rate=1, Current Collector-Electrode
C-rate=3, Current Collector-Electrode
C-rate=5, Current Collector-Electrode

- 10 In the **Plating Susceptibility, C-rate** toolbar, click  **Plot**.

### *Lithium Film Thickness, C-rate*

- 1 In the **Model Builder** window, right-click **Plating Susceptibility, C-rate** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Lithium Film Thickness, C-rate in the **Label** text field.
- 3 Locate the **Plot Settings** section. In the **x-axis label** text field, type Time (s).
- 4 In the **y-axis label** text field, type Film thickness change (nm).

### *Point Graph 1*

- 1 In the **Model Builder** window, expand the **Lithium Film Thickness, C-rate** node, then click **Point Graph 1**.
- 2 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1) > Lithium-Ion Battery > Dissolving–depositing species > liion.sbtot\_pcel - Total film thickness change - m**.
- 3 Locate the **y-Axis Data** section. From the **Unit** list, choose **nm**.
- 4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Time**.
- 5 Click to expand the **Legends** section. In the table, enter the following settings:

<b>Legends</b>
C-rate=1, Thickness
C-rate=3, Thickness
C-rate=5, Thickness

### *Filter 1*

- 1 In the **Model Builder** window, expand the **Point Graph 1** node.
- 2 Right-click **Filter 1** and choose **Delete**.

### *Point Graph 2*

In the **Model Builder** window, right-click **Point Graph 2** and choose **Delete**.

### *Global 1*

- 1 In the **Model Builder** window, right-click **Lithium Film Thickness, C-rate** 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
liion.cdc1.phis0	V	Cell potential

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

5 From the **Color** list, choose **Cycle (reset)**.

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

7 In the table, enter the following settings:

Legends
C-rate=1, Cell voltage
C-rate=3, Cell voltage
C-rate=5, Cell voltage

#### *Lithium Film Thickness, C-rate*

1 In the **Model Builder** window, click **Lithium Film Thickness, C-rate**.

2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.


3 Select the **Two y-axes** checkbox.

4 Select the **Secondary y-axis label** checkbox. In the associated text field, type Cell voltage (V).

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

6 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

7 From the **Position** list, choose **Bottom**.

8 In the **Lithium Film Thickness, C-rate** toolbar, click  **Plot**.

#### *Loss of Lithium Inventory, C-rate*

1 In the **Model Builder** window, right-click **Lithium Plating Current, C-rate** and choose **Duplicate**.

2 In the **Settings** window for **ID Plot Group**, type Loss of Lithium Inventory, C-rate in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type Lithium inventory loss (mAh).

4 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

5 From the **Position** list, choose **Bottom**.

### Global I

- 1 In the **Model Builder** window, expand the **Loss of Lithium Inventory, C-rate** node, then click **Global I**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:



Expression	Unit	Description
<code>negative(liion.c_pce1_LiDead*F_const)*A_cell</code>	mAh	

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

Legends
C-rate=1, Loss
C-rate=3, Loss
C-rate=5, Loss

- 5 In the **Loss of Lithium Inventory, C-rate** toolbar, click  **Plot**.



### ADD STUDY

- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.  
Add a new Study with a parametric sweep to study the impact of temperature.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces > Time Dependent with Initialization**.
- 4 Click the **Add Study** button in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

### STUDY - TEMPERATURE

- 1 In the **Settings** window for **Study**, type Study - Temperature in the **Label** text field.
- 2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

### Parametric Sweep

- 1 In the **Study** toolbar, click  **Parametric Sweep**.
- 2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
- 3 Click  **Add**.



4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
T (Temperature)	298 283 268	K


*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, 100/C\_rate, 3600\*6/C\_rate).

*Solution 7 (sol7)*

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 7 (sol7)** node, then click **Time-Dependent Solver 1**.
- 3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.
- 4 From the **Times to store** list, choose **Steps taken by solver**.
- 5 Right-click **Study - Temperature > Solver Configurations > Solution 7 (sol7) > Time-Dependent Solver 1** and choose **Stop Condition**.
- 6 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.
- 7 Click  **Add**.
- 8 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
comp1.liion.cdc1.phis0<(Vlow*(t>3600/C_rate))	True (>=1)	√	Stop expression 1

- 9 Locate the **Output at Stop** section. Clear the **Add information** checkbox.
- 10 In the **Study** toolbar, click  **Compute**.

**RESULTS**

*Plating Susceptibility, Temperature*

- 1 In the **Model Builder** window, right-click **Plating Susceptibility, C-rate** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type **Plating Susceptibility, Temperature** in the **Label** text field.

- 3 Locate the **Data** section. From the **Dataset** list, choose **Study - Temperature/ Parametric Solutions 2 (sol9)**.

#### *Point Graph 1*

- 1 In the **Model Builder** window, expand the **Plating Susceptibility, Temperature** node, then click **Point Graph 1**.
- 2 In the **Settings** window for **Point Graph**, click to expand the **Legends** section.
- 3 In the table, enter the following settings:

<b>Legends</b>
T=298 K, Electrode-Separator
T=283 K, Electrode-Separator
T=268 K, Electrode-Separator

#### *Point Graph 2*

- 1 In the **Model Builder** window, click **Point Graph 2**.
- 2 In the **Settings** window for **Point Graph**, locate the **Legends** section.
- 3 In the table, enter the following settings:

<b>Legends</b>
T=298 K, Current Collector-Electrode
T=283 K, Current Collector-Electrode
T=268 K, Current Collector-Electrode

- 4 In the **Plating Susceptibility, Temperature** toolbar, click  **Plot**.

#### *Cell Voltage, Temperature*

- 1 In the **Model Builder** window, right-click **Cell Voltage, C-rate** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Cell Voltage, Temperature in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study - Temperature/ Parametric Solutions 2 (sol9)**.

#### *Global 1*

- 1 In the **Model Builder** window, expand the **Cell Voltage, Temperature** node, then click **Global 1**.
- 2 In the **Settings** window for **Global**, click to expand the **Legends** section.

3 In the table, enter the following settings:

---

Legends
T=298 K, Charge
T=283 K, Charge
T=268 K, Charge

---

#### *Global 2*

- 1 In the **Model Builder** window, click **Global 2**.
- 2 In the **Settings** window for **Global**, locate the **Legends** section.
- 3 In the table, enter the following settings:

---

Legends
T=298 K, Discharge
T=283 K, Discharge
T=268 K, Discharge

---

4 In the **Cell Voltage, Temperature** toolbar, click  **Plot**.

#### *Lithium Film Thickness, Temperature*

- 1 In the **Model Builder** window, right-click **Lithium Film Thickness, C-rate** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Lithium Film Thickness, Temperature in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study - Temperature/ Parametric Solutions 2 (sol9)**.

#### *Point Graph 1*

- 1 In the **Model Builder** window, expand the **Lithium Film Thickness, Temperature** node, then click **Point Graph 1**.
- 2 In the **Settings** window for **Point Graph**, click to expand the **Legends** section.
- 3 In the table, enter the following settings:

---

Legends
T=298 K, Thickness
T=283 K, Thickness
T=268 K, Thickness

---

*Global 1*

- 1 In the **Model Builder** window, click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **Legends** section.
- 3 In the table, enter the following settings:

<b>Legends</b>
T=298 K, Cell voltage
T=283 K, Cell voltage
T=268 K, Cell voltage

- 4 In the **Lithium Film Thickness, Temperature** toolbar, click  **Plot**.

*Loss of Lithium Inventory, Temperature*

- 1 In the **Model Builder** window, right-click **Loss of Lithium Inventory, C-rate** and choose **Duplicate**.
- 2 In the **Model Builder** window, click **Loss of Lithium Inventory, C-rate 1**.
- 3 In the **Settings** window for **ID Plot Group**, type Loss of Lithium Inventory, Temperature in the **Label** text field.
- 4 Locate the **Data** section. From the **Dataset** list, choose **Study - Temperature/ Parametric Solutions 2 (sol9)**.

*Global 1*

- 1 In the **Model Builder** window, click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **Legends** section.
- 3 In the table, enter the following settings:

<b>Legends</b>
T=298 K, Loss
T=283 K, Loss
T=268 K, Loss

*Global 2*

- 1 In the **Model Builder** window, click **Global 2**.
- 2 In the **Settings** window for **Global**, locate the **Legends** section.

3 In the table, enter the following settings:

---

**Legends**

---

T=298 K, Cell voltage


---

T=283 K, Cell voltage

---

T=268 K, Cell voltage

---

4 In the **Loss of Lithium Inventory, Temperature** toolbar, click  **Plot**.