Created in COMSOL Multiphysics 6.1

Lithium-Ion Battery Rate Capability

Introduction

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. This way of plotting energy versus power (or current if the cell voltage stays fairly constant throughout the load cycle) is also called a Ragone plot.

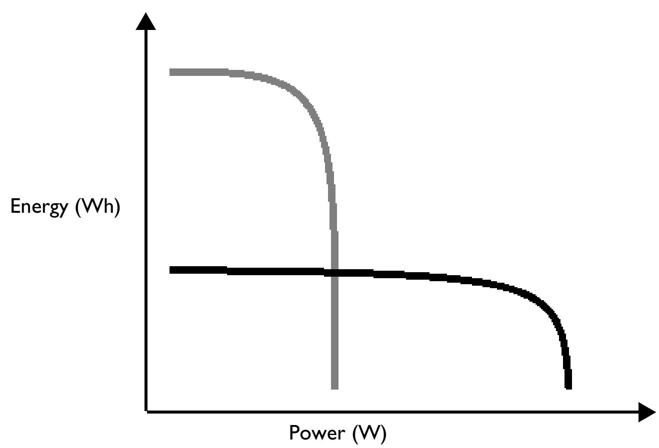


Figure 1: Comparison of energy outputs. Energy optimized cells (gray) can supply more energy but for lower current loads. Power optimized cells (black) work fine for higher power (current loads) but can only provide a fraction of the energy at low power.

This tutorial 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 tutorial, where the individual contributions to the voltage losses are analyzed more in detail.

Model Definition

The model is set up in 1D for a graphite/NMC battery cell. A more detailed description of the model can be found in Lithium-Ion Battery Base Model in 1D. Discharge curves are simulated for a range of current magnitudes (C-rates) for two different battery designs: an energy-optimized cell and a power-optimized cell. Changing from the energy-optimized case to the power-optimized case is done in the model by lowering the cross-sectional charge capacity parameter from 40 Ah/m^2 to 20 Ah/m^2, which results in reducing the electrode thickness in the geometry by half.

The volumetric energy (J/m^3) and power (W/m^3) outputs during the discharge, starting from fully charged conditions, 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.

$$W = \frac{\int_0^t (I \cdot E_{\mathrm{cell}})dt}{L_{\mathrm{cell}}} \tag{1}$$

Where the length L_{cell} of the cell is calculated as

$$L_{\mathrm{cell}} = L_{\mathrm{neg}} + L_{\mathrm{sep}} + L_{\mathrm{pos}} + L_{\mathrm{ccs}}/2 \tag{2}$$

where L_{ccs} is the sum both thickness of the positive and negative current collector foils in jelly roll. (The factor 1/2 stems from the configuration of a typical jelly roll where each metal foil is being coated on both sides by the same electrode layer.)

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

An Event interface is also used for implementing an accurate stop condition in the solver for when the cell voltage goes below a threshold level equal to the open circuit voltage at 0% cell state of charge.

Results and Discussion

Figure 2 shows the discharge curves of the energy optimized 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.

At 10C the capacity utilization decrease is substantial; less than 10% of the available capacity has been utilized.

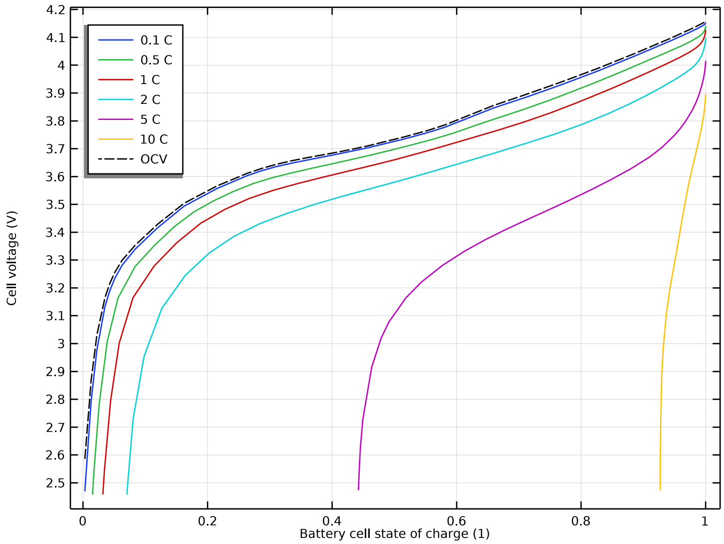


Figure 2: Solid lines: Cell voltages versus SOC during discharge at various C-rates of the energy-optimized cell. Dashed line: Corresponding open circuit voltage (OCV) versus SOC.

To investigate what could be the reason for the large capacity decrease at 10C, we plot the electrolyte salt concentration at the end of this discharge simulation in Figure 3. Toward the right in the figure a noticeable drop in electrolyte concentration is seen, and for the 25 rightmost micrometers, the concentration is close to 0. This region corresponds to the inner parts of the positive electrode in the model, and the reason for the depletion of lithium ions is the prolonged fast lithium intercalation rate, in combination with an insufficient lithium ion transport from the negative electrode through the separator. .

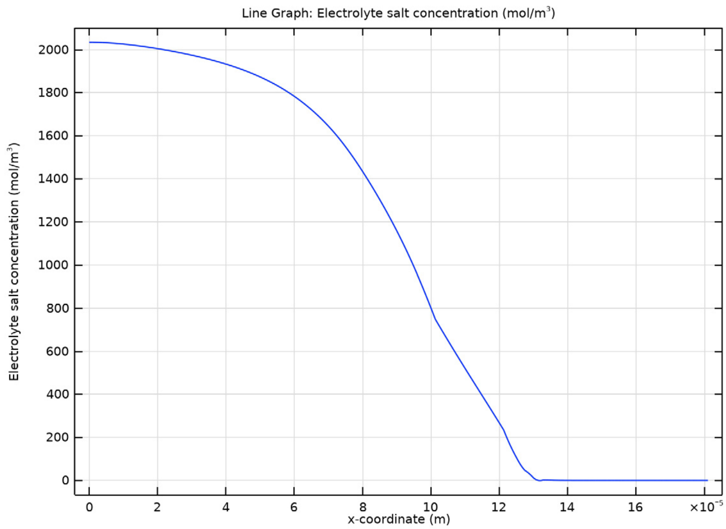


Figure 3: Electrolyte concentration at the end of discharge at 10C of the energy-optimized cell.

The depletion of lithium ions will result in a very low local electrolyte conductivity, and this is manifested in Figure 4 where a corresponding steep potential drop is seen. This steep potential drop will result in the interior of the electrode not being utilized at all toward the end of discharge at high rates for the energy-optimized cell.

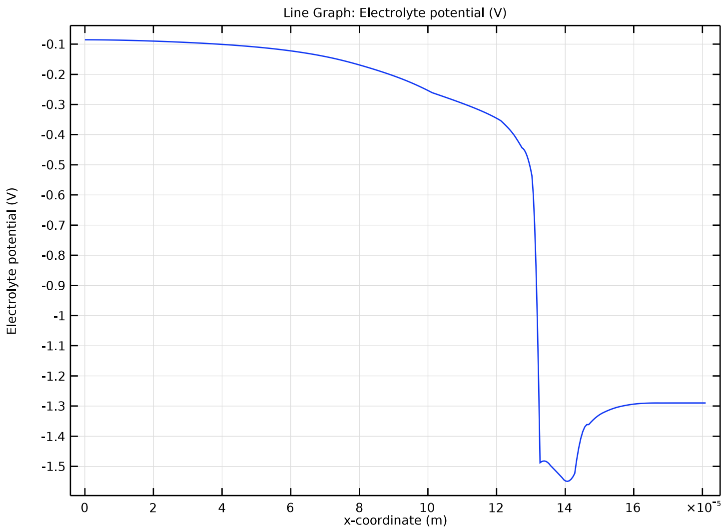


Figure 4: Electrolyte phase potential at the end of discharge at 10C of the energy-optimized cell.

Figure 5 shows the discharge curves for the power-optimized case, using half as thick electrodes as in the energy optimized case. These thinner electrodes now allows for utilizing about 60% of the available charge at the highest 10C discharge rate, as opposed to less than 10% for the energy-optimized case.

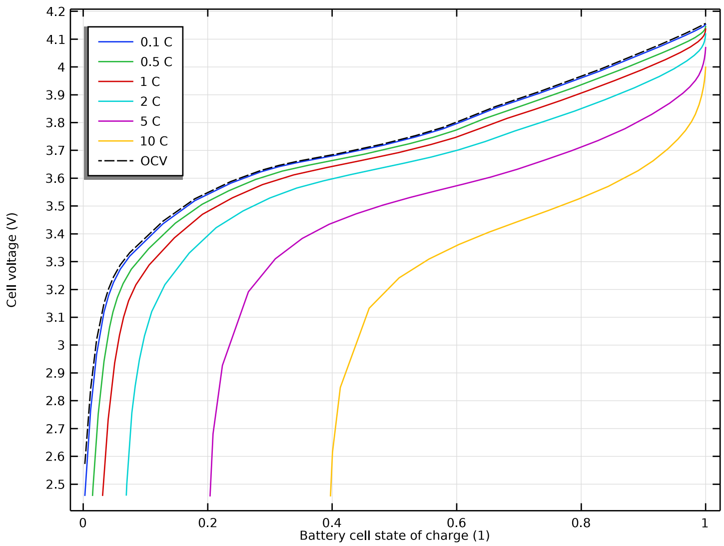


Figure 5: Solid lines: Cell voltages versus SOC during discharge at various C-rates of the power-optimized cell. Dashed line: Corresponding open circuit voltage (OCV) versus SOC.

Finally, the energy versus power Ragone plot is plotted in Figure 6. For power levels above around 200 W/m^3, the power-optimized battery starts to outperform the energy-optimized cell.

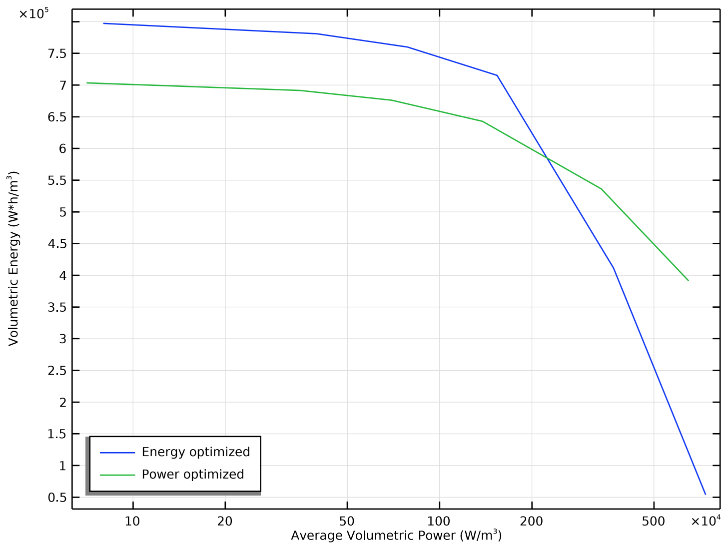


Figure 6: Volumetric energy versus power Ragone plot, comparing the energy optimized to the power optimized cell.

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

Modeling Instructions

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

2 In the **Application Libraries** window, select **Battery Design Module>Batteries, Lithium-Ion>lib_base_model_1d** in the tree.

3 Click **Open**.

In this tutorial we will discharge the battery model you just opened at various C-rates from 100% state of charge. The first simulations will be run for an energy-optimized cell, with a large cross-sectional cell capacity. Those results will then be compared with a power-optimized cell, featuring thinner electrodes.

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. In the table, enter the following settings:

Name	Expression	Value	Description
q_cell	40[A*h/m^2]	1.44E5 C/m^2	Cross-sectional cell capacity
soc_init	100[%]	1	Initial SOC
C_rate	1	1	Discharge rate
I_app	-C_rate*I_1C	-40 A/m^2	Applied cell current density
L_ccs	10[um]	1E-5 m	Thickness of current collectors (for Ragone plot)

COMPONENT 1 (COMP1)

In the **Model Builder** window, expand the **Component 1 (comp1)** node.

LITHIUM-ION BATTERY (LIION)

Electrode Current Density 1

Modify the cell current density boundary condition as follows:

1. In the **Model Builder** window, expand the **Component 1 (comp1)>Lithium-Ion Battery (liion)** node, then click **Electrode Current Density 1**.
2. In the **Settings** window for **Electrode Current Density**, locate the **Electrode Current Density** section.
3. In the $i_{n,\mathrm{s}}$ text field, type `I_app`.

COMPONENT 1 (COMP1)

Add additional physics interfaces for adding an integral equation for accumulated energy, and for setting up an event-based stop condition.

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.

5 In the tree, select **Mathematics>ODE and DAE Interfaces>Events (ev)**.

6 Click **Add to Component 1** in the window toolbar.

7 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

CUMULATIVE ENERGY

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Global ODEs and DAEs (ge)**.

2 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) (1)	Initial value (u_0) (1)	Initial value (u_t0) (1/s)	Description
W	d(W,t)-abs(I_app*E_cell)	0	0	

The above equation sets the time derivative of the accumulated energy to equal the power density output (current density times voltage) of the cell. The expression is marked in orange, indicating unit issues. The equation is formulated per cell area unit (m^2) of the jelly roll. Set the units of the dependent variable W and the equation expression as follows:

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	J/m^2

6 Click **Define Source Term Unit**.

7 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	W/m^2

EVENTS (EV)

Add an indicator state and an implicit event which will be used to control when to stop the simulation. (It is also possible to add stop conditions in the time-dependent solver without the using of events, but that would typically be less accurate).

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Events (ev)**.

Indicator States 1

1 In the **Physics** toolbar, click **Global** and choose **Indicator States**.

The indicator state is defined to turn positive when the cell voltage drops below the OCV voltage at 0% SOC.

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	E_ocv_cell_0-E_cell	0	

Implicit Event 1

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.

STUDY 1

Add a parametric sweep for a range of C-rates as follows:

Parametric Sweep

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

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

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
C_rate (Discharge rate)	0.1 0.5 1 2 5 10	

Step 1: Time Dependent

Set the solver maximum solver time to be inversely proportional to the C-rate as follows:

1 In the **Model Builder** window, click **Step 1: Time Dependent**.

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

3 In the **Output times** text field, type `0 1/C_rate`.

Solution 1 (sol1)

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

The time dependent solver will automatically shorten the time step when needed in order to resolve gradients in the model. In order to get a good resolution in the discharge curves, store the solution every 3rd time step taken by the solver. (Solving the solution every time step would require more disk space when saving the solution.)

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

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

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

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

In order to get the simulation started more easily, set the initial time step to be inversely proportional to the C-rate as follows:

6 Click to expand the **Time Stepping** section.

7 Select the **Initial step** check box. In the associated text field, type `0.001/C_rate`.

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

Finally, add a stop condition based on the event you added previously.

9 In the **Settings** window for **Stop Condition**, locate the **Stop Events** section.

10 In the table, select the **Active** check box for **Events (ev)/Implicit Event 1**.

11 Locate the **Output at Stop** section. Clear the **Add warning** check box.

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

RESULTS

Add a plot of the cell voltages vs the state of charge as follows:

Cell Voltages vs SOC

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

2 In the **Settings** window for **1D Plot Group**, type `Cell Voltages vs SOC` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

Global 1

1 Right-click **Cell Voltages vs SOC** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> E_cell - Point Probe 1 - V**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`E_cell`	`V`	`Cell voltage`

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

5 In the **Expression** text field, type `soc_cell`.

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

7 In the **Legend** text field, type `eval(C_rate) C`.

Global 2

1 In the **Model Builder** window, right-click **Cell Voltages vs SOC** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>E_ocv_cell - Open-circuit cell voltage - V**.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

4 From the **Parameter selection (C_rate)** list, choose **First**.

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

6 In the **Expression** text field, type `soc_cell`.

7 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
`OCV`

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

10 From the **Color** list, choose **Black**.

11 In the **Cell Voltages vs SOC** toolbar, click **Plot**.

Cell Voltages vs SOC

1 In the **Model Builder** window, click **Cell Voltages vs SOC**.

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

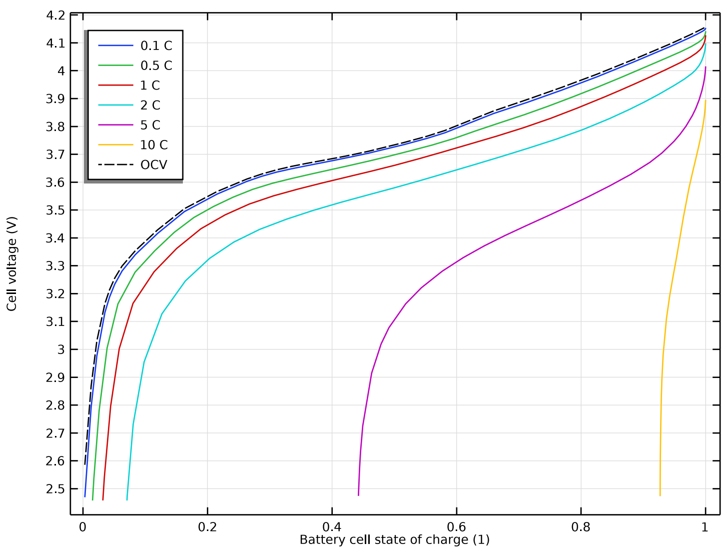
3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

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

6 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

7 In the **Cell Voltages vs SOC** toolbar, click **Plot**.



Global Evaluation 2

To create the Ragone plot (energy density vs average power density), first evaluate the energy variable at the last time point of the simulation.

In the **Results** toolbar, click **Global Evaluation**.

Ragone Plot Data Evaluation

1 In the **Model Builder** window, under **Results>Derived Values** click **Global Evaluation 1**.

2 In the **Settings** window for **Global Evaluation**, type `Ragone Plot Data Evaluation` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

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

Expression	Unit	Description
W/(L_neg+L_sep+L_pos+ L_ccs/2)	W*h/m^3	Volumetric Energy
W/t/(L_neg+L_sep+L_pos+ L_ccs/2)	W/m^3	Average Volumetric Power

Note that we are computing the volumetric values by dividing by the thickness of the cell.

5 Click ▾ next to **Evaluate**, then choose **New Table**.

Ragone Plot Data Energy Optimized Cell

1 In the **Model Builder** window, expand the **Results>Tables** node, then click **Table 2**.

2 In the **Settings** window for **Table**, type `Ragone Plot Data Energy Optimized Cell` in the **Label** text field.

Now plot the table data you just generated.

Ragone Plots

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

2 In the **Settings** window for **1D Plot Group**, type `Ragone Plots` in the **Label** text field.

3 Locate the **Axis** section. Select the **x-axis log scale** check box.

4 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

Table Graph 1

1 Right-click **Ragone Plots** and choose **Table Graph**.

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

3 From the **Table** list, choose **Ragone Plot Data Energy Optimized Cell**.

4 From the **x-axis data** list, choose **Average Volumetric Power (W/m^3)**.

5 From the **Plot columns** list, choose **Manual**.

6 In the **Columns** list, select **Volumetric Energy (W*h/m^3)**.

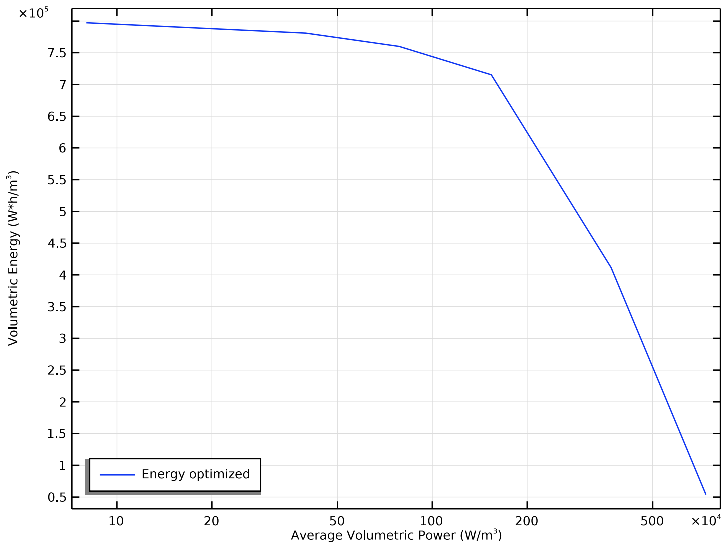
7 Click to expand the **Legends** section. Select the **Show legends** check box.

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

9 In the table, enter the following settings:

Legends
`Energy optimized`

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



The Ragone plot indicates a large decrease in output energy for large power levels (discharge currents). Reviewing the default electrolyte salt (Li ion) concentration plot at the last time point at the highest current level indicates what could be the issue.

Electrolyte Salt Concentration (liion)

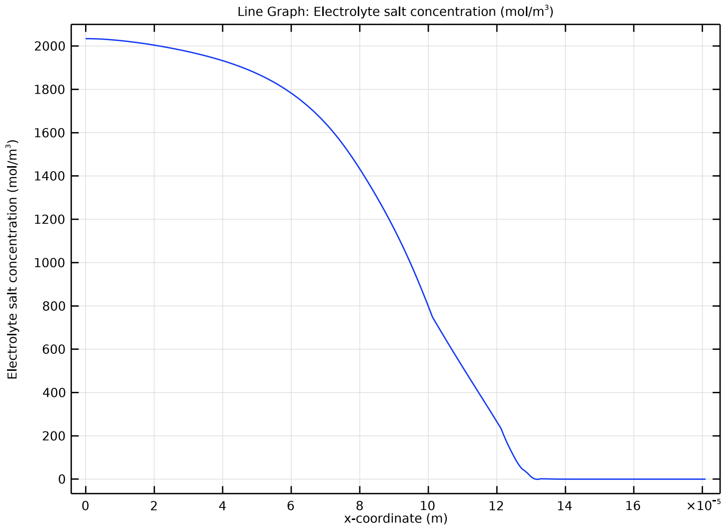
1 In the **Model Builder** window, under **Results** click **Electrolyte Salt Concentration (liion)**.

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

3 From the **Parameter selection (C_rate)** list, choose **Last**.

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

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



The concentration drops to zero in the interior of the positive electrode. Now check out the electrolyte potential plot at the same time.

Electrolyte Potential (liion)

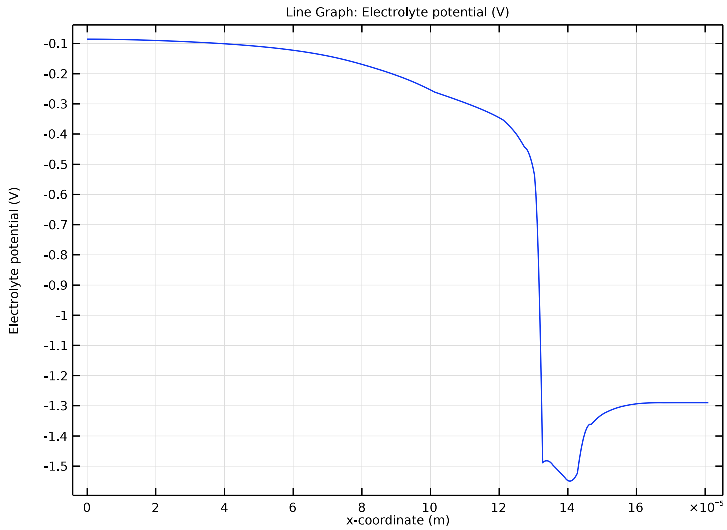
1 In the **Model Builder** window, click **Electrolyte Potential (liion)**.

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

3 From the **Parameter selection (C_rate)** list, choose **Last**.

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

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



A very large electrolyte potential drop is seen in the positive electrode. This is a result of the electrolyte conductivity dropping to essentially zero when the lithium ions are depleted in the electrolyte. As a result of this, the whole electrode cannot be utilized during discharge at high rates. We will now rerun the simulations for a power-optimized cell using thinner electrodes to see if this improves the rate capability at high currents.

GLOBAL DEFINITIONS

Parameters 1

Lower the cross-sectional cell capacity. Note that this also automatically changes the values for the electrode thicknesses (L_neg and L_pos).

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
q_cell	20[A*h/m^2]	72000 C/m²	Cross-sectional cell capacity

STUDY 1

Parametric Solutions 1 (sol2)

Before recomputing, make sure you copy the old solution for future reference.

1 In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Parametric Solutions 1 (sol2)** and choose **Solution>Copy**.

Parametric Solutions - Energy Optimized Cell

1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Parametric Solutions 1 - Copy 1 (sol9)**.

2 In the **Settings** window for **Solution**, type `Parametric Solutions - Energy Optimized Cell` in the **Label** text field.

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

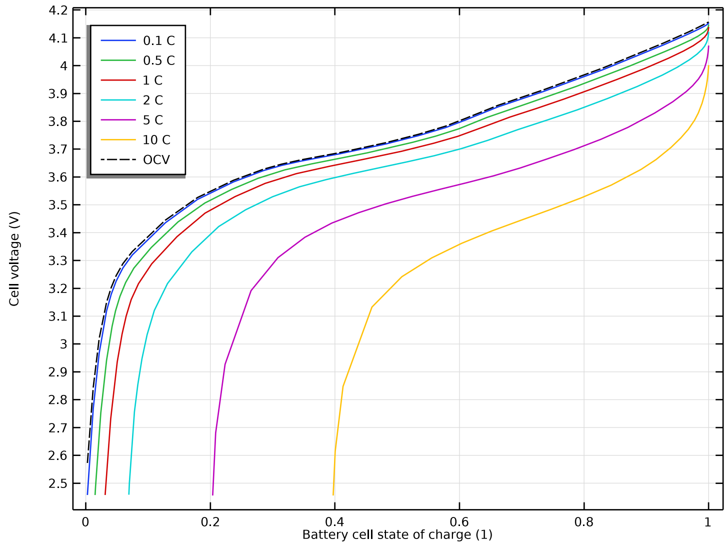
RESULTS

Check out the discharge curves for the power-optimized cell:

Cell Voltages vs SOC

1 In the **Model Builder** window, under **Results** click **Cell Voltages vs SOC**.

2 In the **Cell Voltages vs SOC** toolbar, click **Plot**.



Note that the voltages do not drop as sharply for low SOCs as they did for the energy-optimized cell. (You can do the comparison by changing the **Dataset** to your stored solution for the energy-optimized case.)

Ragone Plot Data Evaluation

Generate new Ragone table data and plot it as follows:

1 In the **Model Builder** window, under **Results>Derived Values** right-click **Ragone Plot Data Evaluation** and choose **Evaluate>New Table**.

Ragone Plot Data for Power Optimized Cell

1 In the **Model Builder** window, under **Results>Tables** click **Table 3**.

2 In the **Settings** window for **Table**, type `Ragone Plot Data for Power Optimized Cell` in the **Label** text field.

Table Graph 2

1 In the **Model Builder** window, under **Results>Ragone Plots** right-click **Table Graph 1** and choose **Duplicate**.

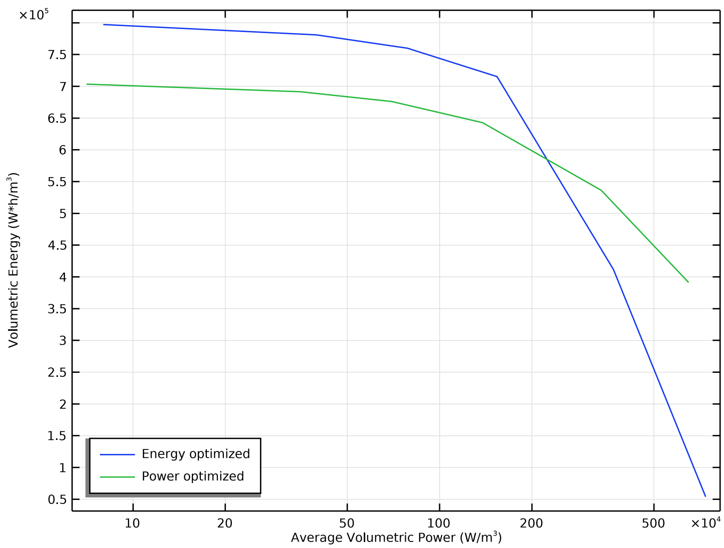
2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Table** list, choose **Ragone Plot Data for Power Optimized Cell**.

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

Legends
`Power optimized`

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



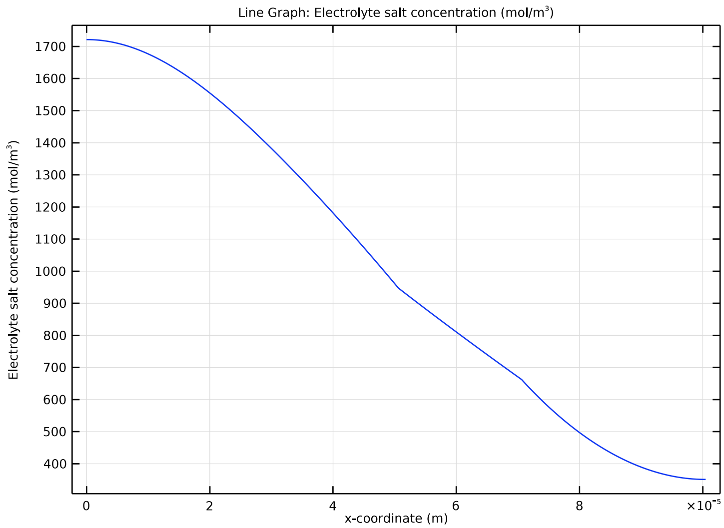
As can be seen, the power-optimized cell is capable of delivering higher energy densities for higher power densities than the energy-optimized cell.

Electrolyte Salt Concentration (liion)

The salt concentration plot for the power-optimized case does not indicate as severe ion depletion as for the energy optimized case:

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

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



Electrolyte Potential (liion)

The absence of ion depletion does not result in the huge electrolyte potential drop as was seen for the energy-optimized case:

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

2 In the **Electrolyte Potential (liion)** toolbar, click **Plot**.