Model created in COMSOL Multiphysics 6.4

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 can deliver a significant amount of power, as it experiences minimal polarization (voltage loss) even under high current loads. However, this comes at the cost of lower energy density. 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 such as cell phones. Power-optimized cells are better suited for power-demanding applications such as hybrid-electric vehicles. 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.

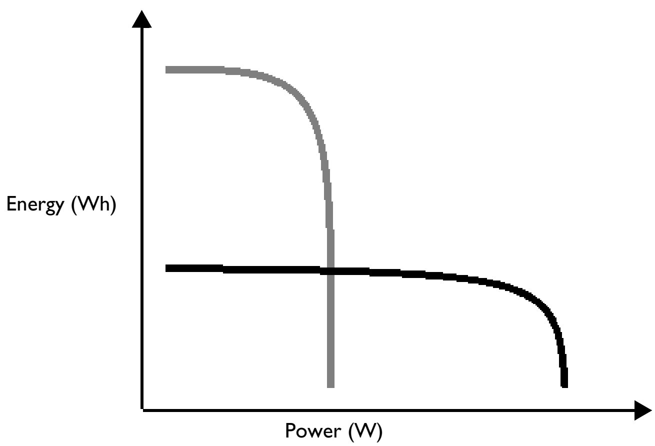


Figure 1: Comparison of energy outputs. Energy optimized cells (gray) can supply more energy but for lower current loads. Power optimized cells (black) work fine for higher power (current loads) but can only provide a fraction of the energy at low power.

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 Power Losses in a Lithium-Ion Battery tutorial, which is build upon this model and analyzes the individual contributions to the power losses in more 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 positive electrode thickness parameter from 60 µm to 25 µm. The negative electrode thickness is automatically reduced based on the correlation discussed in Lithium-Ion Battery Base Model in 1D.

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.

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.

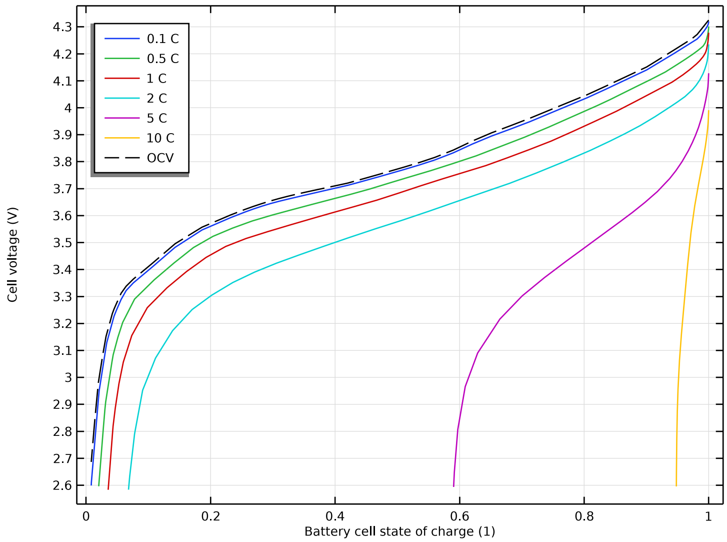


Figure 2: Solid lines: Cell voltages versus SOC during discharge at various C-rates of the energy-optimized cell. Dashed line: Corresponding open circuit voltage (OCV) versus SOC.

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.

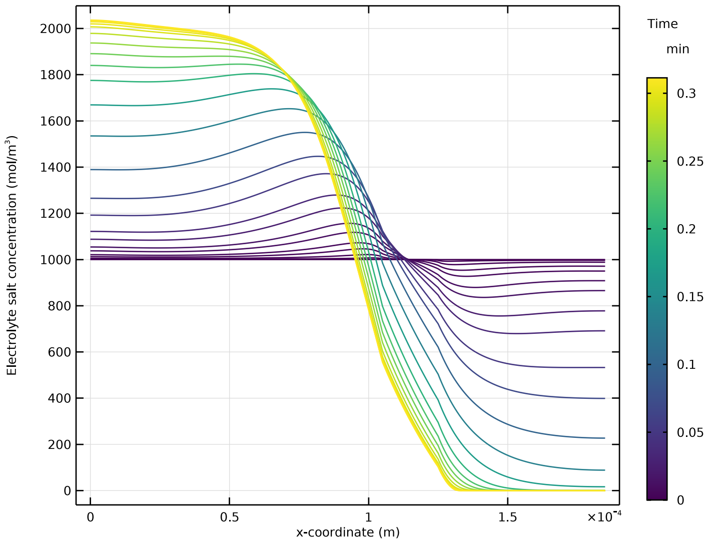


Figure 3: Electrolyte concentration at the end of discharge at 10C of the energy-optimized cell.

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.

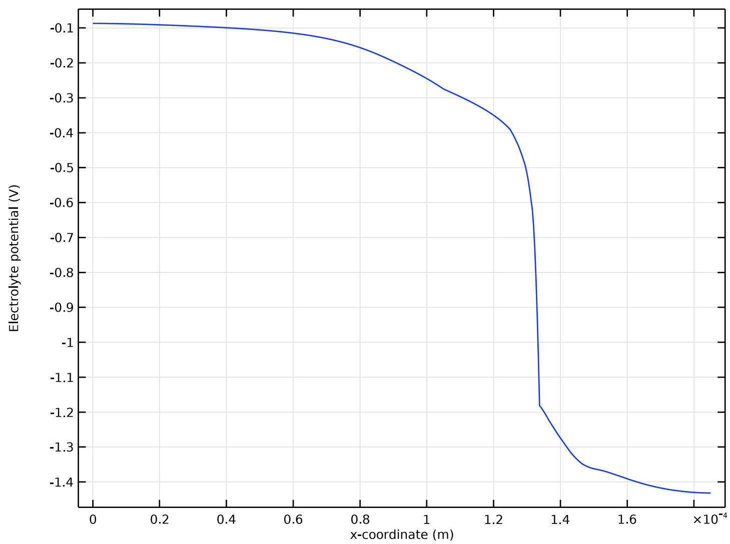


Figure 4: Electrolyte phase potential at the end of discharge at 10C of the energy-optimized cell.

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.

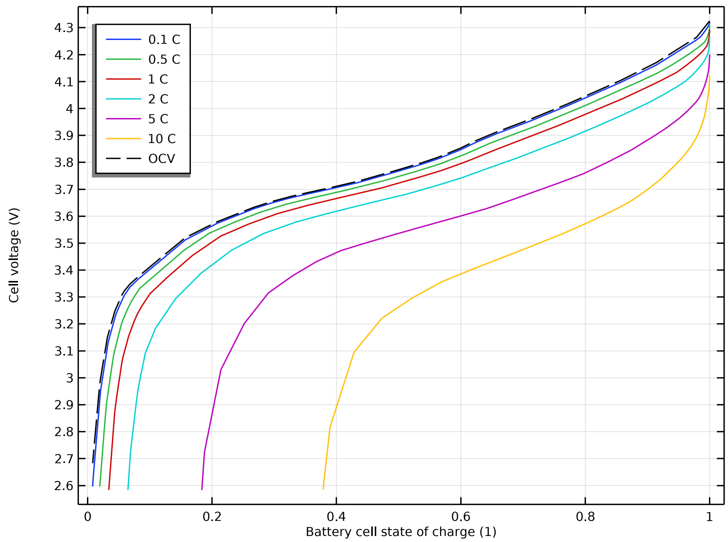


Figure 5: Solid lines: Cell voltages versus SOC during discharge at various C-rates of the power-optimized cell. Dashed line: Corresponding open circuit voltage (OCV) versus SOC.

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.

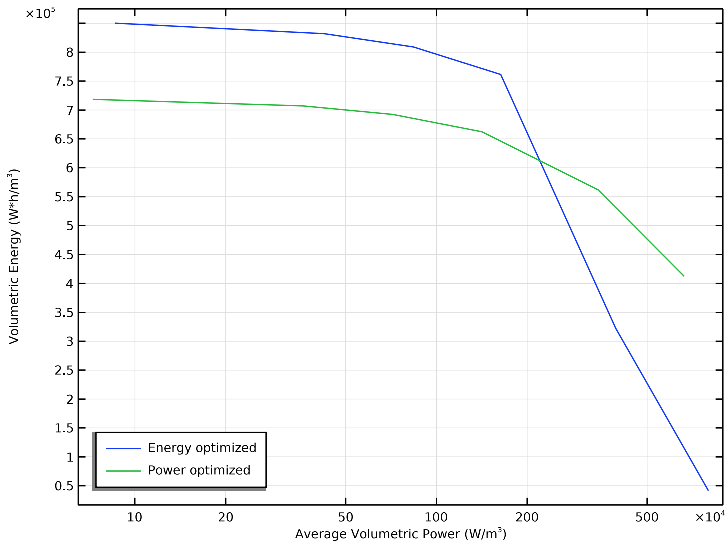


Figure 6: Volumetric energy versus power Ragone plot, comparing the energy optimized to the power optimized cell.

Application Library path: `Battery_Design_Module/Lithium-Ion_Batteries, _Performance/lib_rate_capability`

Modeling Instructions

APPLICATION LIBRARIES

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

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

3 Click **Open**.

In this tutorial you will simulate the discharge of 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 thick electrodes. 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
L_pos	60[um]	6E-5 m	Positive electrode thickness
soc_init	100[%]	1	Initial SOC
C_rate	1	1	Discharge rate
E_stop	2.6[V]	2.6 V	Stop (threshold) voltage

DEFINITIONS (COMP1)

Variables 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node, then click **Variables 1**.

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	liion.lc1.I_app/A_cell	A/m²	Applied cell current density

LITHIUM-ION BATTERY (LIION)

Load Cycle 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Lithium-Ion Battery (liion)** node, then click **Load Cycle 1**.

2 In the **Settings** window for **Load Cycle**, locate the **Cycling Stop Condition** section.

3 From the list, choose **Minimum voltage**.

4 In the E_{min} text field, type E_stop.

C Rate 1

1 In the **Model Builder** window, expand the **Load Cycle 1** node, then click **C Rate 1**.

2 In the **Settings** window for **C Rate**, locate the **C-rate Multiple** section.

3 In the C_{set} text field, type -C_rate.

COMPONENT 1 (COMP1)

Add an additional physics interface for adding an integral equation for accumulated energy.

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 the **Add to Component 1** button in the window toolbar.
5. In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

CUMULATIVE ENERGY

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

Global Equations 1 (ODE1)

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Cumulative Energy (ge)** click **Global Equations 1 (ODE1)**.
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 (ut_0) (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

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: Current Distribution Initialization

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 **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Cumulative Energy (ge)**.

Step 2: 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 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 1/C_rate`.

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.)

Solution 1 (sol1)

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

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

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

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

5 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. In the **Initial step** text field, type `0.001/C_rate`.

7 In the **Study** toolbar, click **=** **Compute**.

RESULTS

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

Cell Voltages vs. SOC

1 In the **Results** toolbar, click **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 (sol3)**.

Global 1

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

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

3 In the table, enter the following settings:

Expression	Unit	Description
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**, locate the **Data** section.

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

4 From the **Parameter selection (C_rate)** 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** > **E_ocv_cell - Open-circuit cell voltage - V**.

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

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

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

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

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

11 In the table, enter the following settings:

Legends
OCV

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.

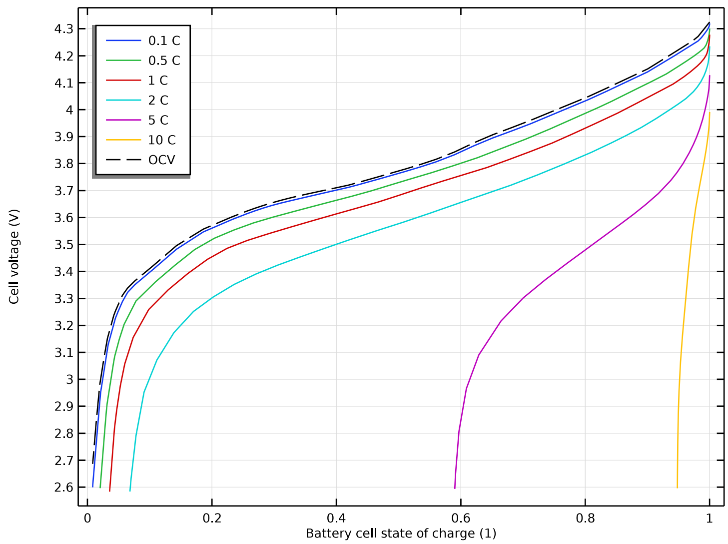
3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** checkbox. 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**.



Ragone Plot Data Evaluation

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

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

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 **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

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

5 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.

6 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** checkbox.

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 box, select **Volumetric Energy (W*h/m^3)**.

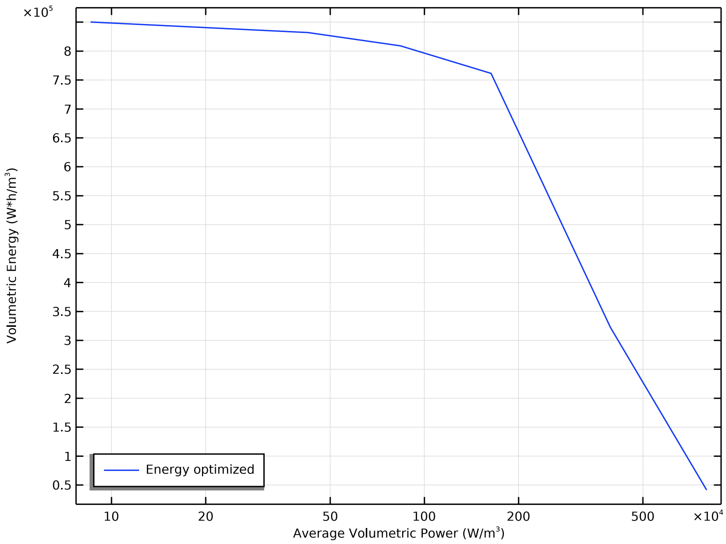
7 Click to expand the **Legends** section. Select the **Show legends** checkbox.

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**.

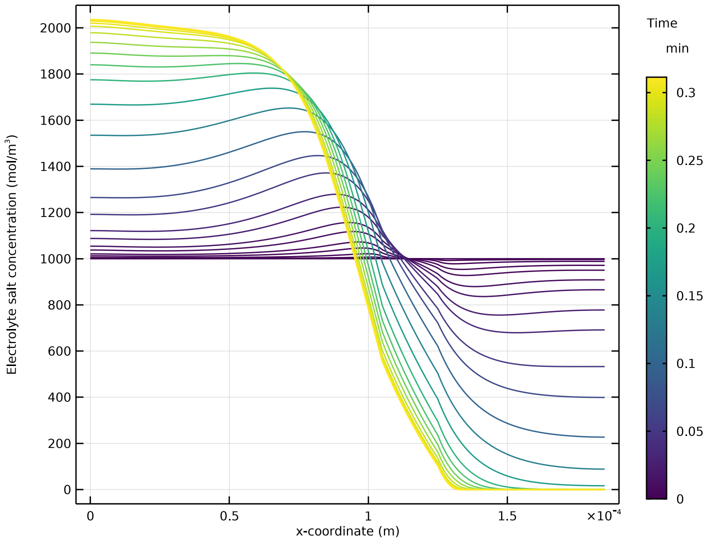


The Ragone plot indicates a large decrease in output energy for large power levels (discharge currents). Reviewing the default electrolyte salt (Li ion) concentration plot at the last time point at the highest current level indicates what could be the issue.

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 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

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

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

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

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

Line Graph 1

1 Right-click **Electrolyte Potential** and choose **Line Graph**.

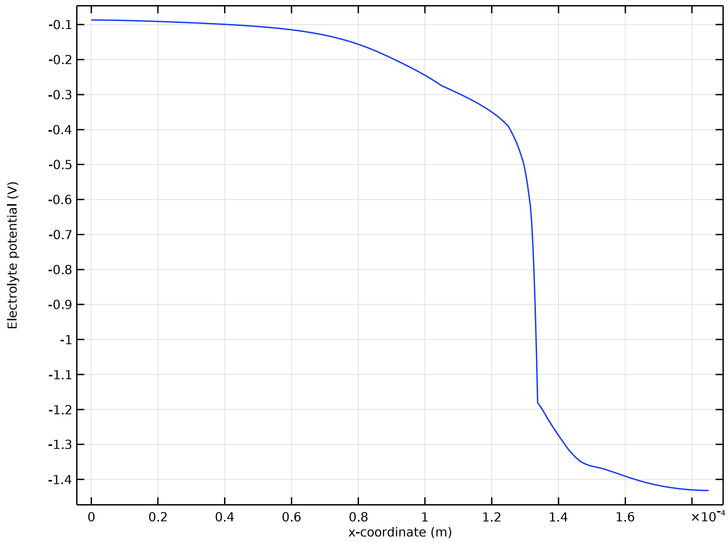
2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

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

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

6 In the **Electrolyte Potential** 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 positive electrode thickness. Note that the negative electrode thickness is automatically reduced based on the correlation defined in the **Parameters 1** node.

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
L_pos	25[um]	2.5E-5 m	Positive electrode thickness

STUDY 1

Parametric Solutions 1 (sol3)

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 (sol3)** 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 (sol10)**.

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

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

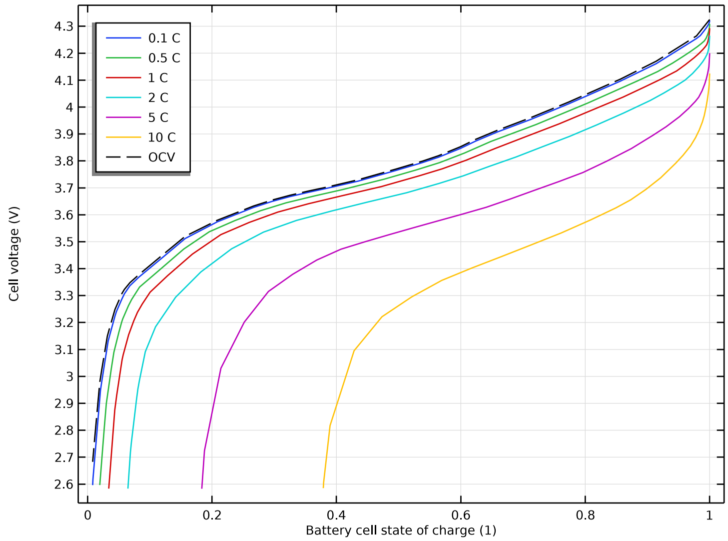
RESULTS

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**.

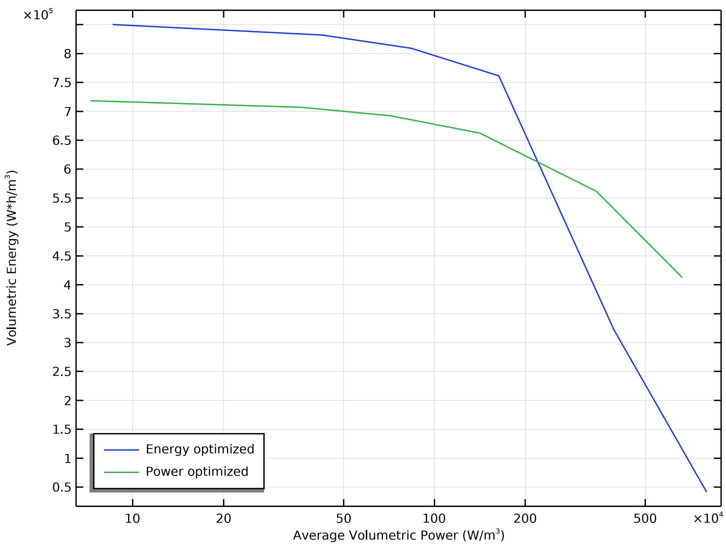
2 In the **Settings** window for **Table Graph**, locate the **Data** section.

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**.



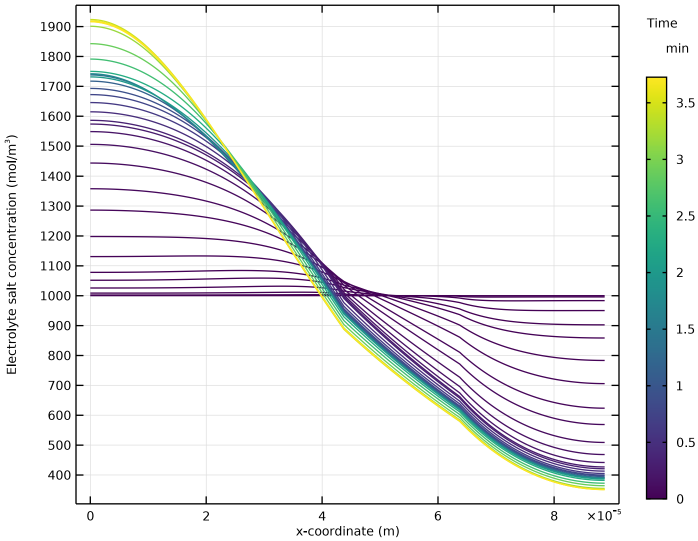
As can be seen, the power-optimized cell is capable of delivering higher energy densities for high power densities than the energy-optimized cell.

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

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**.

2 In the **Electrolyte Potential** toolbar, click **Plot**.