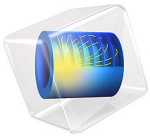


1D Isothermal Lithium-Ion Battery

Introduction

This example 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 sizes of the active materials — in this case, a carbon material in the negative electrode and lithium manganese oxide ($LiMn_2O_4$ spinel) in 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).

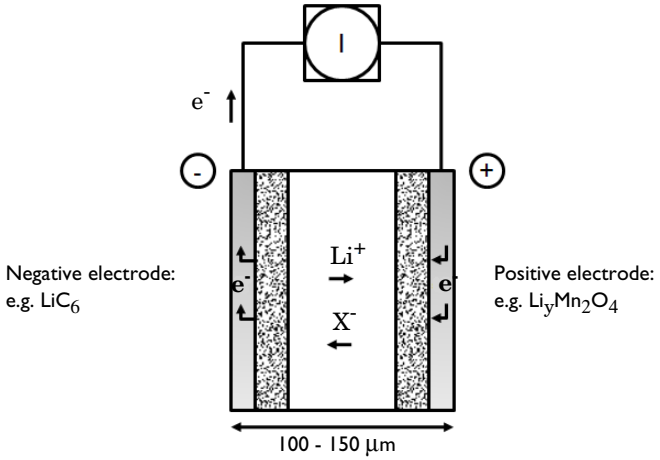


Figure 1: Cross section of a lithium-ion battery showing the electrochemical processes that occur during operation.

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
- Polymer electrolyte: 52 μm
- Positive porous electrode: 174 μm

The ionic charge balances and material balances are modeled according to the equations for binary 1:1 electrolytes (Ref. 1). The material parameters for the electrolyte refer to a plasticized EC/DMC electrolyte residing in a polymer matrix, and the electrolyte volume fraction specified in the model hence refer to the sum of the liquid electrolyte and polymer matrix volume fractions.

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 electrolyte phase of the porous electrodes, effective conductivities, σ_l^{eff}, are used that take porosity and tortuosity into account as given by the following expression:

$$\sigma_l^{\text{eff}} = \sigma_l \varepsilon^{\gamma}$$

where γ is the Bruggeman coefficient, using a value of 3.3. The diffusivity is treated similarly.

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.

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. Insulation boundary 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 consists of 2 M $LiPF_6$ salt in 1:2 EC:DMC (by volume) solvent and p(VDF-HFP). The electrode materials are carbon-based material 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 or the Material library in the model. The properties vary significantly during the charge and discharge phases due to the changes in composition.

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

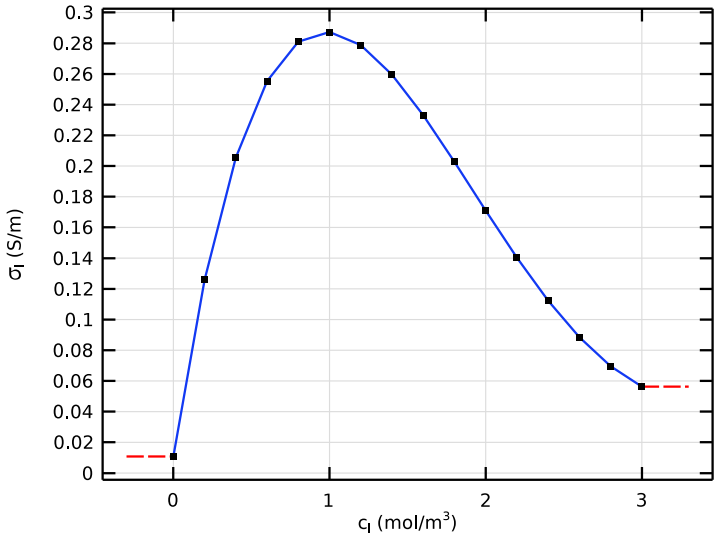


Figure 2: The model specifies the ionic conductivity of the electrolyte using an interpolation function according to this behavior with concentration.

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

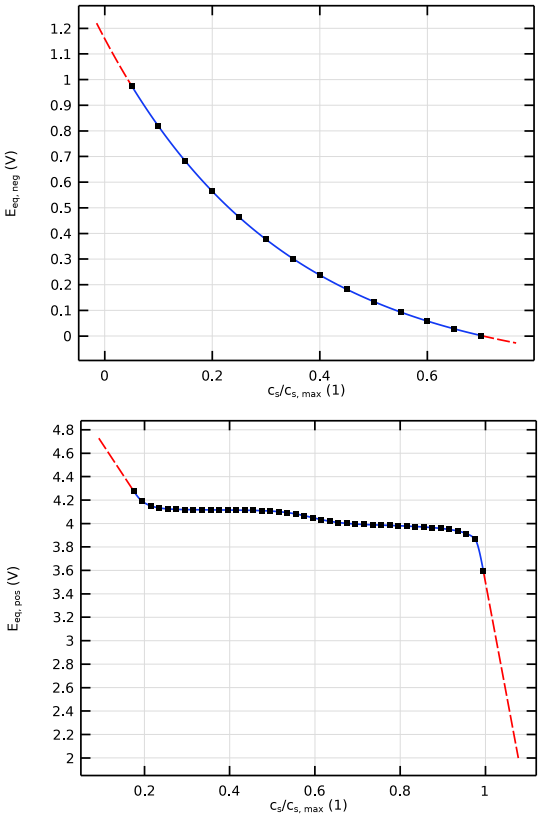


Figure 3: The equilibrium voltage of the electrode materials.

The model uses the following definition of SOC:

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

The initial SOC-values for the positive and negative electrodes are 0.17 and 0.56, respectively, with the concentrations selected initially in the model. 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.

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.

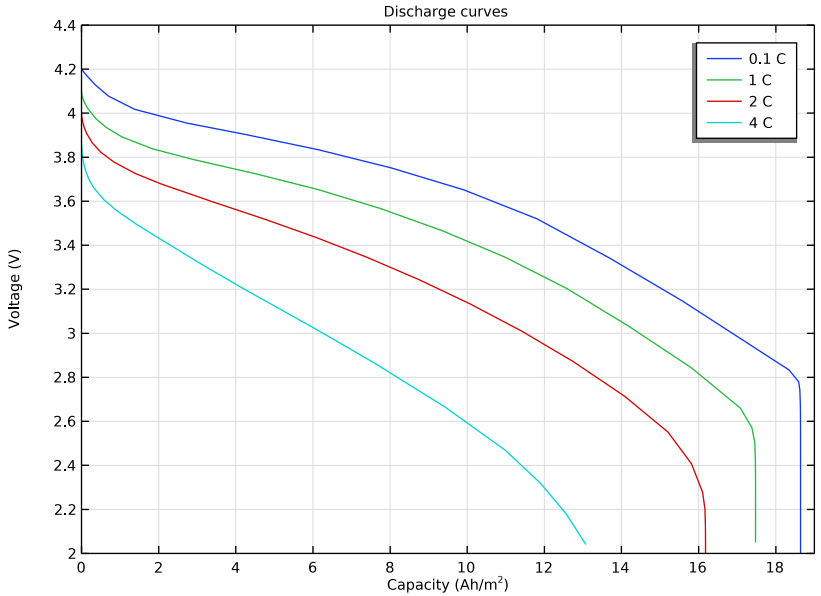


Figure 4: Discharge curves for various discharge rates.

Figure 4 shows that the maximum discharge capacity of 17.5 Ah/m^2 is obtained for 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.

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.

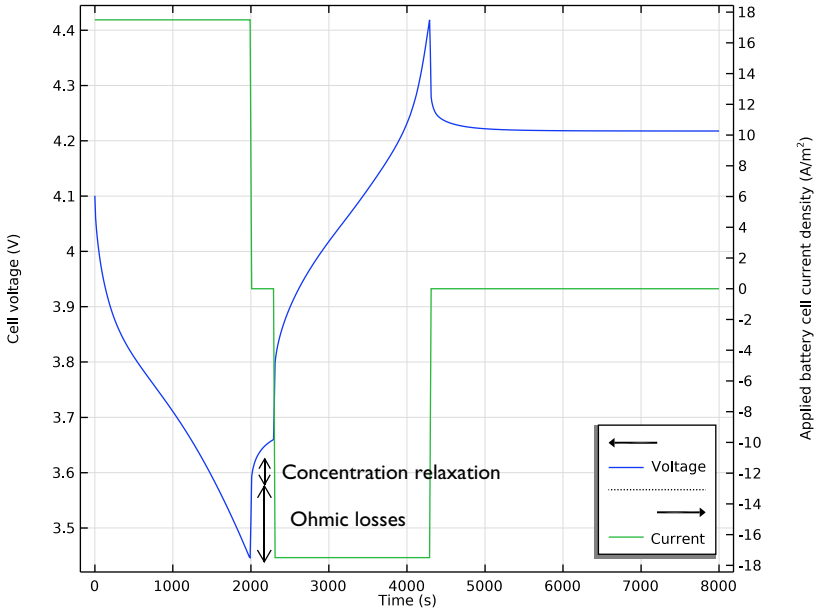


Figure 5: Cell voltage and current during the applied cycle.

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.

It is possible to visualize the contributions of the different losses to the total overpotential. You can plot the contribution as shown in Figure 6 using the following procedure:

1. Plot the electrolyte potential profile at the initial stage of the discharge with a bias of 148 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 558 mV, again in order to get the profile in the same scale as the overpotential.

3 Plot the reaction overpotential profile.

All plots are within similar range of potential.

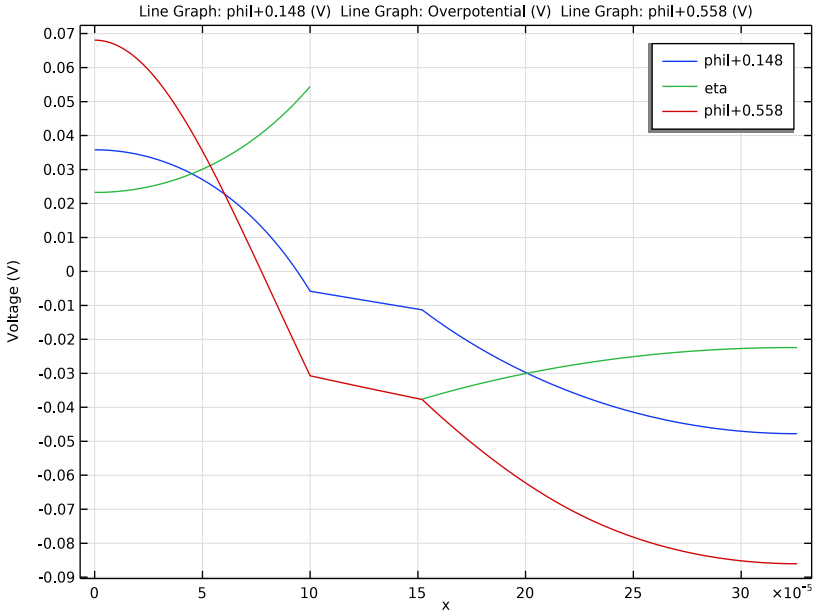


Figure 6: Voltage losses in the battery during discharge.

Figure 6 shows that the two main losses are due to the reaction overpotential and electrolyte resistance. The difference between electrolyte potential profiles initially and toward 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 7 depicts the profile at several stages during the discharge and charge cycle.

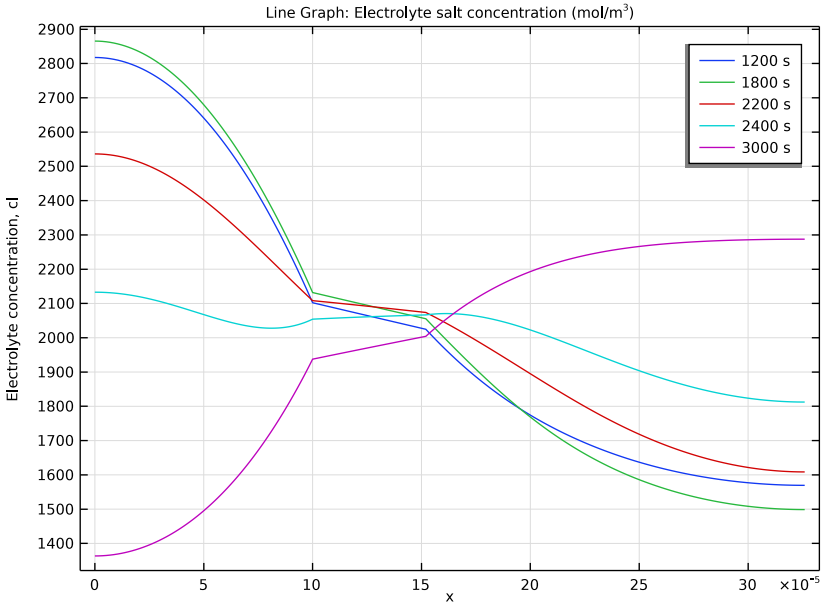


Figure 7: Electrolyte-phase concentration profiles at various times.

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.

The concentration in the solid phase at the surface of the particles also affects the current density. Figure 8 depicts the distribution of the concentration in the solid-phase particles just before the end of the discharge.

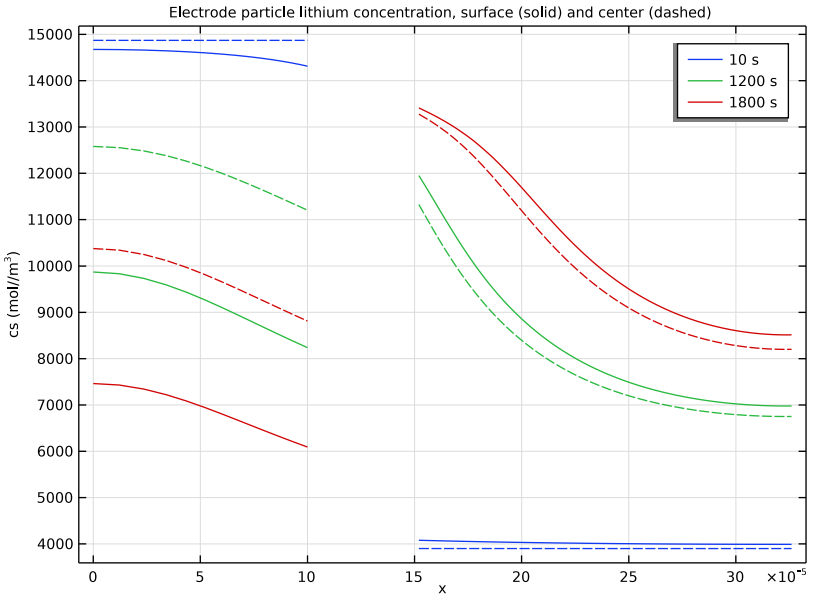


Figure 8: Concentration distribution of lithium in the solid particles during the discharge phase. (Dashed lines: Center of particles. Solid lines: Surface of particles.)

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 8500 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.

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, no. 6, pp. 1890–1903, 1996.

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/li_battery_1d`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.

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**.

(The **Time Dependent with Initialization study** will perform a time-dependent simulation, using a initialization study step to calculate the initial potentials in the cell.)

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 Click **Load from File**.

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

GEOMETRY 1

The geometry contains three domains. Create the geometry by specifying the lengths of the domains.

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:

Lengths (m)
L_neg
L_sep
L_pos

5 Click **Build Selected**.

GLOBAL DEFINITIONS

This model uses an interpolation function, imported from a text file, for the equilibrium potential of the negative electrode material.

Interpolation 1 (int1)

1 In the **Home** toolbar, click **Functions** and choose **Global>Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

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

4 Click **Browse**.

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

6 Click **Import**.

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

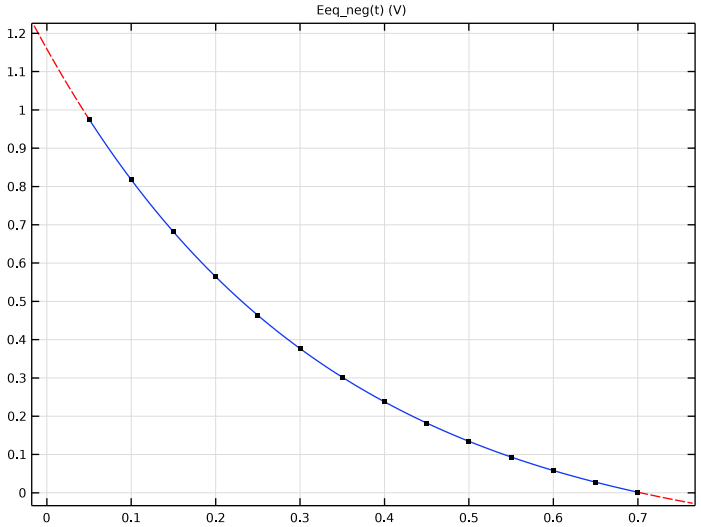
8 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Cubic spline**.

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

10 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
Eeq_neg	V

11 Click **Plot**.



Piecewise 1 (pw1)

The load cycle is set up using a Piecewise function. The data is imported from a text file and smoothing is enabled.

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Piecewise**.

2 In the **Settings** window for **Piecewise**, locate the **Definition** section.

3 In the **Argument** text field, type `t`.

4 From the **Smoothing** list, choose **Continuous second derivative**.

5 From the **Transition zone** list, choose **Absolute size**.

6 In the **Size of transition zone** text field, type `10`.

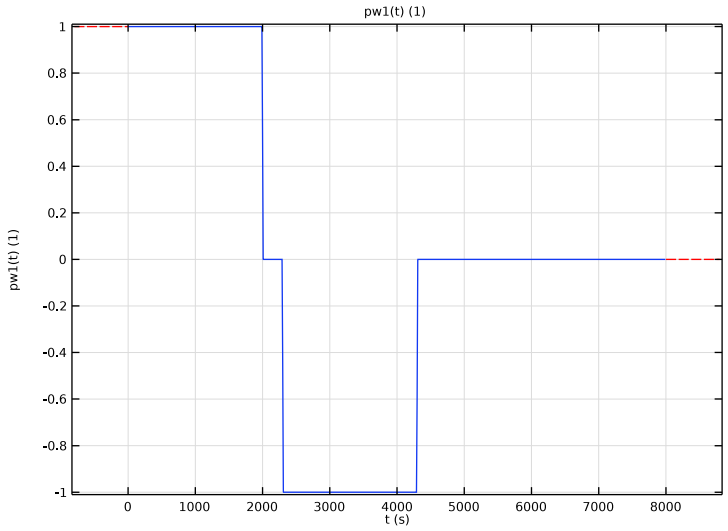
7 Find the **Intervals** subsection. Click **Load from File**.

8 Browse to the model's Application Libraries folder and double-click the file `li_battery_1d_load_cycle.txt`.

9 Locate the **Units** section. In the **Arguments** text field, type `s`.

10 In the **Function** text field, type `1`.

11 Click **Plot**.



DEFINITIONS

Variables (Positive Current Collector)

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, type `Variables (Positive Current Collector)` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

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

Name	Expression	Unit	Description
`i_app`	`pw1(t)*i_1C`	A/m²	`Applied battery cell current density`

MATERIALS

This model also uses battery materials available in the material library.

ADD MATERIAL

LMO is selected as positive electrode material.

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Battery>Electrodes>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery)**.

4 Click **Add to Component** in the window toolbar.

Note: In the Materials node, `cEeqref` denotes the maximum lithium concentration in the active material.

MATERIALS

LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)

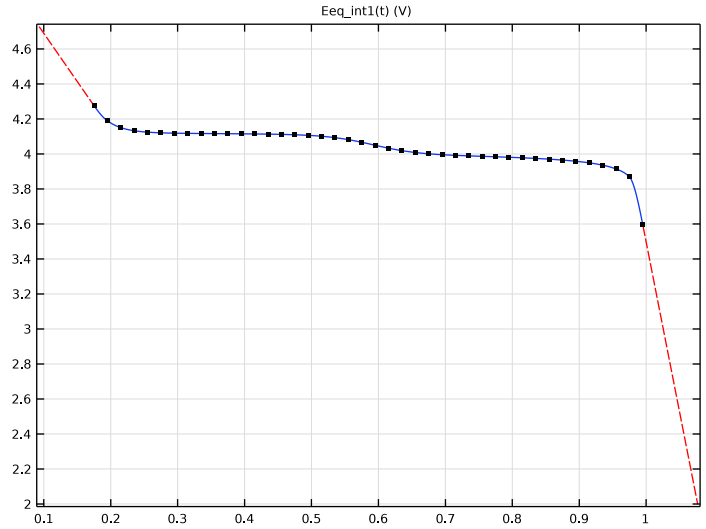
1 Select Domain 3 only.

2 In the **Model Builder** window, expand the **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)** node.

Interpolation 1 (Eeq_int1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)>Equilibrium potential (elpot)** node, then click **Interpolation 1 (Eeq_int1)**.

2 In the **Settings** window for **Interpolation**, click **Plot**.



ADD MATERIAL

LiPF6 in 1:2 EC:DMC and p(VdF-HFP) is selected as electrolyte.

1 Go to the **Add Material** window.

2 In the tree, select **Battery>Electrolytes>LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery)**.

3 Click **Add to Component** in the window toolbar.

4 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery) (mat2)

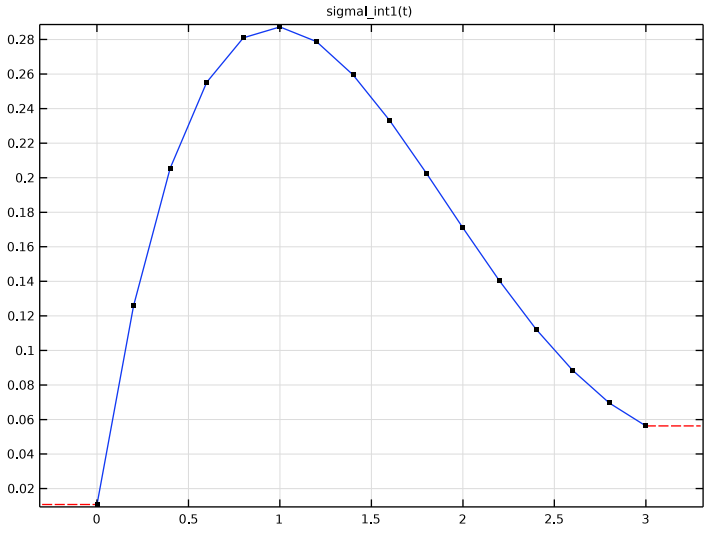
1 Click in the **Graphics** window and then press Ctrl+A to select all domains.

2 In the **Model Builder** window, expand the **LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery) (mat2)** node.

Interpolation 1 (sigmal_int1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials> LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery) (mat2)> Electrolyte conductivity (ionc)** node, then click **Interpolation 1 (sigmal_int1)**.

2 In the **Settings** window for **Interpolation**, click **Plot**.



Porous Electrode 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Lithium-Ion Battery (liion)** and choose **Porous Electrode**.

2 Select Domain 1 only.

3 In the **Settings** window for **Porous Electrode**, locate the **Electrode Properties** section.

4 From the σ_s list, choose **User defined**. In the associated text field, type `Ks_neg`.

5 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsl_neg`.

6 In the ε_s text field, type `epss_neg`.

7 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the f_l text field, type `epsl_neg^brugg`.

8 From the **Electrical conductivity** list, choose **No correction**.

9 From the **Diffusion** list, choose **User defined**. In the f_{Dl} text field, type `epsl_neg^brugg`.

Particle Intercalation 1

1 In the **Model Builder** window, click **Particle Intercalation 1**.

2 In the **Settings** window for **Particle Intercalation**, locate the **Species Settings** section.

3 In the $c_{s,init}$ text field, type `cs0_neg`.

4 From the $c_{s,max}$ list, choose **User defined**. In the associated text field, type `csmax_neg`.

5 Locate the **Particle Transport Properties** section. From the D_s list, choose **User defined**. In the associated text field, type `Ds_neg`.

6 In the r_p text field, type `rp_neg`.

7 Click to expand the **Operational SOCs for Initial Cell Charge Distribution** section. From the soc_{min} list, choose **User defined**. From the soc_{max} list, choose **User defined**.

Porous Electrode Reaction 1

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

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.

3 From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_neg(liion.cs_surface/csmax_neg)`.

4 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Rate constant**.

5 In the k text field, type `k_neg`.

6 In the $c_{l,ref}$ text field, type `cl_ref`.

7 Click to expand the **Heat of Reaction** section. From the list, choose **User defined**.

Porous Electrode 2

1 In the **Physics** toolbar, click — **Domains** and choose **Porous Electrode**.

2 Select Domain 3 only.

In the **Materials** node, the electrolyte material has been assigned to all domains. You hence need to set the electrode material selection manually, which in this case is LMO electrode material.

3 In the **Settings** window for **Porous Electrode**, locate the **Electrode Properties** section.

4 From the **Electrode material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)**.

5 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsl_pos`.

6 In the ε_s text field, type `epss_pos`.

7 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the f_l text field, type `epsl_pos^brugg`.

8 From the **Electrical conductivity** list, choose **No correction**.

9 From the **Diffusion** list, choose **User defined**. In the f_{Dl} text field, type `epsl_pos^brugg`.

Particle Intercalation 1

1 In the **Model Builder** window, click **Particle Intercalation 1**.

2 In the **Settings** window for **Particle Intercalation**, locate the **Material** section.

3 From the **Particle material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)**.

4 Locate the **Species Settings** section. In the $c_{s,init}$ text field, type `cs0_pos`.

5 Locate the **Particle Transport Properties** section. From the D_s list, choose **User defined**. In the associated text field, type `Ds_pos`.

6 In the r_p text field, type `rp_pos`.

Changing to quadratic elements in the particle dimension improves accuracy.

7 Click to expand the **Particle Discretization** section. In the N_{ord} text field, type `2`.

Porous Electrode Reaction 1

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

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Material** section.

3 From the **Material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)**.

4 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Rate constant**.

5 In the k text field, type `k_pos`.

6 In the $c_{l,ref}$ text field, type `cl_ref`.

Electric Ground 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Ground**.

2 Select Boundary 1 only.

Electrode Current Density 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current Density**.

2 Select Boundary 4 only.

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

4 In the $i_{n,s}$ text field, type `-i_app`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the cl text field, type `cl_0`.

GLOBAL DEFINITIONS

Default Model Inputs

Set up the temperature value used in the entire model.

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`.

STUDY 1

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

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(0,10,8000)`.

4 In the **Home** toolbar, click **Compute**.

RESULTS

Boundary Electrode Potential with Respect to Ground (liion)

A number of plots are created by default. The first plot shows the electrode potential versus time on the boundary where you applied the current density condition. Since you grounded the other electrode, this equals the cell voltage. Modify this plot to also plot the battery current on a second y-axis. (Figure 5):

1 In the **Model Builder** window, under **Results** click **Boundary Electrode Potential with Respect to Ground (liion)**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

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

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** check box. In the associated text field, type `Cell voltage (V)`.

6 Select the **Two y-axes** check box.

7 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Point Graph 1

1 In the **Model Builder** window, expand the **Boundary Electrode Potential with Respect to Ground (liion)** node, then click **Point Graph 1**.

2 In the **Settings** window for **Point Graph**, click to expand the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
Voltage

Point Graph 2

1 Right-click **Results>Boundary Electrode Potential with Respect to Ground (liion)> Point Graph 1** and choose **Duplicate**.

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)> Definitions>Variables>i_app - Applied battery cell current density - A/m²**.

3 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** check box.

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

Legends
Current

5 In the **Boundary Electrode Potential with Respect to Ground (liion)** toolbar, click **Plot**.

1D Plot Group 6

Now reproduce the rest of the plots in the model documentation for the discharge/charge cycle, starting with a plot for comparing the different voltage losses (Figure 6).

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

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

3 From the **Dataset** list, choose **None**.

Line Graph 1

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

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

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

5 In the **Times (s)** list, select **10**.

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

7 Locate the **y-Axis Data** section. In the **Expression** text field, type `phil+0.148`.

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

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

10 In the table, enter the following settings:

Legends
phil+0.148

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `liion.eta_per1`.

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

Legends
eta

Line Graph 3

1 Right-click **Line Graph 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 In the **Times (s)** list, select **1990**.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `phil+0.558`.

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

Legends
phil+0.558

1D Plot Group 6

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

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box. In the associated text field, type `x`.

4 Select the **y-axis label** check box. In the associated text field, type `Voltage (V)`.

5 In the **1D Plot Group 6** toolbar, click  **Plot**.

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 7).

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

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

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

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electrolyte Salt Concentration (liion)** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **Legends** section.

3 Select the **Show legends** check box.

Electrolyte Salt Concentration (liion)

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

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box. In the associated text field, type `x`.

4 Select the **y-axis label** check box. In the associated text field, type `Electrolyte concentration, cl`.

5 In the **Electrolyte Salt Concentration (liion)** toolbar, click **Plot**.

1D Plot Group 7

This plot shows the concentration profile within the particles in the electrodes (Figure 8).

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

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

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

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

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.

8 Select the **x-axis label** check box. In the associated text field, type `x`.

9 Select the **y-axis label** check box. In the associated text field, type `cs (mol//m<sup>3</sup>)`.

Line Graph 1

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

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>Particle intercalation> liion.cs_surface - Insertion particle concentration, surface - mol/m³**.

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

Line Graph 2

1 In the **Model Builder** window, right-click **1D Plot Group 7** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>Particle intercalation> liion.cs_center - Insertion particle concentration, center - mol/m³**.

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

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

7 In the **1D Plot Group 7** toolbar, click **Plot**.

8 Click the **Zoom Extents** button in the **Graphics** toolbar.

GLOBAL DEFINITIONS

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 2.0 V.

Parameters 1

Begin by adding a global current variable.

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
C	1	1	C-rate factor for the parametric study

DEFINITIONS (COMP1)

Also, add a variable for the discharge current.

Variables (Positive Current Collector)

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Variables (Positive Current Collector)**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
i_app_p	C*i_1C	A/m²	Discharge current for the parametric study

Integration 1 (intop1)

Using a integration operator you can access the cell voltage at the positive current collector boundary during the computation.

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 **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

5 In the **Operator name** text field, type `PositiveCC`.

LITHIUM-ION BATTERY (LIION)

Electrode Current Density 1

Now add a second Electrode Current Density boundary condition node, by duplicating the existing one, for use in a second study.

Electrode Current Density 2 - Study 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** right-click **Electrode Current Density 1** and choose **Duplicate**.

2 In the **Settings** window for **Electrode Current Density**, type `Electrode Current Density 2 - Study 2` in the **Label** text field.

3 Locate the **Electrode Current Density** section. In the $i_{n,\mathrm{s}}$ text field, type `-i_app_p`.

Electrode Current Density 1 - Study 1

1 In the **Model Builder** window, click **Electrode Current Density 1**.

2 In the **Settings** window for **Electrode Current Density**, type `Electrode Current Density 1 - Study 1` in the **Label** text field.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Time Dependent with Initialization**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 2** 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 `0 40000`.

Disable the first Electrode Current Density node in this study.

4 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

5 In the tree, select **Component 1 (comp1)>Lithium-Ion Battery (liion)> Electrode Current Density 1 - Study 1**.

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

Similarly, if you choose to run Study 1 again later, you need to disable the second Electrode Current Density node in that study.

Parametric Sweep

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

Modify the default solver.

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 (C-rate factor for the parametric study)	`0.1 1 2 4`	

Solution 3 (sol3)

1 In the **Study** toolbar, click **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 **Solution 3 (sol3)** node.

3 Right-click **Study 2>Solver Configurations>Solution 3 (sol3)>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.PositiveCC(comp1.phis)<2.0	True (>=1)	√	Stop expression 1

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 better resolution for the discharge curves.

Store the actual steps taken by the solver to make sure to capture any sudden steep voltage changes.

9 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 3 (sol3)** click **Time-Dependent Solver 1**.

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

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

Store only every 3rd time step. This reduces the size of the stored solution and the size of model file.

12 In the **Store every Nth step** text field, type 3.

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

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

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

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

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

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

3 From the **Dataset** list, choose **Study 2/Parametric Solutions 1 (sol5)**.

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

Point Graph 1

1. Right-click **1D Plot Group 8** and choose **Point Graph**.
2. Select Boundary 4 only.
3. 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>phis - Electric potential - V**.
4. 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.
5. In the **Expression** text field, type `(t[s]/1[h])*i_app_p`.
6. Locate the **Legends** section. Select the **Show legends** check box.
7. From the **Legends** list, choose **Evaluated**.
8. In the **Legend** text field, type `eval(C) C`.
9. In the **1D Plot Group 8** toolbar, click **Plot**.

1D Plot Group 8

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

1. In the **Model Builder** window, click **1D Plot Group 8**.
2. In the **Settings** window for **1D Plot Group**, locate the **Title** section.
3. From the **Title type** list, choose **Manual**.
4. In the **Title** text area, type `Discharge curves`.
5. Locate the **Plot Settings** section.
6. Select the **x-axis label** check box. In the associated text field, type `Capacity (Ah/m<sup>2</sup>)`.
7. Select the **y-axis label** check box. In the associated text field, type `Voltage (V)`.
8. Locate the **Axis** section. Select the **Manual axis limits** check box.
9. In the **x minimum** text field, type `0`.
10. In the **x maximum** text field, type `19`.
11. In the **y minimum** text field, type `2.0`.
12. In the **y maximum** text field, type `4.4`.
13. In the **1D Plot Group 8** toolbar, click **Plot**.