



# Lithium-Ion Battery Rate Capability

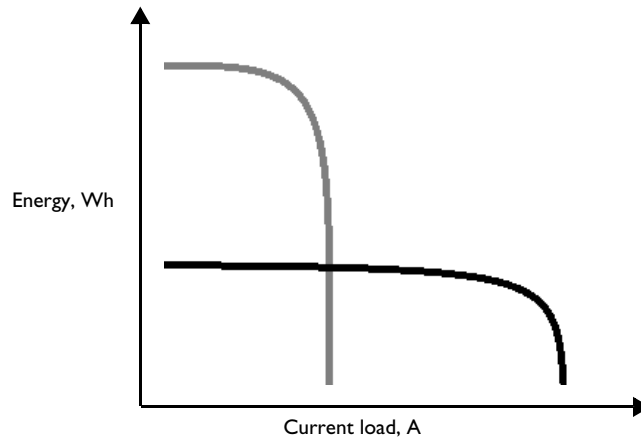
## Introduction

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A battery's possible energy and power outputs are critical to consider when deciding in which type of device it can be used.

A cell with high rate capability is able to generate a considerable amount of power, as it suffers from little polarization (voltage loss) even at high current loads. In contrast, a low rate-capability cell has the opposite behavior. The former cell type is said to be power optimized, while the latter type is energy optimized.

Characteristic for energy-optimized cells is that these have more capacity, and are thus able to supply more energy, but only for mild loads. Therefore, energy-optimized batteries are more suitable for portable electronics, for example, cell phones. The power energy-optimized ones fits, for example, power-demanding hybrid-electric vehicles better. The difference between these two types of cells is illustrated in [Figure 1](#).



*Figure 1: Comparison of energy outputs. Energy optimized cells (gray) can supply more energy but for lower current loads. Power optimized cells (black) work fine for higher current loads but can only provide a fraction of the energy.*

This application performs a rate capability investigation of two lithium-ion battery cell designs using the Lithium-Ion Battery interface. You can also learn more about how to study rate capability with the [Lithium-Ion Battery Internal Resistance](#) application.

## *Model Definition*

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The model is set up for both MCMB/LMO and LTO/NMC battery cells. The materials are available from the Battery Material Library and mainly default settings are selected.

The model domains consist of:

- Negative porous electrode:
  - Cell 1) Graphite, MCMB ( $\text{Li}_x\text{C}_6$  graphite) active material and electronic conductor.
  - Cell 2) Lithium–titanate, LTO ( $\text{Li}_4\text{Ti}_5\text{O}_{12}$ ) active material and electronic conductor.
- Separator.
- Positive porous electrode:
  - Cell 1) LMO ( $\text{LiMn}_2\text{O}_4$  spinel) active material, electronic conductor, and filler.
  - Cell 2) NMC ( $\text{LiNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$ ) active material, electronic conductor, and filler.
- Electrolyte: 1.0 M  $\text{LiPF}_6$  in EC:DEC (1:1 by weight)

The upper and lower cut-off voltages are set to 4.1 V and 3.3 V, respectively, for MCMB/LMO and 3.3 V and 0.5 V, respectively, for LTO/NMC. The cut-off voltages correspond to the potential difference between the open-circuit potentials of the positive and negative electrode active materials when the battery is either completely charged or fully discharged.

The Lithium-Ion Battery interface accounts for:

- Electronic 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
- Material transport within the spherical particles that form the electrodes
- Butler-Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium potential.

To investigate the rate capability, the battery is discharged from its fully charged state and charged from its fully discharge state. This is done for different current loads, defined in terms of C-rate with 1C being the current load to discharge a fully charged battery completely in 1 hour. This model bases the C-rate on the battery capacity,  $Q_B$ . For a 12 Ah battery 1C is thus equal to 12 A. The same definition is used in the Initial Cell Charge Distribution feature that is used in this model. It is also this feature that allows you to have initial cell state-of-charge (SOC) as a model input.

The energy and power outputs during the discharge are calculated and investigated in a Ragone plot. A Global ODEs and DAEs interface is used to calculate the energy output according to [Equation 1](#).

$$W = \int_0^t (I \cdot E_{\text{cell}}) dt \quad (1)$$

The power output is computed by dividing the energy with the total discharge time.

An Event interface is also used to restrict the operation of the battery within the upper and lower cut-off voltages.

More battery parameters and additional variable definitions used here are found in the [Lithium-Ion Battery Seed](#) application.

#### **STUDY SETTINGS**

A parametric sweep where the current load is varied is included in the existing study.

#### *Results and Discussion*

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The current loads applied on the cell are 0.01C, 0.1C, 0.5C, 1C, 2C, 5C, and 10C. At discharge the initial cell voltage is set at the upper cut-off voltage, 4.1 V, and at charge to the lower cut-off voltage, 3.3 V, for the MCMB/LMO battery cell. In [Figure 2](#), the cell voltage for the discharge loads is shown for the MCMB/LMO cell. A clear increase in

polarization (voltage drop) with increased load is observed. Compared to the open-circuit voltage curve, the capacity utilization decreases considerably with increased load as well.

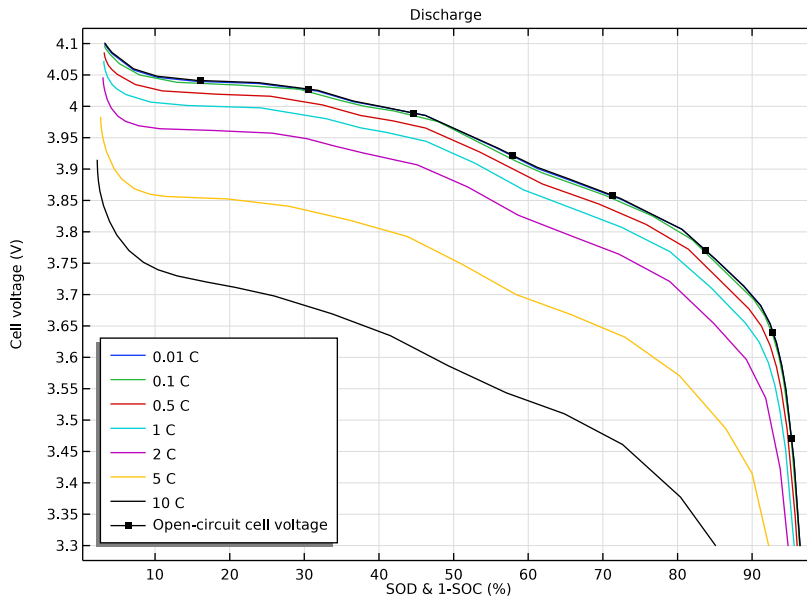


Figure 2: Cell voltage during 0.01C, 0.1C, 1C, 2C, 5C, and 10C discharge current load for the MCMB/LMO battery cell.

For the LTO/NMC battery cell, the initial cell voltage is set to the upper cut-off voltage, 3.2 V, at discharge and to the lower cut-off voltage, 0.5 V, at charge. In Figure 3, the cell voltage for the discharge loads is shown for the LTO/NMC cell. The observed increase in

polarization with current load is slightly higher for this battery design. Less capacity is also discharged.

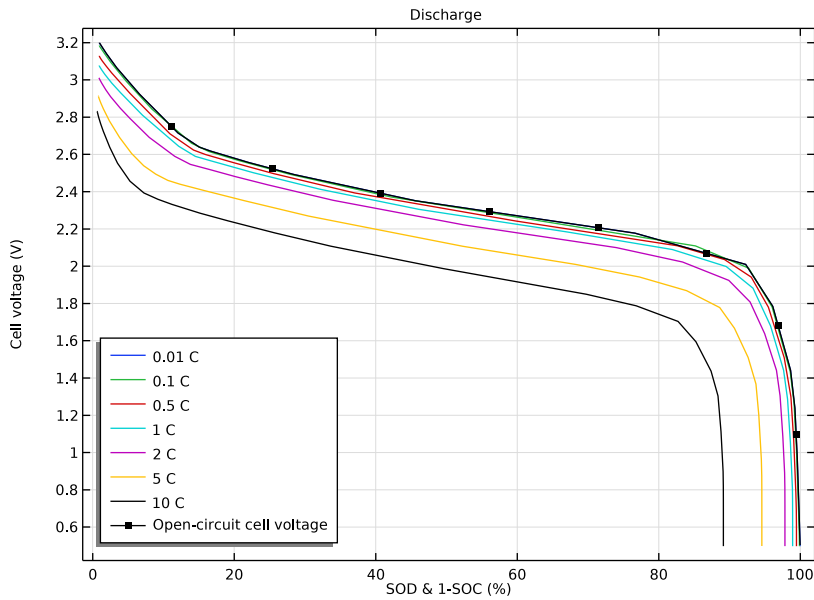
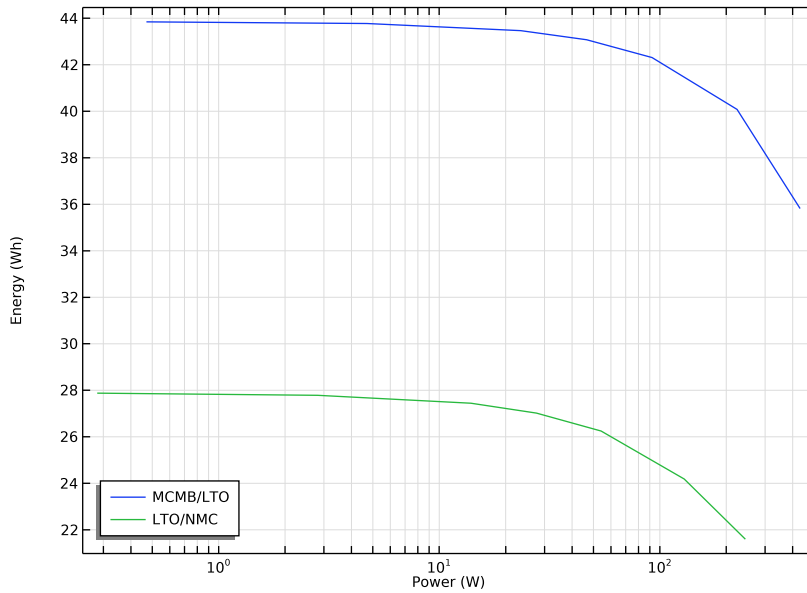


Figure 3: Cell voltage during 0.01C, 0.1C, 1C, 2C, 5C, and 10C discharge current load for the LTO/NMC battery cell.

Figure 4 is a Ragone plot displaying both battery designs' energy versus power output. The shape of the plot is characteristic for batteries. With increased energy output less power is obtained and vice versa. The shape of the Ragone plot can change drastically if the battery design is altered. A comparison of the MCMB/LMO and LTO/NMC data shows that the energy density is considerably lower in the LTO/NMC cell. This is mainly explained by the lower cell voltage of the cell (see Figure 2 and Figure 3). Improved rate capability would shift the slope further to the right along the x-axis, at the same time as the whole curve is shifted downward. The LTO/NMC cell has, despite the lower energy density, also worse rate capability. The rather small change in energy density with current load (~10%) for both cells indicates that both are rather power-optimized. To achieve

better rate capability other design features than electrode chemistry can be changed, this is described in the [Lithium-Ion Battery Internal Resistance](#) application.



*Figure 4: Ragone plot for the MCMB/LMO and LTO/NMC battery cells.*

The charge behavior is normally harder to put into the context of rate capability. This is illustrated for the MCMB/LMO battery cell in [Figure 5](#). The polarization is slightly more pronounced compared to discharge. However, most striking is that the charged capacity is considerably lower than the discharged capacity (less of SOC window is utilized). This mainly has to do with the shape of the open-circuit potential curves of the electrode active materials. The low capacity usage normally means that the active electrode material can handle peaks of medium-high current load, where the cell voltage exceeds that of a fully

charged cell ( $>4.1$  V), given that the voltage is within the stability window of the electrolyte.

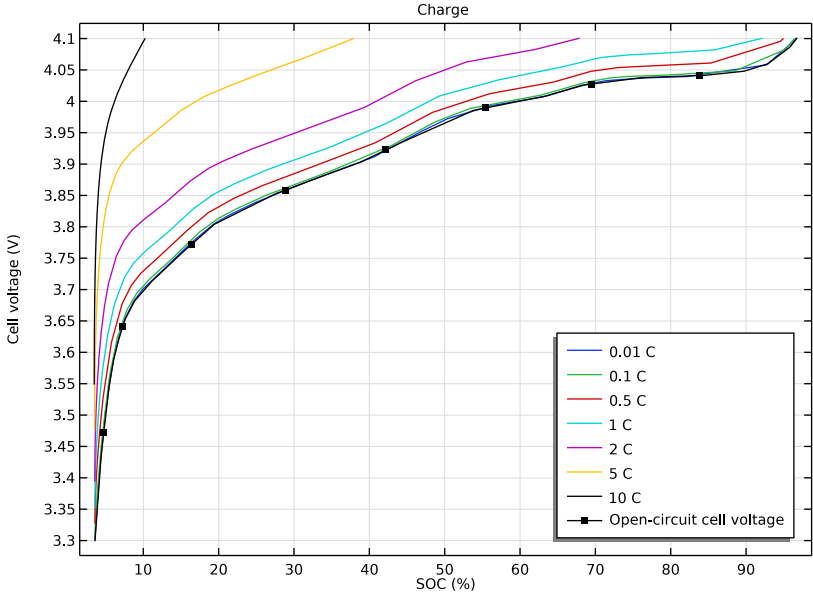


Figure 5: Cell voltage during 0.01C, 0.1C, 1C, 2C, 5C, and 10C charge current load for the MCMB/LMO battery cell.



The cell voltage at charge load for the LTO/NMC cell is displayed in Figure 6. The charged capacity is also lower than the discharged capacity for this cell design, however, the polarization is in the same magnitude as for the discharge.

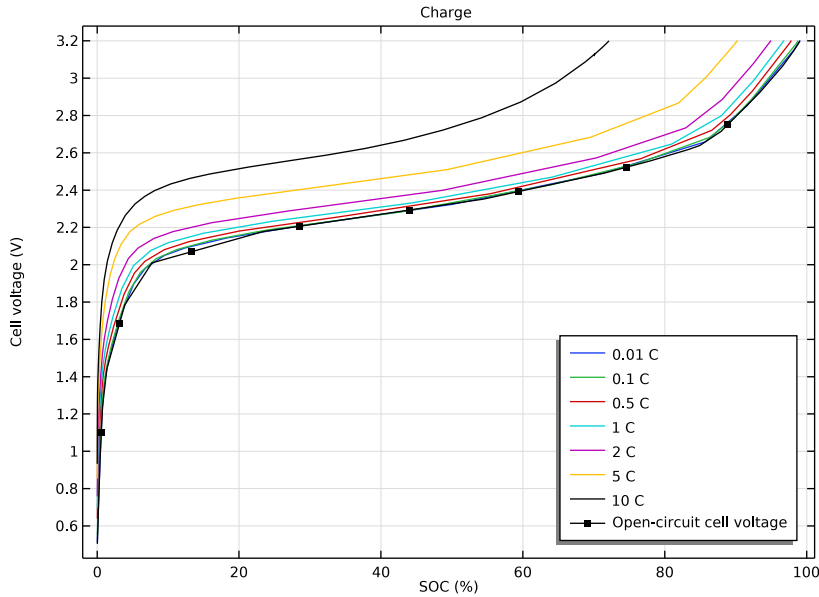


Figure 6: Cell voltage during 0.01C, 0.1C, 1C, 2C, 5C, and 10C charge current load for the LTO/NMC battery cell.

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**Application Library path:** Battery\_Design\_Module/Batteries,\_Lithium-Ion/  
li\_battery\_rate\_capability

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### *Modeling Instructions*

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#### **ROOT**

- 1 From the **File** menu, choose **Open**.
- 2 Browse to the model's Application Libraries folder and double-click the file `li_battery_seed.mph`.

## GLOBAL DEFINITIONS

Add parameters for controlling the C-rate as well as the upper and lower cut-off voltages for the battery cell.

### 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 In the table, enter the following settings:

Name	Expression	Value	Description
a	1	1	C-factor for C-rate calculation
Ecell_up	4.1[V]	4.1 V	Upper cut-off voltage
Ecell_low	3.3[V]	3.3 V	Lower cut-off voltage

Also modify the parameter value for Ecell\_init as follows:


- 4 In the table, enter the following settings:

Name	Expression	Value	Description
Ecell_init	if(a>0,Ecell_low, Ecell_up)	3.3 V	Initial cell voltage

## DEFINITIONS (COMPI)

Load the variables from a text file.

### Variables 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `li_battery_management_variables.txt`.

## LITHIUM-ION BATTERY (LIION)

### Electrode Current -Current Load Rates

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **Electrode Current 1**.
- 2 In the **Settings** window for **Electrode Current**, type Electrode Current -Current Load Rates in the **Label** text field.

**3** Locate the **Electrode Current** section. In the  $I_{s,total}$  text field, type `li.ion.I_1C*a`.

#### *Porous Electrode 1*

In the **Particle Intercalation** nodes of the **Porous Electrode** features, it is useful to enable fast assembly in the particle dimension option. This option enables an alternative method for assembling of the diffusion equation in the particle dimension, that typically decreases computation time for 1D models. Note that the same diffusion equations are solved for regardless of assembly method. Additionally, specify the reference exchange current density for the electrode kinetics in the **Porous Electrode Reaction** nodes.

#### *Particle Intercalation 1*

- 1** In the **Model Builder** window, expand the **Porous Electrode 1** node, then click **Particle Intercalation 1**.
- 2** In the **Settings** window for **Particle Intercalation**, click to expand the **Particle Discretization** section.
- 3** Select the **Fast assembly in particle dimension** check box.

#### *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 **Electrode Kinetics** section.
- 3** In the  $i_{0,ref}(T)$  text field, type `i0ref_neg`.

#### *Particle Intercalation 2*

- 1** In the **Model Builder** window, expand the **Porous Electrode 2** node, then click **Particle Intercalation 1**.
- 2** In the **Settings** window for **Particle Intercalation**, locate the **Particle Discretization** section.
- 3** Select the **Fast assembly in particle dimension** check box.


#### *Porous Electrode Reaction 2*

- 1** In the **Model Builder** window, click **Porous Electrode Reaction 1**.
- 2** In the **Settings** window for **Porous Electrode Reaction**, locate the **Electrode Kinetics** section.
- 3** In the  $i_{0,ref}(T)$  text field, type `i0ref_pos`.

### **COMPONENT 1 (COMP1)**

For the rate capability investigation a Global equation that calculates the cumulative energy is set up.

## ADD PHYSICS

- 1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.
- 3 In the tree, select **Mathematics>ODE and DAE Interfaces>Global ODEs and DAEs (ge)**.
- 4 Click **Add to Component 1** in the window toolbar.

## CUMULATIVE ENERGY

In the **Settings** window for **Global ODEs and DAEs**, type **Cumulative Energy** in the **Label** text field.


### *Global Equations 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Cumulative Energy (ge)** click **Global Equations 1**.
- 2 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.
- 3 In the table, enter the following settings:

Name	f(u,ut,utt,t) (I)	Initial value (u_0) (I)	Initial value (u_t0) (I/s)	Description
W	Wt-abs(pos_cc(liion.I ts_ec1))*Ecell	0	0	

- 4 Locate the **Units** section. Click  **Define Dependent Variable Unit**.
- 5 In the **Dependent variable quantity** table, enter the following settings:

Dependent variable quantity	Unit
Custom unit	A*V*s

- 6 Click  **Define Source Term Unit**.
- 7 In the **Source term quantity** table, enter the following settings:


Source term quantity	Unit
Custom unit	A*V

## COMPONENT 1 (COMP1)

Add an **Events** interface to control the cut-off voltages.

## ADD PHYSICS

- 1 Go to the **Add Physics** window.

- 2 In the tree, select **Mathematics>ODE and DAE Interfaces>Events (ev)**.
- 3 Click **Add to Component I** in the window toolbar.
- 4 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

## EVENTS (EV)


### *Implicit Event 1*

Define the cut-off at charge, STOP\_CH.

- 1 Right-click **Component I (comp1)>Events (ev)** and choose **Implicit Event**.
- 2 In the **Settings** window for **Implicit Event**, locate the **Event Conditions** section.
- 3 In the **Condition** text field, type STOP\_CH>0.


### *Implicit Event 2*

Define the cut-off at discharge, STOP\_DCH.

- 1 In the **Physics** toolbar, click  **Global** and choose **Implicit Event**.
- 2 In the **Settings** window for **Implicit Event**, locate the **Event Conditions** section.
- 3 In the **Condition** text field, type STOP\_DCH>0.

### *Indicator States 1*

Define the values of cell voltage, Ecell, for the cut-offs.

- 1 In the **Physics** toolbar, click  **Global** and choose **Indicator States**.
- 2 In the **Settings** window for **Indicator States**, locate the **Indicator Variables** section.
- 3 In the table, enter the following settings:

Name	$g(v,vt,vtt,t)$	Initial value (u0)	Description
STOP_DCH	Ecell_low-comp1.Ecell	0	
STOP_CH	comp1.Ecell-Ecell_up	0	


## STUDY 1

Start by adding a Parametric sweep to the Study node.

In order to investigate several current loads, use a number of high initial voltages with discharge currents, and a number of low initial voltages with charge currents. Voltages and current loads are available in a text file.

### *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  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `li_battery_rate_capability_parametric_sweep.txt`.

#### *Step 1: Current Distribution Initialization*

Shut off the Events and Cumulative Energy Density interfaces in the first study step.

- 1 In the **Model Builder** window, click **Step 1: Current Distribution Initialization**.
- 2 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.
- 3 In the table, clear the **Solve for** check boxes for **Cumulative Energy (ge)** and **Events (ev)**.


#### *Step 2: Time Dependent*

Enter the times the model should be solved for in the Time Dependent (second) study step.

- 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 0 500000.

#### *Solution 1 (sol1)*

Select the following time-dependent settings to speed up the simulation and to save the solution.


- 1 In the **Study** toolbar, click  **Show Default Solver**.  
Store the actual steps taken by the solver to make sure to capture any sudden steep voltage changes.
- 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**.  
Store only every 3rd time step. This reduces the solution and resulting file size.
- 5 In the **Store every Nth step** text field, type 3.
- 6 Click to expand the **Time Stepping** section. Select the **Initial step** check box.
- 7 In the **Event tolerance** text field, type 1e-3.
- 8 Select the **Nonlinear controller** check box.

- 9 Click to expand the **Output** section. Right-click **Time-Dependent Solver 1** and choose **Stop Condition**.  
Add a Stop Condition defined by the Events interface.
- 10 In the **Settings** window for **Stop Condition**, locate the **Stop Events** section.
- 11 In the table, select the **Active** check boxes for **Events (ev)/Implicit Event 1** and **Events (ev)/Implicit Event 2**.
- 12 Locate the **Output at Stop** section. Clear the **Add warning** check box.


#### **MESH 1**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
- 2 In the **Settings** window for **Mesh**, locate the **Mesh Settings** section.
- 3 From the **Sequence type** list, choose **User-controlled mesh**.

#### *Size 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size 1**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Predefined** list, choose **Extremely fine**.
- 4 Click  **Build All**.

#### **STUDY 1**

- 1 In the **Model Builder** window, click **Study 1**.
- 2 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 3 Clear the **Generate default plots** check box.
- 4 Clear the **Generate convergence plots** check box.
- 5 In the **Study** toolbar, click  **Compute**.

#### *Parametric Solutions 1 (sol3)*


In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Parametric Solutions 1 (sol3)** and choose **Solution>Copy**.

#### *Copied Parametric Solutions MCBM/LMO*

- 1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Parametric Solutions 1 - Copy 1 (sol18)**.
- 2 In the **Settings** window for **Solution**, type Copied Parametric Solutions MCBM/LMO in the **Label** text field.

## RESULTS

### *Cell Voltages Discharge MCMB/LMO*

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Cell Voltages Discharge MCMB/LMO in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **None**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 5 In the **Title** text area, type Discharge.
- 6 Locate the **Plot Settings** section. Select the **x-axis label** check box.
- 7 In the associated text field, type SOD & 1-SOC (%).
- 8 Select the **y-axis label** check box.
- 9 In the associated text field, type Cell voltage (V).
- 10 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

### *Global I*

- 1 Right-click **Cell Voltages Discharge MCMB/LMO** and choose **Global**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study I/Copied Parametric Solutions MCMB/LMO (sol18)**.
- 4 From the **Parameter selection (a)** list, choose **From list**.
- 5 In the **Parameter values (a (C))** list, choose **-0.01, -0.1, -0.5, -1, -2, -5, and -10**.
- 6 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (comp1)>Definitions>Variables>Ecell - Battery cell voltage - V**.
- 7 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Inner solutions**.
- 8 From the **Parameter** list, choose **Expression**.
- 9 In the **Expression** text field, type  $(1-SOC_{cell}) * 100$ .
- 10 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
- 11 In the table, enter the following settings:

<b>Legends</b>
0.01 C
0.1 C
0.5 C
1 C



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**Legends**

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2 C

5 C

10 C

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### *Global 2*

- 1 In the **Model Builder** window, right-click **Cell Voltages Discharge MCMB/LMO** and choose **Global**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Copied Parametric Solutions MCMB/LMO (sol18)**.
- 4 From the **Parameter selection (a)** list, choose **First**.
- 5 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>EOCVcell - Open-circuit cell voltage, coulombic - V**.
- 6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Inner solutions**.
- 7 From the **Parameter** list, choose **Expression**.
- 8 In the **Expression** text field, type  $(1 - SOC_{cell}) * 100$ .
- 9 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Black**.
- 10 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.
- 11 Locate the **Legends** section. From the **Legends** list, choose **Manual**.
- 12 In the table, enter the following settings:

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**Legends**

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Open-circuit cell voltage

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- 13 In the **Cell Voltages Discharge MCMB/LMO** toolbar, click  **Plot**.

### *Global Evaluation 2*

Create a Ragone plot as follows:


- 1 In the **Results** toolbar, click  **Global Evaluation**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.
- 4 From the **Parameter selection (a)** list, choose **Manual**.
- 5 In the **Parameter indices (1-14)** text field, type range (1, 1, 7).
- 6 From the **Time selection** list, choose **Last**.

7 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
W	W*h	Energy
W/t	W	Power

8 Click  next to  **Evaluate**, then choose **New Table**.


#### *Ragone Plot*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Ragone Plot in the **Label** text field.
- 3 Locate the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Plot Settings** section. Select the **x-axis label** check box.
- 5 In the associated text field, type Power (W).
- 6 Select the **y-axis label** check box.
- 7 In the associated text field, type Energy (Wh).
- 8 Locate the **Axis** section. Select the **x-axis log scale** check box.

#### *Table Graph 1*

- 1 Right-click **Ragone Plot** and choose **Table Graph**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Table** list, choose **Table 2**.
- 4 From the **x-axis data** list, choose **Power (W)**.
- 5 From the **Plot columns** list, choose **Manual**.
- 6 In the **Columns** list, select **Energy (W\*h)**.
- 7 Click to expand the **Legends** section. Select the **Show legends** check box.
- 8 From the **Legends** list, choose **Manual**.
- 9 In the table, enter the following settings:

Legends
MCMB/LTO



10 In the **Ragone Plot** toolbar, click  **Plot**.

#### **GLOBAL DEFINITIONS**

Benchmark the MCMB/LMO cell against a LTO/NMC cell.

Add the two materials from the Battery Material Library.

## ADD 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>LTO Electrode, Li4Ti5O12 (Negative, Li-ion Battery)**.
- 4 Click the right end of the **Add to Component** split button in the window toolbar.
- 5 From the menu, choose **Add to Global Materials**.
- 6 In the tree, select **Battery>Electrodes>NMC III Electrode, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery)**.
- 7 Click the right end of the **Add to Component** split button in the window toolbar.
- 8 From the menu, choose **Add to Global Materials**.
- 9 In the **Home** toolbar, click  **Add Material** to close the **Add Material** window.

## MATERIALS

### *Material Link 2 (matlnk2)*

- 1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials** node, then click **Material Link 2 (matlnk2)**.
- 2 In the **Settings** window for **Material Link**, locate the **Link Settings** section.
- 3 From the **Material** list, choose **LTO Electrode, Li4Ti5O12 (Negative, Li-ion Battery) (mat4)**.

### *Material Link 3 (matlnk3)*

- 1 In the **Model Builder** window, click **Material Link 3 (matlnk3)**.
- 2 In the **Settings** window for **Material Link**, locate the **Link Settings** section.
- 3 From the **Material** list, choose **NMC III Electrode, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat5)**.

## GLOBAL DEFINITIONS

Adjust the upper and lower cut-off voltages to the new chemistry.

### *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 In the table, enter the following settings:

Name	Expression	Value	Description
Ecell_up	3.2[V]	3.2 V	Upper cut-off voltage
Ecell_low	0.5[V]	0.5 V	Lower cut-off voltage


## LITHIUM-ION BATTERY (LIION)

### *Initial Cell Charge Distribution 1*

The negative LTO electrode material does not cause as pronounced SEI layer formation. This means that the cyclable lithium loss at assemble and excess negative electrode material can both be set to zero.

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **Initial Cell Charge Distribution 1**.
- 2 In the **Settings** window for **Initial Cell Charge Distribution**, locate the **Battery Cell Electrode Balancing** section.
- 3 In the  $f_{\text{host,neg,ex}}$  text field, type 0.
- 4 In the  $f_{\text{cycl,loss}}$  text field, type 0.

### STUDY 1

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

### RESULTS


### *Cell Voltages Discharge LTO/NMC*

- 1 In the **Model Builder** window, right-click **Cell Voltages Discharge MCMB/LMO** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Cell Voltages Discharge LTO/NMC in the **Label** text field.

### *Global 1*

- 1 In the **Model Builder** window, expand the **Cell Voltages Discharge LTO/NMC** node, then click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.

### *Global 2*

- 1 In the **Model Builder** window, click **Global 2**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.
- 4 In the **Cell Voltages Discharge LTO/NMC** toolbar, click  **Plot**.

### *Global Evaluation 2*

Update the Ragone plot as follows:

In the **Model Builder** window, right-click **Global Evaluation 2** and choose **Evaluate>New Table**.


#### *Table Graph 2*

- 1 In the **Model Builder** window, under **Results>Ragone Plot** right-click **Table Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Table** list, choose **Table 3**.
- 4 Locate the **Legends** section. In the table, enter the following settings:


---

<b>Legends</b>
LTO/NMC

---

- 5 In the **Ragone Plot** toolbar, click  **Plot**.

#### *Ragone Plot*

- 1 In the **Model Builder** window, click **Ragone Plot**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Lower left**.
- 4 In the **Ragone Plot** toolbar, click  **Plot**.

#### *Cell Voltages Charge MCMB/LMO*

- 1 In the **Model Builder** window, right-click **Cell Voltages Discharge MCMB/LMO** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Cell Voltages Charge MCMB/LMO in the **Label** text field.
- 3 Locate the **Title** section. In the **Title** text area, type Charge.
- 4 Locate the **Plot Settings** section. In the **x-axis label** text field, type SOC (%).

#### *Global 1*


- 1 In the **Model Builder** window, expand the **Cell Voltages Charge MCMB/LMO** node, then click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 In the **Parameter values (a (C))** list, choose **0.01, 0.1, 0.5, 1, 2, 5, and 10**.
- 4 Locate the **x-Axis Data** section. In the **Expression** text field, type  $SOC_{cell} * 100$ .

#### *Global 2*

- 1 In the **Model Builder** window, click **Global 2**.

- 2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.
- 3 In the **Expression** text field, type `SOCcell*100`.

#### *Cell Voltages Charge MCMB/LMO*

- 1 In the **Model Builder** window, click **Cell Voltages Charge MCMB/LMO**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Lower right**.
- 4 In the **Cell Voltages Charge MCMB/LMO** toolbar, click  **Plot**.


#### *Cell Voltages Charge LTO/NMC*

- 1 Right-click **Cell Voltages Charge MCMB/LMO** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type `Cell Voltages Charge LTO/NMC` in the **Label** text field.

#### *Global 1*

- 1 In the **Model Builder** window, expand the **Cell Voltages Charge LTO/NMC** node, then click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.

#### *Global 2*

- 1 In the **Model Builder** window, click **Global 2**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.
- 4 In the **Cell Voltages Charge LTO/NMC** toolbar, click  **Plot**.