1D Isothermal Lithium-Ion Battery

Introduction

This model demonstrates the Lithium-Ion Battery interface for studying the discharge and charge of a lithium-ion battery for a given set of material properties. The geometry is in one dimension and the model is isothermal. Battery developers can use the model to investigate the influence of various design parameters such as the choice of materials, dimensions, and the particle size distribution of the active materials, in this case carbon on the negative electrode and lithium manganese oxide ($LiMn_2O_4$) on the positive electrode. You can also benefit from simulating battery performance under different operating conditions and in different devices, for example, cell phones or laptop computers.

The example treats a detailed model of a discharge-recharge cycle for a lithium-ion battery. The model is based on a study by J. Newman and others (Ref. 1).

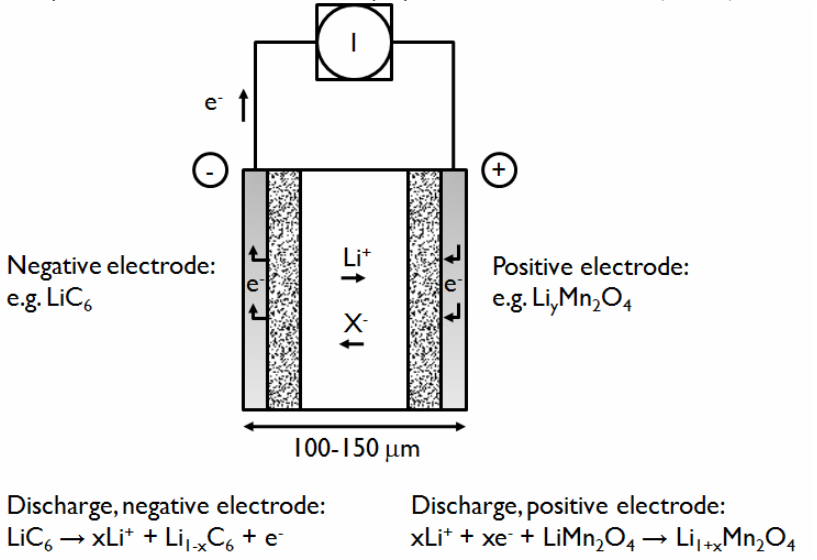

Figure 1: Cross section of a lithium-ion battery showing the electrochemical processes that occur during operation.

The model includes the following processes:

- Electronic current conduction in the electrodes

- Ionic charge transport in the electrodes and electrolyte/separator
- Material transport in the electrolyte, allowing for the introduction of the effects of concentration on ionic conductivity and concentration overpotential, which in this case are obtained from experimental data
- Material transport within the spherical particles that form the electrodes
- Butler-Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium potential.

Model Definition

This example models the battery cross section in 1D, which implies that edge effects in the length and height of the battery are neglected. The example uses the following domains:

- Negative porous electrode: 100 μm
- Separator (electrolyte): 52 μm
- Positive porous electrode: 183 μm

The electric potential in the electron conducting phase, ϕ_s, is calculated using a charge balance based on Ohm's law where the charge transfer reactions result in source or sink term. For the porous electrodes effective conductivities, σ_s^{eff}, are used that take porosity and tortuosity into account as given by the following expression:

$$\sigma_s^{\text{eff}} = \sigma_s \varepsilon^{\gamma} \quad (1)$$

where γ is the Bruggeman coefficient, which is set to 1.5 in this model, corresponding to a packed bed of spherical particles.

The ionic charge balances and material balances are modeled according to the equations for binary 1:1 electrolytes (Ref. 1).

Fickian diffusion describes the transport in the spherical particles. The diffusion equation is expressed in spherical coordinates for the material balance of lithium in the particles.

Butler-Volmer electrode kinetics describes the local charge transfer current density in the electrodes. The Butler-Volmer expressions are introduced as source or sink terms in the charge balances and material balances.

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BOUNDARY CONDITIONS

For the electronic current balance, a potential of 0 V is set on the negative electrode's current collector/feeder boundary. At the positive electrode current collector/feeder, the current density is specified. In this model, the current density is cycled through a discharge, followed by an interval of zero current, and a final charging stage. The inner boundaries facing the separator are insulating for electric currents.

For the ionic charge balance in the electrolyte, the current collector/feeder boundaries are insulating. Insulating conditions also apply to the material balances.

At the particle surface in the local particle model, the material flux is determined by the local electrochemical reaction rate.

MATERIAL PROPERTIES

The material properties are those of a typical lithium-ion battery. The electrolyte is based on 1:2 EC:DMC and p(VDF-HFP) as the solvent mixture, and $LiPF_6$ as the salt. The electrode materials are graphite (Li_xC_6) for the negative electrode and $Li_yMn_2O_4$ for the positive electrode.

The electrolyte conductivity and the equilibrium potential of the negative and positive electrodes are composition dependent through experimentally measured data. This data is tabulated in interpolating functions in the model and the properties vary significantly during charge and discharge due to the changes in composition.

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The model specifies the electrolyte conductivity according to the function in Figure 2.

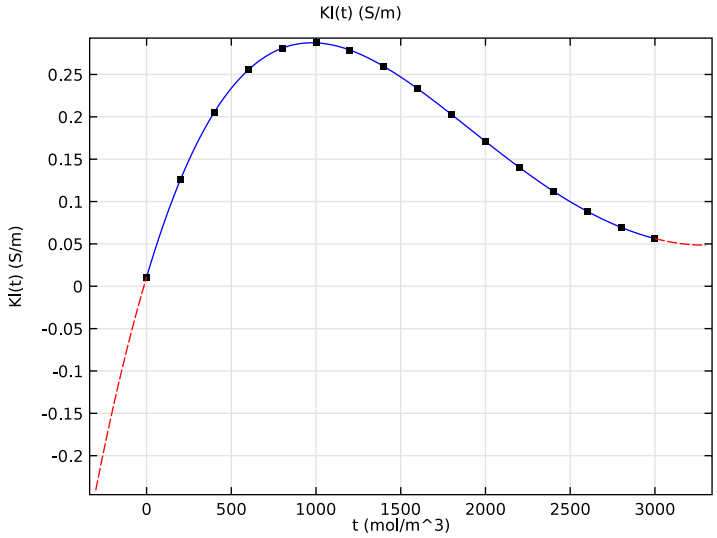

Figure 2: The model specifies the ionic conductivity of the electrolyte using an interpolation function according to this behavior with concentration.

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Figure 3 displays the equilibrium potentials for the negative and positive electrodes as functions of the measured state of charge (SOC).

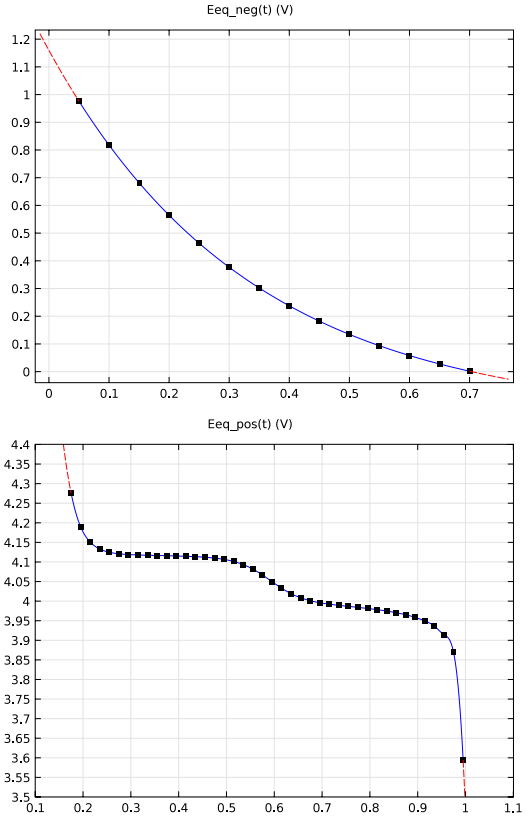

Figure 3: The equilibrium voltage of the electrode materials.

The model uses the following definition of SOC:

$$\mathrm{SOC} = \frac{c_{s,\mathrm{Li}}^{\mathrm{surf}}}{c_{s,\mathrm{Li}}^{\mathrm{max}}} \tag{2}$$

The initial SOC-values for the negative and positive electrodes are 0.17 and 0.56, respectively. This corresponds to an open circuit cell voltage of approximately 4.22 V, which corresponds to a fully charged battery.

For complete details on the material properties and constants, see Ref. 1.

Results and Discussion

DISCHARGE CURVES

The battery is initially at a fully charged state. A first modeling approach is to simulate discharge at various current densities and then display the discharge curves. The results show the capacity of the battery at different discharge rates. This model defines end-of-discharge as the time when the cell voltage drops below 3 V. The nominal discharge current density, corresponding to case 1C below (a current density corresponding to a theoretical full discharge in one hour), is 17.5 A/m^2.

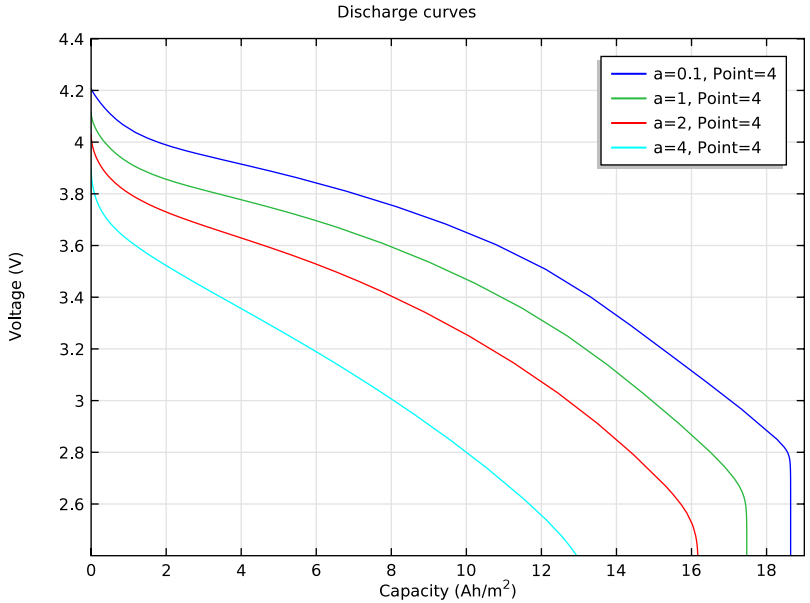

Figure 4: Discharge curves for various discharge rates.

Figure 4 shows that the maximum discharge capacity of 17.5 Ah/m^2 is obtained for the a current density of 1.75 A/m^2 (0.1 C). It can also be seen that the 3 V discharge capacity decreases slightly when applying a 1C discharge current and dramatically when going above that. At 4C, the battery delivers approximately 50% of the theoretical capacity before it reaches a cell voltage of 3 V. The discharge curves are identical to those presented in Ref. 1.

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DISCHARGE AND CHARGE CYCLE

Figure 5 depicts the discharge-charge cycle applied in the next step of the simulation. The cycle applies 2000 s of discharge at nominal current density (case 1C above), 300 s at open circuit, then 2000 s of charge at nominal current density, and finally open-circuit conditions.

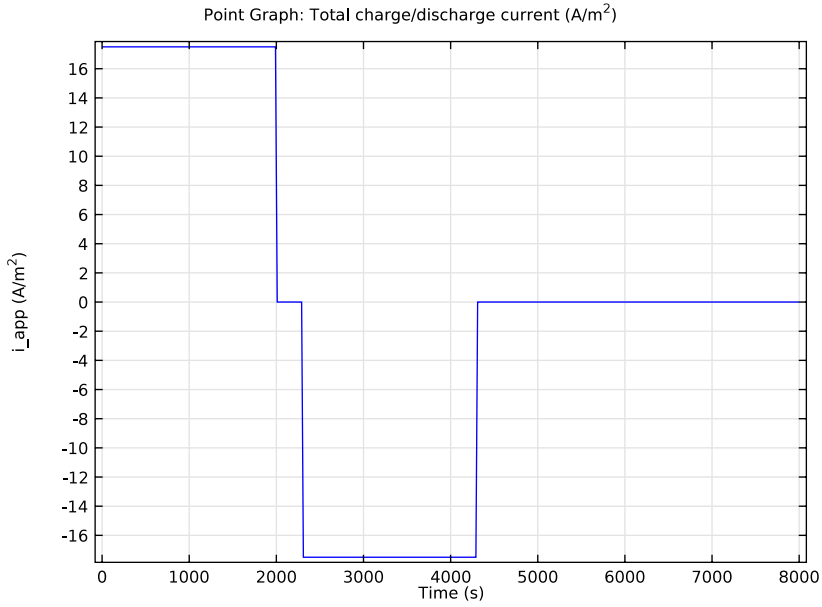

Figure 5: The applied current density as a function of time.

The time-dependent cell voltage predicted by the model is shown in Figure 6.

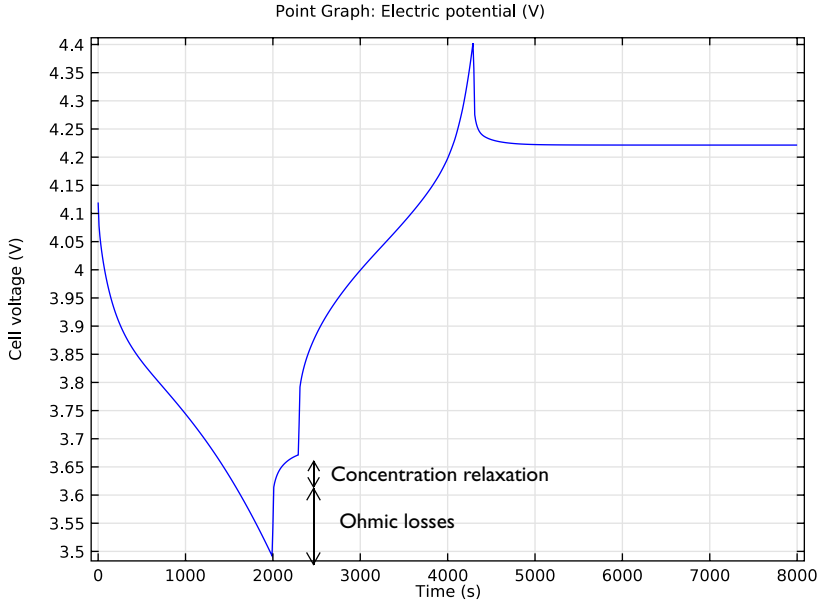

Figure 6: Cell voltage during the applied cycle.

During both discharge and charge, the cell voltage experiences ohmic losses of approximately 100 mV and a concentration overpotential of about 50 mV. These losses are clearly visible in the plot when the current is set to 0, where you can see an immediate relaxation of the voltage due to the relaxation of ohmic losses followed by a slower relaxation of the concentration overpotential (see Figure 6 above).

It is possible to visualize the contributions of the different losses to the total overpotential. You can plot the contribution as shown in Figure 7 using the following procedure:

1. Plot the electrolyte potential profile at the initial stage of the discharge with a bias of 144 mV to get all the plots in the same range of potential.
2. Plot the electrolyte potential profile at the end of the discharge adding a bias of 560 mV, again in order to get the profile in the same scale as the overpotential.
3. Plot the reaction overpotential profile.

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All plots are within similar range of potential.

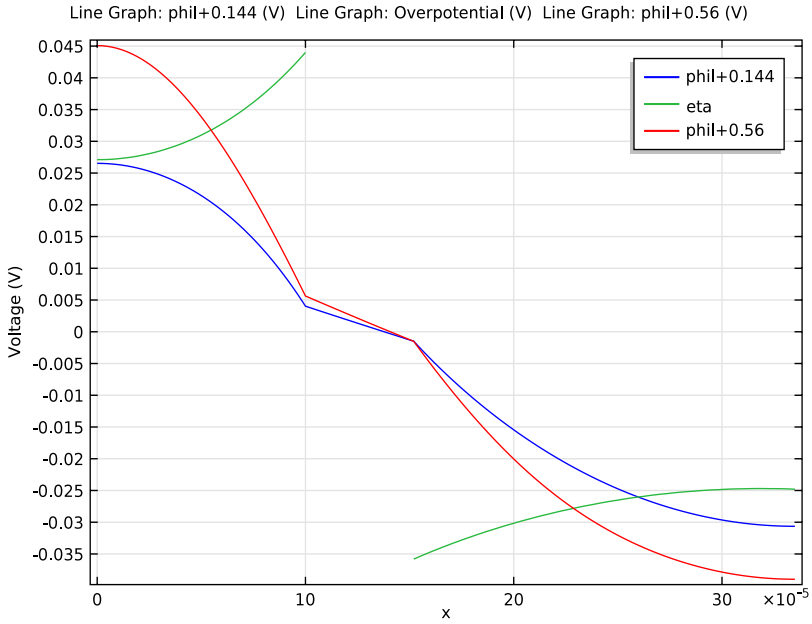

Figure 7: Voltage losses in the battery during discharge.

Figure 7 shows that the two main losses are due to the reaction overpotential and electrolyte resistance. The difference between electrolyte potential profiles initially and at the end of the discharge stage indicates the influence of the concentration polarization; it is approximately half the magnitude of the two previous losses and is thus also important to consider. The figure does not include the electronic potential profile in the solid phase, but the simulations show that contributions from the ohmic losses in the electronic conductors are negligible.

To further investigate the reason for the steep voltage decrease, you can plot the concentration profile in the electrolyte. Figure 8 depicts the profile at several stages during the discharge and charge cycle.

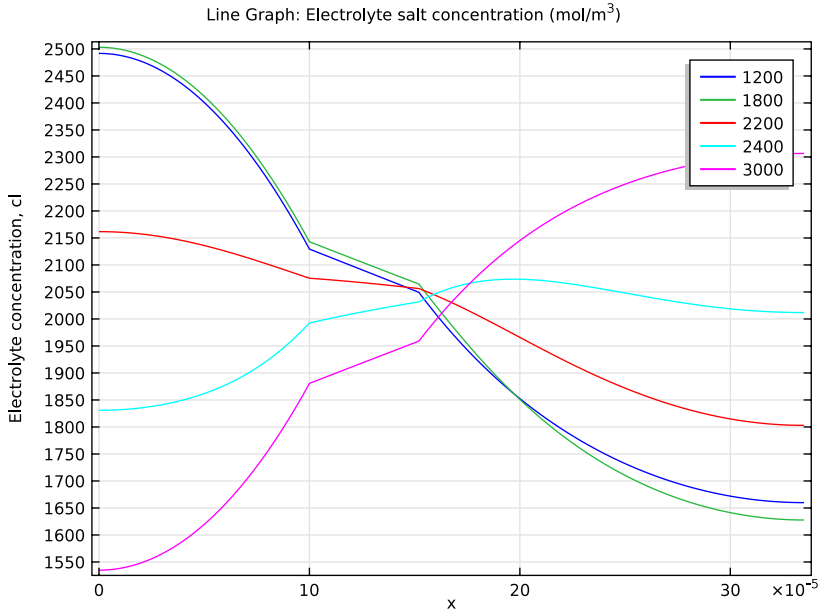

Figure 8: Electrolyte-phase concentration profiles at various times.

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The cell experiences significant concentration polarization due to the low effective diffusion coefficient in the electrolyte, which in turn leads to variations in ionic conductivity and concentration overpotential.

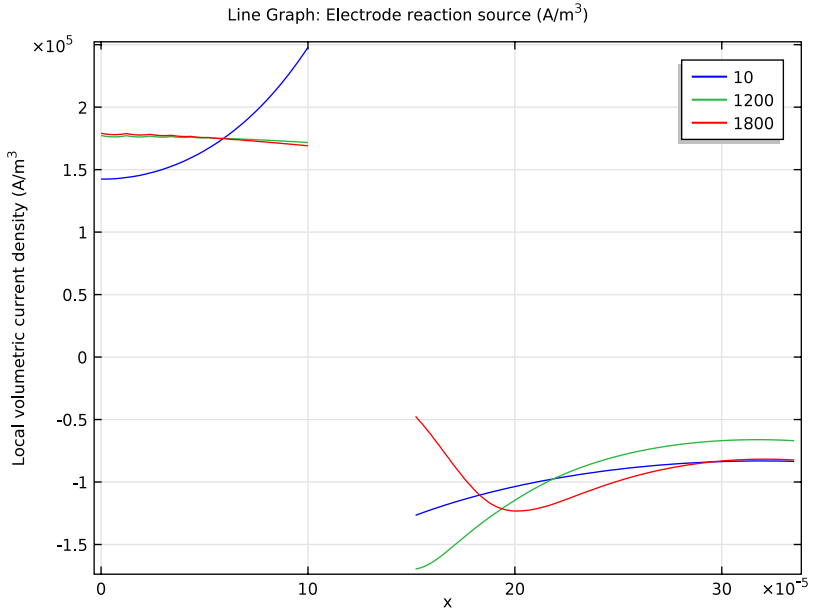

Figure 9: Local current-density distribution within the battery at various stages during the discharge.

The concentration in the solid phase at the surface of the particles also affects the current density. Figure 10 depicts the distribution of the concentration in the solid-phase particles just before the end of the discharge.

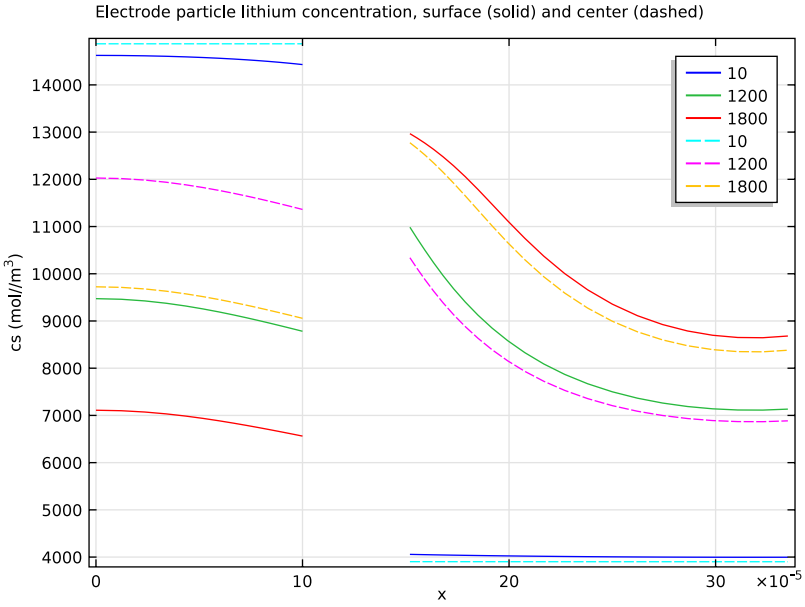

Figure 10: Concentration distribution of lithium in the solid particles during the discharge phase.

At 1800 s the concentration in the negative electrode varies from 9500 mol/m^3 in the particle center to approximately 7000 mol/m^3 at the surface, with moderate variation along the width of the cell. At the positive electrode, the variation along the width is much more pronounced with a surface concentration of approximately 13,000 mol/m^3 at the electrolyte interface and only 8000 mol/m^3 at the positive current collector/feeder. This large variation arises due to the nonuniform current distribution, which in turn is caused mainly by the poor electrolyte conductivity (due to low porosity) but also by the concentration polarization.

As the surface concentration changes, the equilibrium voltage also varies, causing a lower reaction overpotential and a decrease in the local current density. This effect tends to even out the local charge transfer current density to some extent but results in a larger overall voltage loss in the battery.

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Reference

1. M. Doyle, J. Newman, A.S. Gozdz, C.N. Schmutz, and J.M. Tarascon, "Comparison of Modeling Predictions with Experimental Data from Plastic Lithium Ion Cells," *J. Electrochem. Soc.*, vol. 143, p. 1890, 1996.

Model Library path: `Batteries_and_Fuel_Cells_Module/Batteries/li_battery_1d`

Modeling Instructions

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Click the **1D** button.

3 Click **Next**.

4 In the **Add physics** tree, select **Electrochemistry>Battery Interfaces>Lithium-Ion Battery (liion)**.

5 Click **Add Selected**.

6 Click **Next**.

7 Find the **Studies** subsection. In the tree, select **Preset Studies>Time Dependent**.

8 Click **Finish**.

GLOBAL DEFINITIONS

Parameters

1 In the **Model Builder** window, right-click **Global Definitions** and choose **Parameters**.

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `li_battery_1d_parameters.txt`.

GEOMETRY 1

The geometry contains three domains. Create the geometry by specifying the coordinates of the boundaries.

Interval 1

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

2 In the **Interval** settings window, locate the **Interval** section.

3 From the **Number of intervals** list, choose **Many**.

4 In the **Points** edit field, type `0,L_neg,L_neg+L_sep,L_neg+L_sep+L_pos`.

5 Click the **Build Selected** button.

GLOBAL DEFINITIONS

This model uses interpolation functions, imported from text files, for the equilibrium potentials and electrolyte conductivity.

Interpolation 1

1 In the **Model Builder** window, right-click **Global Definitions** and choose **Functions>Interpolation**.

2 In the **Interpolation** settings window, locate the **Definition** section.

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

4 Click the **Browse** button.

5 Browse to the model's Model Library folder and double-click the file `li_battery_1d_Eeq_neg.txt`.

6 Click the **Import** button.

7 In the **Function name** edit field, type `Eeq_neg`.

8 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Cubic spline**.

9 From the **Extrapolation** list, choose **Nearest function**.

10 Locate the **Units** section. In the **Function** edit field, type `V`.

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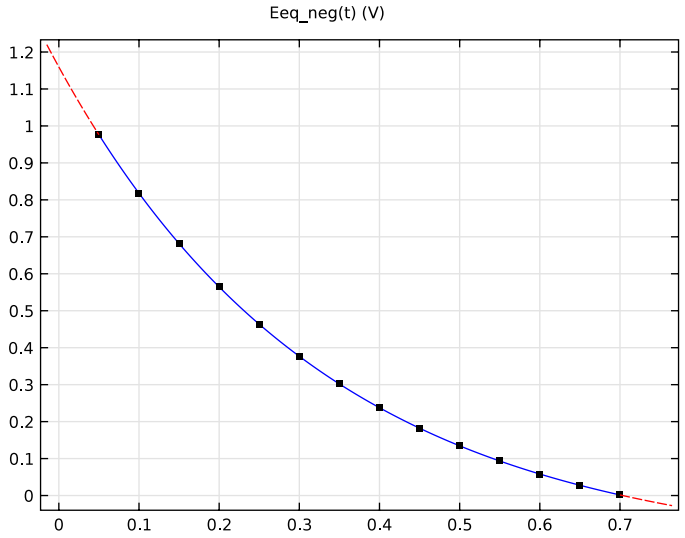
11 Click the **Plot** button.



Interpolation 2

1 Right-click **Global Definitions** and choose **Functions>Interpolation**.

2 In the **Interpolation** settings window, locate the **Definition** section.

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

4 Click the **Browse** button.

5 Browse to the model's Model Library folder and double-click the file `li_battery_1d_Eeq_pos.txt`.

6 Click the **Import** button.

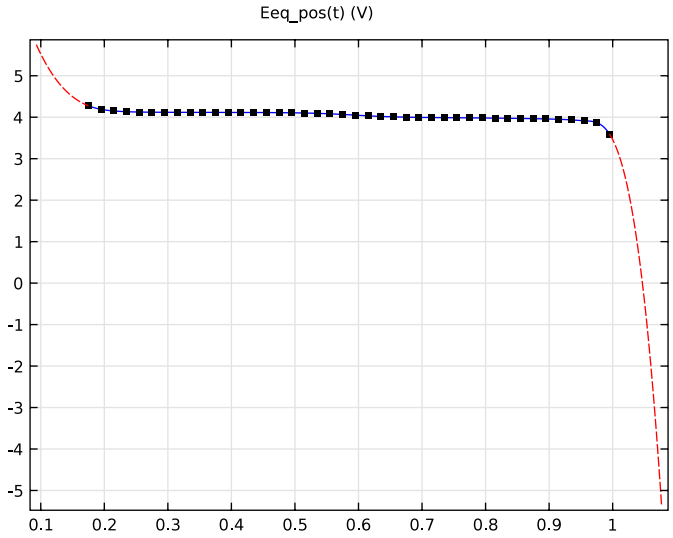
7 In the **Function name** edit field, type `Eeq_pos`.

8 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Cubic spline**.

9 From the **Extrapolation** list, choose **Nearest function**.

10 Locate the **Units** section. In the **Function** edit field, type `V`.

11 Click the **Plot** button.



Interpolation 3

1 Right-click **Global Definitions** and choose **Functions>Interpolation**.

2 In the **Interpolation** settings window, locate the **Definition** section.

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

4 Click the **Browse** button.

5 Browse to the model's Model Library folder and double-click the file `li_battery_1d_Kl.txt`.

6 Click the **Import** button.

7 In the **Function name** edit field, type `Kl`.

8 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Cubic spline**.

9 From the **Extrapolation** list, choose **Nearest function**.

10 Locate the **Units** section. In the **Arguments** edit field, type `mol/m^3`.

11 In the **Function** edit field, type `S/m`.

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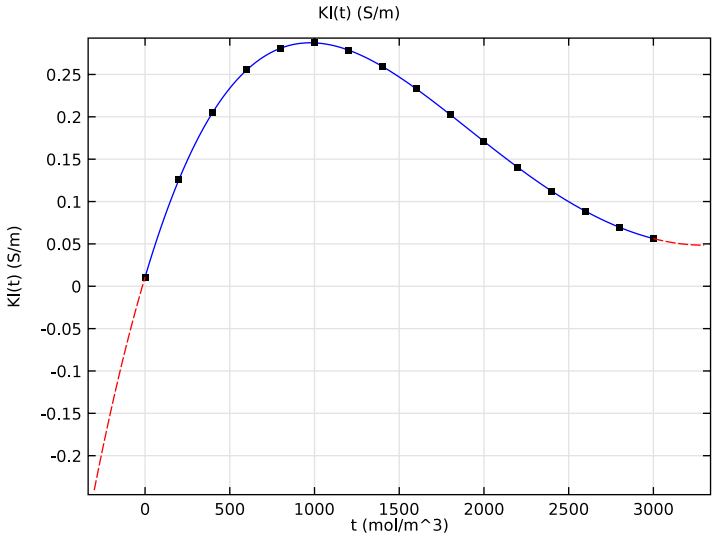
12 Click the **Plot** button.



Step 1

Add a step function that you will use when defining variables for the load cycle.

1 Right-click **Global Definitions** and choose **Functions>Step**.

2 In the **Step** settings window, click to expand the **Smoothing** section.

3 In the **Size of transition zone** edit field, type 10.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Model 1** right-click **Definitions** and choose **Variables**.

2 Right-click **Variables 1** and choose **Rename**.

3 Go to the **Rename Variables** dialog box and type `Variables (Positive End Terminal)` in the **New name** edit field.

4 Click **OK**.

5 In the **Variables** settings window, locate the **Geometric Entity Selection** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundary 4 only.

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

Name	Expression	Description
i_app	i_disch*disch_on+i_charge*charge_on	Total charge/discharge current
disch_on	step1((t_disch_stop-t)[1/s])	Discharge on/off function
charge_on	step1((t-t_disch_stop-t_ocp)[1/s])*step1((t_charge_stop+t_disch_stop+t_ocp-t)[1/s])	Charge on/off function

LITHIUM-ION BATTERY

Porous Electrode 1

1 In the **Model Builder** window, under **Model 1** right-click **Lithium-Ion Battery** and choose **Porous Electrode**.

2 Select Domain 1 only.

3 In the **Porous Electrode** settings window, locate the **Model Inputs** section.

4 In the T edit field, type `T`.

5 Locate the **Electrolyte Properties** section. From the σ_l list, choose **User defined**. In the associated edit field, type `Kl(cl)`.

6 From the D_l list, choose **User defined**. In the associated edit field, type `Dl`.

7 From the t_+ list, choose **User defined**. In the associated edit field, type `t_plus`.

8 Locate the **Electrode Properties** section. From the σ_s list, choose **User defined**. In the associated edit field, type `Ds_neg`.

9 Locate the **Particle Intercalation** section. From the D_s list, choose **User defined**. In the associated edit field, type `Ds_neg`.

10 Locate the **Electrode Properties** section. In the σ_s edit field, type `Ks_neg`.

11 Locate the **Particle Intercalation** section. From the $c_{s,max}$ list, choose **User defined**. In the associated edit field, type `csmax_neg`.

12 In the $c_{s,init}$ edit field, type `cs0_neg`.

13 In the r_p edit field, type `rp_neg`.

14 Locate the **Volume Fractions** section. In the ε_s edit field, type `epss_neg`.

15 In the ε_l edit field, type `epsl_neg`.

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16 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **Bruggeman**.

17 From the **Electrical conductivity** list, choose **Bruggeman**.

18 From the **Diffusion** list, choose **Bruggeman**.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Porous Electrode 1** node, then click **Porous Electrode Reaction 1**.

2 In the **Porous Electrode Reaction** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T`.

4 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq},ref}$ edit field, type `Eeq_neg(liion.cs_surface/csmax_neg)`.

5 Locate the **Electrode Kinetics** section. In the k_{a} edit field, type `k_neg`.

6 In the k_{c} edit field, type `k_neg`.

Electrolyte 1

1 In the **Model Builder** window, under **Model 1>Lithium-Ion Battery** click **Electrolyte 1**.

2 In the **Electrolyte** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T`.

4 Locate the **Electrolyte** section. From the σ_{l} list, choose **User defined**. In the associated edit field, type `Kl(cl)`.

5 From the D_{l} list, choose **User defined**. In the associated edit field, type `Dl`.

6 From the t_+ list, choose **User defined**. In the associated edit field, type `t_plus`.

Porous Electrode 2

1 In the **Model Builder** window, right-click **Lithium-Ion Battery** and choose **Porous Electrode**.

2 Select Domain 3 only.

3 In the **Porous Electrode** settings window, locate the **Model Inputs** section.

4 In the T edit field, type `T`.

5 Locate the **Electrolyte Properties** section. From the σ_{l} list, choose **User defined**. In the associated edit field, type `Kl(cl)`.

6 From the D_{l} list, choose **User defined**. In the associated edit field, type `Dl`.

7 From the t_+ list, choose **User defined**. In the associated edit field, type `t_plus`.

8 Locate the **Electrode Properties** section. From the σ_s list, choose **User defined**. In the associated edit field, type `Ks_pos`.

9 Locate the **Particle Intercalation** section. From the D_s list, choose **User defined**. In the associated edit field, type `Ds_pos`.

10 From the $c_{s,max}$ list, choose **User defined**. In the associated edit field, type `csmax_pos`.

11 In the $c_{s,init}$ edit field, type `cs0_pos`.

12 In the r_p edit field, type `rp_pos`.

13 Locate the **Volume Fractions** section. In the ε_s edit field, type `epss_pos`.

14 In the ε_l edit field, type `epsl_pos`.

15 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **Bruggeman**.

16 From the **Electrical conductivity** list, choose **Bruggeman**.

17 From the **Diffusion** list, choose **Bruggeman**.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Porous Electrode 2** node, then click **Porous Electrode Reaction 1**.

2 In the **Porous Electrode Reaction** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T`.

4 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}$ edit field, type `Eeq_pos(liion.cs_surface/csmax_pos)`.

5 Locate the **Electrode Kinetics** section. In the k_a edit field, type `k_pos`.

6 In the k_c edit field, type `k_pos`.

Electric Ground 1

1 In the **Model Builder** window, right-click **Lithium-Ion Battery** and choose **Electrode>Electric Ground**.

2 Select Boundary 1 only.

Electrode Current Density 1

1 Right-click **Lithium-Ion Battery** and choose **Electrode>Electrode Current Density**.

2 Select Boundary 4 only.

3 In the **Electrode Current Density** settings window, locate the **Electrode Current Density** section.

4 In the $\mathbf{i}_{n,s}$ edit field, type `-i_app`.

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Initial Values 2

1 Right-click **Lithium-Ion Battery** and choose **Initial Values**.

2 Select Domain 3 only.

3 In the **Initial Values** settings window, locate the **Initial Values** section.

4 In the *phil* edit field, type `-Eeq_neg(cs0_neg/csmax_neg)`.

5 In the *cl* edit field, type `cl_0`.

6 In the *phis* edit field, type `Eeq_pos(cs0_pos/csmax_pos)-Eeq_neg(cs0_neg/csmax_neg)`.

Initial Values 1

1 In the **Model Builder** window, under **Model 1>Lithium-Ion Battery** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the *phil* edit field, type `-Eeq_neg(cs0_neg/csmax_neg)`.

4 In the *cl* edit field, type `cl_0`.

STUDY 1

First set up a study to investigate the defined discharge/charge cycle.

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

2 In the **Time Dependent** settings window, locate the **Study Settings** section.

3 In the **Times** edit field, type `range(0,10,8000)`.

4 Select the **Relative tolerance** check box.

5 In the associated edit field, type `1e-4`.

6 In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

RESULTS

Reproduce the plots in the model documentation for the discharge/charge cycle, starting with the current load profile (Figure 5).

1D Plot Group 3

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 Right-click **1D Plot Group 3** and choose **Point Graph**.

3 Select Boundary 4 only.

4 In the **Point Graph** settings window, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Definitions>Total charge/discharge current (i_app)**.

5 In the **Model Builder** window, click **1D Plot Group 3**.

6 In the **1D Plot Group** settings window, locate the **Plot Settings** section.

7 Select the **x-axis label** check box.

8 In the associated edit field, type `Time (s)`.

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

10 In the associated edit field, type `i_app (A/m<sup>2</sup>)`.

11 Click the **Plot** button.

1D Plot Group 4

The following steps are for plotting the cell voltage during the discharge/charge cycle (Figure 6):

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 Right-click **1D Plot Group 4** and choose **Point Graph**.

3 Select Boundary 4 only.

4 In the **Point Graph** settings window, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Lithium-Ion Battery>Electric potential (phis)**.

5 In the **Model Builder** window, click **1D Plot Group 4**.

6 In the **1D Plot Group** settings window, locate the **Plot Settings** section.

7 Select the **x-axis label** check box.

8 In the associated edit field, type `Time (s)`.

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

10 In the associated edit field, type `Cell voltage (V)`.

11 Click the **Plot** button.

1D Plot Group 5

Next create a plot for comparing the different voltage losses (Figure 7).

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 In the **1D Plot Group** settings window, locate the **Data** section.

3 From the **Data set** list, choose **None**.

4 Right-click **Results>1D Plot Group 5** and choose **Line Graph**.

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5 In the **Line Graph** settings window, locate the **Data** section.

6 From the **Data set** list, choose **Solution 1**.

7 From the **Time selection** list, choose **From list**.

8 In the **Times** list, select **10**.

9 Locate the **Selection** section. From the **Selection** list, choose **All domains**.

10 Locate the **y-Axis Data** section. In the **Expression** edit field, type `phil+0.144`.

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

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

13 In the table, enter the following settings:

Legends
phil+0.144

14 In the **Model Builder** window, right-click **1D Plot Group 5** and choose **Line Graph**.

15 In the **Line Graph** settings window, locate the **Data** section.

16 From the **Data set** list, choose **Solution 1**.

17 From the **Time selection** list, choose **From list**.

18 In the **Times** list, select **10**.

19 Locate the **Selection** section. From the **Selection** list, choose **All domains**.

20 Locate the **y-Axis Data** section. In the **Expression** edit field, type `liion.eta_per1`.

21 Locate the **Legends** section. Select the **Show legends** check box.

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

23 In the table, enter the following settings:

Legends
eta

24 Right-click **1D Plot Group 5** and choose **Line Graph**.

25 In the **Line Graph** settings window, locate the **Data** section.

26 From the **Data set** list, choose **Solution 1**.

27 From the **Time selection** list, choose **From list**.

28 In the **Times** list, select **1990**.

29 Locate the **Selection** section. From the **Selection** list, choose **All domains**.

30 Locate the **y-Axis Data** section. In the **Expression** edit field, type `phil+0.56`.

31 Locate the **Legends** section. Select the **Show legends** check box.

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

33 In the table, enter the following settings:

Legends
phil+0.56

34 In the **Model Builder** window, click **1D Plot Group 5**.

35 In the **1D Plot Group** settings window, locate the **Plot Settings** section.

36 Select the **x-axis label** check box.

37 In the associated edit field, type `x`.

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

39 In the associated edit field, type `Voltage (V)`.

40 Click the **Plot** button.

Electrolyte Salt Concentration (liion)

Modify the default plot of the electrolyte concentration to compare the profile at various times during the discharge/charge cycle (Figure 8):

1 In the **Model Builder** window, under **Results** click **Electrolyte Salt Concentration (liion)**.

2 In the **1D Plot Group** settings window, locate the **Data** section.

3 From the **Time selection** list, choose **From list**.

4 In the **Times** list, choose **1200**, **1800**, **2200**, **2400**, and **3000**.

5 In the **Model Builder** window, under **Results>Electrolyte Salt Concentration (liion)** click **Line Graph 1**.

6 In the **Line Graph** settings window, locate the **Selection** section.

7 From the **Selection** list, choose **All domains**.

8 Locate the **Legends** section. Select the **Show legends** check box.

9 In the **Model Builder** window, click **Electrolyte Salt Concentration (liion)**.

10 In the **1D Plot Group** settings window, locate the **Plot Settings** section.

11 Select the **x-axis label** check box.

12 In the associated edit field, type `x`.

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

14 In the associated edit field, type `Electrolyte concentration, cl`.

15 Click the **Plot** button.

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1D Plot Group 6

You can plot the local current density for various times in the following way (Figure 9):

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 In the **1D Plot Group** settings window, locate the **Data** section.

3 From the **Time selection** list, choose **From list**.

4 In the **Times** list, choose **10**, **1200**, and **1800**.

5 Right-click **Results>1D Plot Group 6** and choose **Line Graph**.

6 In the **Line Graph** settings window, locate the **Selection** section.

7 From the **Selection** list, choose **All domains**.

8 Locate the **y-Axis Data** section. In the **Expression** edit field, type `liion.ivtot`.

9 Locate the **Legends** section. Select the **Show legends** check box.

10 In the **Model Builder** window, click **1D Plot Group 6**.

11 In the **1D Plot Group** settings window, locate the **Plot Settings** section.

12 Select the **x-axis label** check box.

13 In the associated edit field, type `x`.

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

15 In the associated edit field, type `Local volumetric current density (A/m<sup>3</sup>`.

16 Click the **Plot** button.

1D Plot Group 7

This plot shows the concentration profile within the particles in the electrodes (Figure 10).

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 In the **1D Plot Group** settings window, locate the **Data** section.

3 From the **Time selection** list, choose **From list**.

4 In the **Times** list, select **1900**.

5 Locate the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Electrode particle lithium concentration, surface (solid) and center (dashed)`.

7 Locate the **Plot Settings** section. Select the **x-axis label** check box.

8 In the associated edit field, type `x`.

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

10 In the associated edit field, type `cs (mol//m<sup>3</sup>)`.

11 Right-click **Results>1D Plot Group 7** and choose **Line Graph**.

12 In the **Line Graph** settings window, locate the **Selection** section.

13 From the **Selection** list, choose **All domains**.

14 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Lithium-Ion Battery>Insertion particle concentration, surface (liion.cs_surface)**.

15 Locate the **Legends** section. Select the **Show legends** check box.

16 In the **Model Builder** window, click **1D Plot Group 7**.

17 In the **1D Plot Group** settings window, locate the **Data** section.

18 From the **Time selection** list, choose **From list**.

19 In the **Times** list, choose **10**, **1200**, and **1800**.

20 Right-click **1D Plot Group 7** and choose **Line Graph**.

21 In the **Line Graph** settings window, locate the **Selection** section.

22 From the **Selection** list, choose **All domains**.

23 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Lithium-Ion Battery>Insertion particle concentration, center (liion.cs_center)**.

24 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

25 Locate the **Legends** section. Select the **Show legends** check box.

26 Click the **Plot** button.

27 Click the **Zoom Extents** button on the Graphics toolbar.

To reproduce the discharge curves in Figure 4, modify the problem formulation slightly to use a constant discharge current only, and then set up a parametric study that solves for four different discharge currents. Use a stop condition to stop the solver if the cell voltage drops below 2.4 V.

GLOBAL DEFINITIONS

Begin by adding a global current variable.

Parameters

1 In the **Model Builder** window, under **Global Definitions** click **Parameters**.

2 In the **Parameters** settings window, locate the **Parameters** section.

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3 In the table, enter the following settings:

Name	Expression	Description
a	1	Multiplicative factor for the parametric study

DEFINITIONS

Also, add a variable for the discharge current.

Variables (Positive End Terminal)

1 In the **Model Builder** window, under **Model 1>Definitions** click **Variables (Positive End Terminal)**.

2 In the **Variables** settings window, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Description
i_app_p	a*i_1C	Discharge current for the parametric study

Integration 1

Using a boundary integration variable you can access the cell voltage at the end terminal during the computation.

1 In the **Model Builder** window, right-click **Definitions** and choose **Model Couplings>Integration**.

2 In the **Integration** settings window, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

5 Locate the **Operator Name** section. In the **Operator name** edit field, type EndTerminal.

LITHIUM-ION BATTERY

Electrode Current Density 1

1 In the **Model Builder** window, under **Model 1>Lithium-Ion Battery** click **Electrode Current Density 1**.

2 In the **Electrode Current Density** settings window, locate the **Electrode Current Density** section.

3 In the $\mathbf{i}_{n,s}$ edit field, type -i_app_p.

ROOT

In the **Model Builder** window, right-click the root node and choose **Add Study**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Find the **Studies** subsection. In the tree, select **Preset Studies>Time Dependent**.

3 Click **Finish**.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 2** node, then click **Step 1: Time Dependent**.

2 In the **Time Dependent** settings window, locate the **Study Settings** section.

3 In the **Times** edit field, type `0 40000`.

4 Select the **Relative tolerance** check box.

5 In the associated edit field, type `1e-4`.

Parametric Sweep

1 In the **Model Builder** window, right-click **Study 2** and choose **Parametric Sweep**.

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

3 Click **Add**.

4 In the table, enter the following settings:

Parameter names	Parameter value list
a	`0.1 1 2 4`

Solver 2

Modify the default solver.

1 Right-click **Study 2** and choose **Show Default Solver**.

Introduce a stop condition to stop the solver and move on to the next parameter value if the cell voltage drops below a certain level.

2 In the **Model Builder** window, expand the **Study 2>Solver Configurations>Solver 2** node.

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

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

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5 Click **Add**.

6 In the table, enter the following settings:

Stop expression
`mod1.EndTerminal(mod1.phis)<2.4`

Specify that the solution is to be stored both before and after the stop condition is reached.

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

8 Clear the **Add warning** check box.

Change the output of the solver to store all solver steps to get enough datapoints for the discharge curves.

9 In the **Model Builder** window, under **Study 2>Solver Configurations>Solver 2** click **Time-Dependent Solver 1**.

10 In the **Time-Dependent Solver** settings window, click to expand the **Output** section.

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

12 In the **Model Builder** window, click **Study 2**.

13 In the **Study** settings window, locate the **Study Settings** section.

14 Clear the **Generate default plots** check box.

15 Click the **Compute** button.

RESULTS

You can now plot the discharge curves for the parametric study by performing the following steps (Figure 4):

1D Plot Group 8

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 Right-click **1D Plot Group 8** and choose **Point Graph**.

3 In the **Point Graph** settings window, locate the **Data** section.

4 From the **Data set** list, choose **Solution 3**.

This data set contains the battery model solutions for the parametric sweep in Study 2.

5 Select Boundary 4 only.

6 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Lithium-Ion Battery>Electric potential (phis)**.

This choice corresponds to the time interval, while the outer solutions correspond to the parametric sweep.

7 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

To obtain the capacity along the horizontal axis, multiply the time in hours by the discharge current.

8 In the **Expression** edit field, type `(t/1[h])*i_app_p`.

9 Locate the **Legends** section. Select the **Show legends** check box.

10 Click the **Plot** button.

Finish the plot by adding a title and axis labels and adjusting the axis ranges.

11 In the **Model Builder** window, click **1D Plot Group 8**.

12 In the **1D Plot Group** settings window, locate the **Title** section.

13 From the **Title type** list, choose **Manual**.

14 In the **Title** text area, type `Discharge curves`.

15 Locate the **Plot Settings** section. Select the **x-axis label** check box.

16 In the associated edit field, type `Capacity (Ah/m<sup>2</sup>)`.

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

18 In the associated edit field, type `Voltage (V)`.

19 Click to expand the **Axis** section. Select the **Manual axis limits** check box.

20 In the **x minimum** edit field, type `0`.

21 In the **x maximum** edit field, type `19`.

22 In the **y minimum** edit field, type `2.4`.

23 In the **y maximum** edit field, type `4.4`.

24 Click the **Plot** button.

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