

# Electrode Utilization in a Large Format Lithium-Ion Battery Pouch Cell

# Introduction

Large lithium-ion batteries are widely employed in electric vehicles and for stationary energy storage applications. In the (stacked) pouch battery cell design, all current exits the cell on the cell "tabs", and as the cell size and power increases, the voltage gradients in the highly conductive metal foil current collectors may come into play, resulting in a nonuniform current distribution and electrode utilization in the cell. A nonuniform utilization results in suboptimal use of the battery electrodes and may also result in nonuniform and accelerated electrode aging.

This tutorial models the current distribution and electrode utilization in a large format lithium-ion battery pouch cell, and how it depends on the cell current.

The model is in 3D. Note that all plots are scaled 100 times in the z direction due to the high aspect ratio of the geometric features.

# Model Definition

Figure 1 shows the model geometry. The geometry defines one foil-to-foil unit cell, stacking five layers in the z direction:

- Negative metal current collector foil: 10 µm, Cu (due to symmetry, half of this thickness is used in the model geometry)
- Negative electrode: 60 μm, graphite
- Separator: 30 μm
- Positive electrode: 60 μm, LMO
- Positive metal current collector foil: 10 µm, Al (due to symmetry, half of this thickness is used in the model geometry)
- The electrolyte is LiPF6 in 3:7 EC:EMC
- Symmetry is assumed along the center of the cell

The positive and negative current terminals are located opposite to each other (but may easily be placed on the same side by altering the Geometry node in the model).

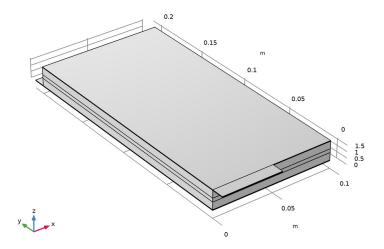


Figure 1: Model geometry, scaled 100 times in the z direction.

The Lithium-Ion Battery interface is used to set up the physics, using Material data from the Battery Material Library.

The Particle Intercalation subnodes to the Porous Electrode nodes model the solid lithium concentration in an additional particle dimension (extra dimension). The model hence defines a fully coupled "pseudo-4D" model.

The battery is charged from 20% to 90% cell state of charge (SOC). The SOC and Initial Cell Charge Distribution node is used to set the initial cell state of charge.

An Electrode Ground boundary condition is used on the negative tab whereas an Electrode Current boundary condition defines the cell current exiting the cell on the positive tab.

A Parametric Sweep is used to solve for two different charge rates (1C and 4C).

# Results and Discussion

Figure 2 and Figure 3 show the potential distribution in the negative and positive metal foils (current collector and tab), respectively, at the beginning of the 4C charge. The potential variation is about 5 mV in the negative current collector and 9 mV in the positive current collector at a 4C charge current.

For a 1C charge current the corresponding potential variation is below 2 mV (results not shown here).

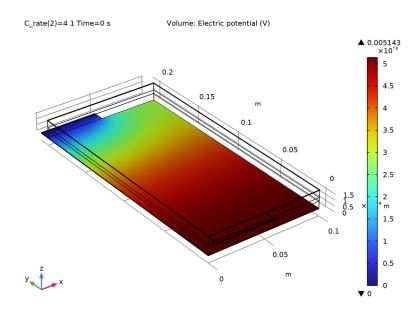


Figure 2: Potential distribution in the negative metal foil (current collector and tab) at the beginning of the 4C charge.

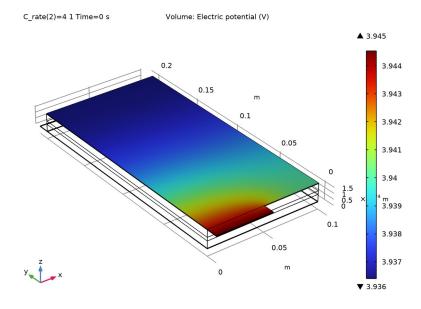


Figure 3: Potential distribution in the positive metal foil (current collector and tab) at the beginning of the 4C charge.

Figure 4 and Figure 5 show the current distribution for a cross section in the middle of the separator at the beginning and end of the 4C charge, respectively. This provides a measure of the electrode utilization for a given time. The current distribution varies about 6% in the separator plane over time. For 1C, the variation is generally smaller (results not shown here). Initially, the separator current density is higher close to the tabs whereas toward the end of the charge, the current density is higher in the central parts of the cell.



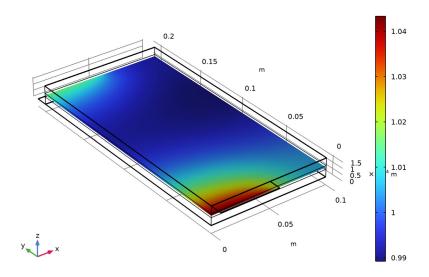


Figure 4: Current distribution in the middle of the separator at the beginning of the 4C charge.

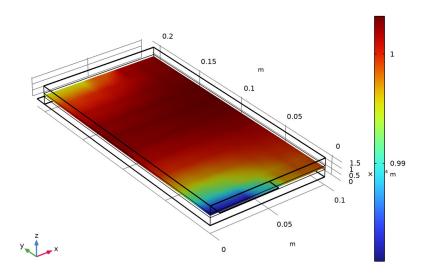


Figure 5: Current distribution in the middle of the separator at the end of the 4C charge.

To get a measure of the relative utilization over the whole charge period, General Projection operators are used to integrate the amount of lithium  $(c_{\mathrm{s,avg}})$  along the electrode depth (the z direction). Dividing the projected change of intercalated lithium by the average for the whole electrode gives a measure of the relative utilization (capacity throughput)  $U_t$ , as a function of the spatial independent variables x and y, at any time t.

$$U(x, y, t) = \frac{\varepsilon_s F \int_0^t (c_{s, \text{avg}}(x, y, z, t) - c_{s, \text{avg}}(x, y, z, 0)) dz}{\frac{1}{W_{\text{cell}} H_{\text{cell}}} \int_0^t I_{\text{cell}}(t) dt}$$

Figure 6 and Figure 7 show the relative utilization over the whole charge period for the 1C and 4C charges, respectively for the positive electrode. The utilization varies between 99.5% and 102% for the 4C charge and between 100% and 101% for the 1C charge. The cycle-averaged utilization is lower than the instantaneous utilization shown in Figure 4 and Figure 5.

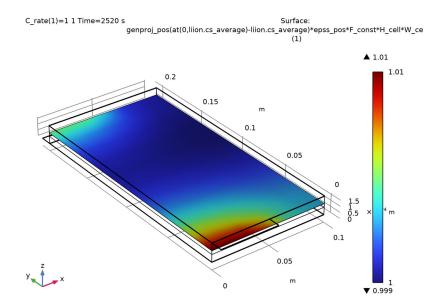


Figure 6: Relative electrode utilization during the 1C charge.

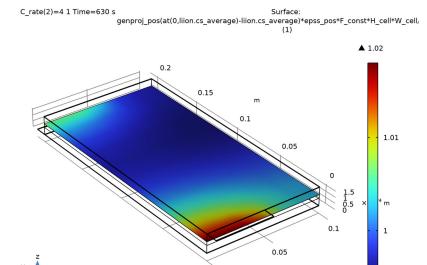


Figure 7: Relative electrode utilization during the 4C charge.

The tutorial demonstrates that the local electrode utilization along the metal foil (current collector and tab) changes over the course of a charge cycle. For this configuration, utilization is fairly uniform during a 1C charge, but a higher charge of 4C results in a slightly nonuniform utilization.

▼ 0.995

Application Library path: Battery\_Design\_Module/Batteries,\_Lithium-Ion/ pouch\_cell\_utilization

# Modeling Instructions

From the File menu, choose New.

#### NEW

In the New window, click Model Wizard.

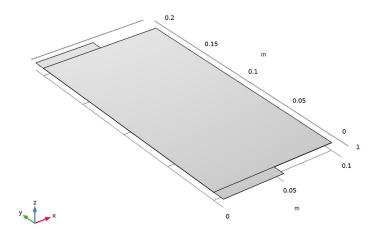
#### MODEL WIZARD

- I In the Model Wizard window, click **1** 3D.
- 2 In the Select Physics tree, select Electrochemistry>Batteries>Lithium-lon 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.
- 6 Click M Done.

#### **GEOMETRY I**

The model geometry is available as a parameterized geometry sequence in a separate MPH-file. If you want to build it from scratch, follow the instructions in the section Appendix - Geometry Modeling Instructions. Otherwise load it from file with the following steps.

- I In the Geometry toolbar, click Insert Sequence and choose Insert Sequence.
- **2** Browse to the model's Application Libraries folder and double-click the file pouch cell utilization geom sequence.mph.
- 3 In the Geometry toolbar, click **Build All**.
- 4 In the Model Builder window, under Component I (compl) click Geometry I.



**5** In the **Model Builder** window, collapse the **Geometry I** node.

#### DEFINITIONS

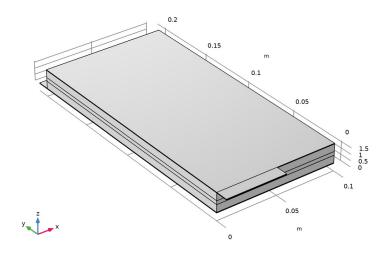
The cell geometry has a high aspect ratio, with the cell thicknesses being very small in relation to the cross-sectional area. To facilitate setting up the physics, change the scaling in the z direction as follows:

#### View 1

In the Model Builder window, expand the Component I (compl)>Definitions node.

#### Camera

- I In the Model Builder window, expand the View I node, then click Camera.
- 2 In the Settings window for Camera, locate the Camera section.
- 3 From the View scale list, choose Manual.
- 4 In the z scale text field, type 100.
- 5 Click ( Update.



#### **GLOBAL DEFINITIONS**

# **Geometry Parameters**

Some parameters were loaded with the geometry sequence.

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, type Geometry Parameters in the Label text field.

# **Physics Parameters**

Add some more parameters from a text file.

- I In the Home toolbar, click Pi Parameters and choose Add>Parameters.
- 2 In the Settings window for Parameters, type Physics Parameters in the Label text field.
- 3 Locate the Parameters section. Click **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file pouch cell utilization physics parameters.txt.

#### MATERIALS

Most of the required material parameters are available in the material libraries. First add Copper and Aluminum for the current conductors.

#### ADD MATERIAL

- I 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 Built-in>Aluminum and Built-in>Copper.
- 4 Click Add to Component in the window toolbar.

#### ADD MATERIAL

Next add the material properties for the electrolyte and electrode materials.

- I Go to the Add Material window.
- 2 In the tree, select Battery>Electrodes>Graphite, LixC6 MCMB (Negative, Li-ion Battery) and Battery>Electrodes>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery).
- **3** Click **Add to Component** in the window toolbar.
- 4 In the tree, select Battery>Electrolytes>LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery).
- 5 Click Add to Component in the window toolbar.
- 6 In the Home toolbar, click **‡** Add Material to close the Add Material window.

# MATERIALS

Aluminum (mat I)

Assign the materials to the corresponding battery domains.

- I In the Model Builder window, click Aluminum (matl).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.

3 From the Selection list, choose Positive Current Collector and Tab.

Copper (mat2)

- I In the Model Builder window, click Copper (mat2).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Negative Current Collector and Tab.

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat3)

- I In the Model Builder window, click Graphite, LixC6 MCMB (Negative, Liion Battery) (mat3).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Negative Electrode.

LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4)

- I In the Model Builder window, click LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat4).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Positive Electrode.

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5)

- I In the Model Builder window, click LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Separator.

# LITHIUM-ION BATTERY (LIION)

Porous Electrode - Negative

The **Separator** node was added to the interface by default. Keep the default settings for the **Separator**, and proceed to add and set up the physics in the porous electrodes and current collectors.

- I In the Model Builder window, under Component I (compl) right-click Lithium-Ion Battery (liion) and choose Porous Electrode.
- 2 In the Settings window for Porous Electrode, type Porous Electrode Negative in the Label text field.
- 3 Locate the Domain Selection section. From the Selection list, choose Negative Electrode.
- 4 Locate the Electrolyte Properties section. From the Electrolyte material list, choose LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5).
- **5** Locate the **Electrode Properties** section. In the  $\sigma_s$  text field, type sigmas\_neg.

- 6 Locate the Porous Matrix Properties section. In the  $\varepsilon_s$  text field, type epss\_neg.
- 7 In the  $\varepsilon_1$  text field, type 1-epss\_neg.

#### Particle Intercalation 1

Leave the settings of the **Species Settings** section as is for now. The initial species concentration setting will be made inactive later when we define the cell state of charge (SOC) on a different node.

- I In the Model Builder window, click Particle Intercalation I.
- 2 In the Settings window for Particle Intercalation, locate the Particle Transport Properties section.
- 3 In the  $r_p$  text field, type rp\_neg.

#### Porous Electrode Reaction 1

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

# Porous Electrode - Positive

- I In the Physics toolbar, click **Domains** and choose Porous Electrode.
- 2 In the Settings window for Porous Electrode, type Porous Electrode Positive in the Label text field.
- 3 Locate the Domain Selection section. From the Selection list, choose Positive Electrode.
- 4 Locate the Electrolyte Properties section. From the Electrolyte material list, choose LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5).
- **5** Locate the **Electrode Properties** section. In the  $\sigma_s$  text field, type sigmas\_pos.
- **6** Locate the **Porous Matrix Properties** section. In the  $\varepsilon_s$  text field, type epss\_pos.
- 7 In the  $\varepsilon_1$  text field, type 1-epss\_pos.

#### Particle Intercalation 1

- I In the Model Builder window, click Particle Intercalation I.
- 2 In the Settings window for Particle Intercalation, locate the Particle Transport Properties section.
- **3** In the  $r_p$  text field, type  $rp_pos$ .

#### Porous Electrode Reaction I

I In the Model Builder window, click Porous Electrode Reaction I.

- 2 In the Settings window for Porous Electrode Reaction, locate the Electrode Kinetics section.
- **3** In the  $i_{0,ref}(T)$  text field, type iOref\_pos.

#### Current Conductor I

- I In the Physics toolbar, click **Domains** and choose Current Conductor.
- 2 In the Settings window for Current Conductor, locate the Domain Selection section.
- 3 From the Selection list, choose Metal Foil Domains.

#### Electric Ground 1

- I In the Physics toolbar, click **Boundaries** and choose **Electric Ground**.
- 2 In the Settings window for Electric Ground, locate the Boundary Selection section.
- 3 From the Selection list, choose Negative Tab End. Enable the Define cell state of charge (SOC) and initial charge inventory on the interface top node. This will allow us to set the initial SOC of the battery cell.
- 4 In the Model Builder window, click Lithium-Ion Battery (liion).
- 5 In the Settings window for Lithium-Ion Battery, locate the Cell Settings section.
- 6 Select the Define cell state of charge (SOC) and initial charge inventory check box.

# SOC and Initial Charge Distribution I

- I In the Model Builder window, click SOC and Initial Charge Distribution 1.
- 2 In the Settings window for SOC and Initial Charge Distribution, locate the **Initial Cell Charge Distribution** section.
- **3** In the  $SOC_0$  text field, type SOC start.

#### Negative Electrode Selection I

- I In the Model Builder window, click Negative Electrode Selection I.
- 2 In the Settings window for Negative Electrode Selection, locate the Domain Selection section.
- 3 From the Selection list, choose Negative Electrode.

#### Positive Electrode Selection I

- I In the Model Builder window, click Positive Electrode Selection I.
- 2 In the Settings window for Positive Electrode Selection, locate the Domain Selection section.
- 3 From the Selection list, choose Positive Electrode.

#### **DEFINITIONS (COMPI)**

Variables 1

I In the Model Builder window, under Component I (compl) right-click Definitions and choose Variables.

An internal 1C current variable (liion.I\_10\_cell), based on the cyclable lithium capacity, is computed automatically by the **SOC and Initial Charge Distribution** node. Use this variable to set up a variable for the applied C rate current.

- 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.I_1C_cell*C_rate	Α	Applied current

# LITHIUM-ION BATTERY (LIION)

Electrode Current I

- I In the Physics toolbar, click **Boundaries** and choose **Electrode Current**.
- 2 In the Settings window for Electrode Current, locate the Boundary Selection section.
- 3 From the Selection list, choose Positive Tab End.
- **4** Locate the **Electrode Current** section. In the  $I_{s,total}$  text field, type I\_app.

#### MESH I

Set up the mesh for the model. Use a mapped mesh on the top boundaries, and a swept mesh for remaining of the geometry.

# Mapped I

- I In the Mesh toolbar, click More Generators and choose Mapped.
- 2 Select Boundary 20 only.

#### Swept I

- I In the Mesh toolbar, click A Swept.
- 2 In the Settings window for Swept, locate the Domain Selection section.
- **3** Click to clear the **Activate Selection** toggle button.

#### Distribution I

I Right-click Swept I and choose Distribution.

By the use of **Distribution** nodes you can control the resolution in the z direction of the individual layers of the cell.

- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 From the Selection list, choose Negative Electrode.
- 4 Locate the Distribution section. From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 15.
- 6 In the Element ratio text field, type 3.

#### Distribution 2

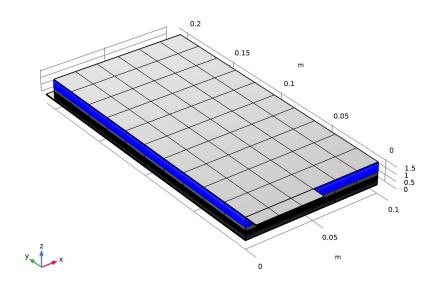
- I In the Model Builder window, right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 From the Selection list, choose Separator.
- 4 Locate the Distribution section. In the Number of elements text field, type 4.

#### Distribution 3

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 From the Selection list, choose Positive Electrode.
- 4 Locate the Distribution section. From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 15.
- 6 In the Element ratio text field, type 3.
- 7 Select the Reverse direction check box.

# 8 Click III Build All.

The finalized mesh should now look as follows.



# **DEFINITIONS (COMPI)**

Before solving, add also a probe for an automatically defined voltage variable created by the **Electrode Current** condition at the positive tab. Since the negative tab is grounded, this voltage corresponds to the cell voltage. The probe will store the cell voltage for every time step taken by the solver in a table, and a dynamically updated plot of the cell voltage will also be available while solving.

# Cell Voltage Probe

- I In the Definitions toolbar, click Probes and choose Global Variable Probe.
- 2 In the Settings window for Global Variable Probe, type Cell Voltage Probe in the Label text field.
- 3 Click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>Lithium-lon Battery>liion.phis0\_ecl -Electric potential on boundary - V.
- 4 Locate the Expression section.
- **5** Select the **Description** check box. In the associated text field, type **Cell Voltage**.

#### STUDY I

Use a **Parametric Sweep** to solve for two different C rates.

# Parametric Sweep

- I 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 (C-rate during simulation)	1 4	1

# Step 2: Time Dependent

- I 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 range(0, sim\_time/2, sim\_time).
- 4 In the Study toolbar, click **Compute**.

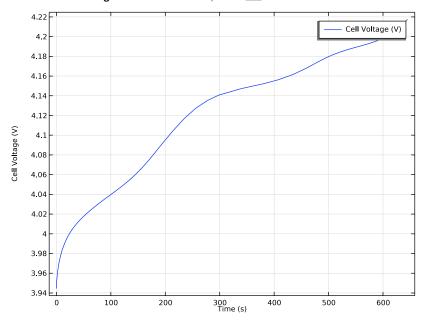
#### RESULTS

A plot of the battery voltage vs time is created automatically by the probe you added earlier.

# Cell Voltage Probe Plot

- I In the Model Builder window, under Results click Probe Plot Group I.
- 2 In the Settings window for ID Plot Group, type Cell Voltage Probe Plot in the Label text field.

3 In the Cell Voltage Probe Plot toolbar, click Plot.



Potential in Negative Current Collector and Tab

The following steps create a plot of the potential at the negative current collector and tab.

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Potential in Negative Current Collector and Tab in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 1/ Parametric Solutions I (sol3).
- 4 From the Time (s) list, choose 0.
- 5 Locate the Color Legend section. Select the Show maximum and minimum values check
- 6 Click to expand the Number Format section. Select the Manual color legend settings check box.
- 7 In the Precision text field, type 4.

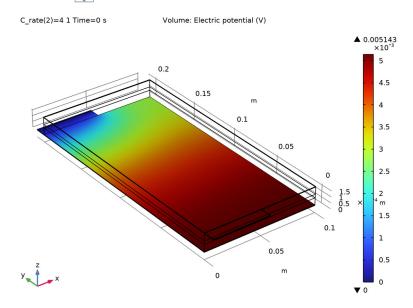
#### Volume 1

- I Right-click Potential in Negative Current Collector and Tab and choose Volume.
- 2 In the Settings window for Volume, locate the Expression section.

3 In the Expression text field, type phis.

Selection I

- I Right-click Volume I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Negative Current Collector and Tab.
- 4 In the Potential in Negative Current Collector and Tab toolbar, click Plot.
- 5 Click the **Zoom Extents** button in the **Graphics** toolbar.



Potential in Negative Current Collector and Tab

Duplicate the plot and modify the copy in order to view the potential at the positive current collector and tab.

In the Model Builder window, under Results right-click Potential in Negative Current Collector and Tab and choose Duplicate.

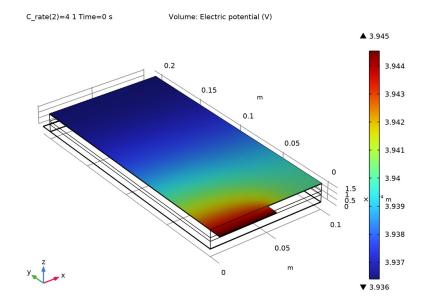
Potential in Positive Current Collector and Tab

- I In the Model Builder window, under Results click Potential in Negative Current Collector and Tab I.
- 2 In the Settings window for 3D Plot Group, type Potential in Positive Current Collector and Tab in the Label text field.

3 In the Model Builder window, expand the Potential in Positive Current Collector and Tab node.

# Selection I

- I In the Model Builder window, expand the Results> Potential in Positive Current Collector and Tab>Volume I node, then click Selection I.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Positive Current Collector and Tab.
- 4 In the Potential in Positive Current Collector and Tab toolbar, click Plot.
- 5 Click the **Zoom Extents** button in the **Graphics** toolbar.



Relative Current Density Across Separator

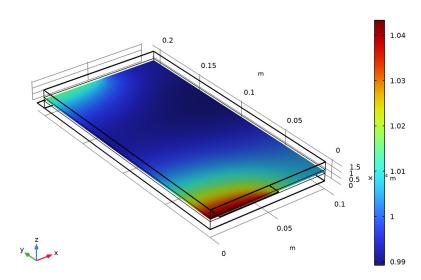
Plot the relative current density across the separator using a slice plot.

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Relative Current Density Across Separator in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 1/ Parametric Solutions I (sol3).
- 4 From the Time (s) list, choose 0.

# Slice 1

- I Right-click Relative Current Density Across Separator and choose Slice.
- 2 In the Settings window for Slice, locate the Expression section.
- 3 In the Expression text field, type liion.IlMag/(I\_app/(H\_cell\*W\_cell)).
- 4 Locate the Plane Data section. From the Plane list, choose XY-planes.
- 5 From the Entry method list, choose Coordinates.
- 6 In the **Z-coordinates** text field, type L\_neg\_cc/2+L\_neg+L\_sep/2.
- 7 In the Relative Current Density Across Separator toolbar, click  **Plot**.
- 8 Click the **Zoom Extents** button in the **Graphics** toolbar.

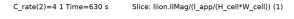
C rate(2)=4 1 Time=0 s Slice: liion.IIMag/(I\_app/(H\_cell\*W\_cell)) (1)

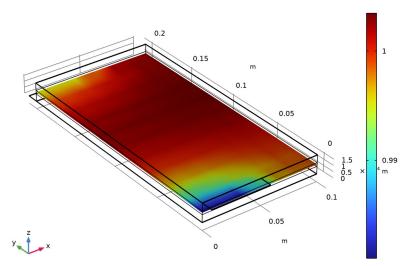


# Relative Current Density Across Separator

- I In the Model Builder window, click Relative Current Density Across Separator.
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Time (s) list, choose 630.

4 In the Relative Current Density Across Separator toolbar, click Plot.





# **DEFINITIONS (COMPI)**

As a final step we will evaluate the relative utilization of the electrodes during the whole charge.

First add two General Projection operators that will be used to integrate the amount of lithium along the electrode depth (the z direction).

# General Projection - Negative

- I In the Definitions toolbar, click Nonlocal Couplings and choose General Projection.
- 2 In the Settings window for General Projection, type General Projection Negative in the Label text field.
- 3 In the Operator name text field, type genproj neg.
- 4 Locate the Source Selection section. From the Selection list, choose Negative Electrode.
- **5** Right-click **General Projection Negative** and choose **Duplicate**.

#### General Projection - Positive

I In the Model Builder window, under Component I (compl)>Definitions click General Projection - Negative I (genproj\_neg2).

- 2 In the Settings window for General Projection, type General Projection Positive in the Label text field.
- 3 In the Operator name text field, type genproj pos.
- 4 Locate the Source Selection section. From the Selection list, choose Positive Electrode.

#### STUDY I

In order to make the operators available in the solution, you need to update the solution.

In the Study toolbar, click C Update Solution.

#### RESULTS

Utilization (Relative Capacity Throughput)

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Utilization (Relative Capacity Throughput) in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 1/ Parametric Solutions I (sol3).
- 4 From the Parameter value (C\_rate) list, choose 1.
- 5 Locate the Color Legend section. Select the Show maximum and minimum values check box.

Surface 1

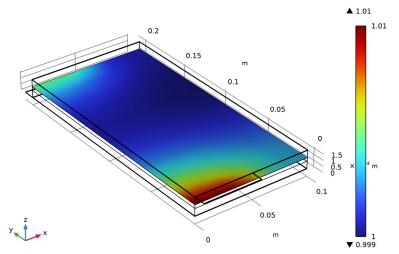
- I Right-click Utilization (Relative Capacity Throughput) and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- 3 In the Expression text field, type genproj pos(at(0,liion.cs average)liion.cs\_average)\*epss\_pos\*F\_const\*H\_cell\*W\_cell/(I\_app\*t).

Selection 1

- I Right-click Surface I and choose Selection.
- **2** Select Boundary 16 only.

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

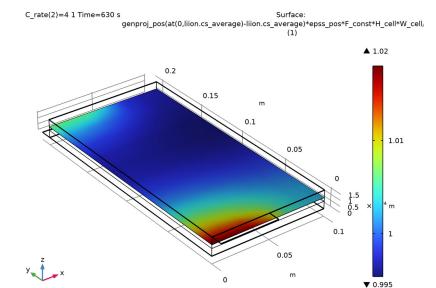




Utilization (Relative Capacity Throughput)

- I In the Model Builder window, under Results click **Utilization (Relative Capacity Throughput)**.
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Parameter value (C\_rate) list, choose 4.

# 4 In the Utilization (Relative Capacity Throughput) toolbar, click **1** Plot.



# Appendix - Geometry Modeling Instructions

From the File menu, choose New.

#### NEW

In the New window, click Model Wizard.

#### MODEL WIZARD

- I In the Model Wizard window, click 1 3D.
- 2 Click **Done**.

# **GLOBAL DEFINITIONS**

# Parameters 1

Import the parameter file.

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 pouch cell utilization geometry parameters.txt.

#### **GEOMETRY I**

Set up the model geometry using the following steps.

Work Plane I (wbl)

In the Geometry toolbar, click Swork Plane.

Work Plane I (wp I)>Plane Geometry

In the Model Builder window, click Plane Geometry.

Work Plane I (wp I)>Rectangle I (r I)

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type W cell.
- 4 In the Height text field, type H cell.

Extrude I (ext I)

- I In the Model Builder window, right-click Geometry I and choose Extrude.
- 2 In the Settings window for Extrude, locate the Distances section.
- **3** In the table, enter the following settings:

```
Distances (m)
L neg cc/2
L_neg_cc/2+L_neg
L neg cc/2+L neg+L sep
L_neg_cc/2+L_neg+L_sep+L_pos
L neg cc/2+L neg+L sep+L pos+L pos cc/2
```

Block I (blk I)

- I In the Geometry toolbar, click Block.
- 2 In the Settings window for Block, locate the Size and Shape section.
- 3 In the Width text field, type W tab.
- 4 In the **Depth** text field, type H tab.
- 5 In the **Height** text field, type L\_neg\_cc/2.
- 6 Locate the **Position** section. In the y text field, type H cell.

- 7 Click | Build Selected.
- 8 Click the Zoom Extents button in the Graphics toolbar.

# Block 2 (blk2)

- I In the **Geometry** toolbar, click **Block**.
- 2 In the Settings window for Block, locate the Size and Shape section.
- 3 In the Width text field, type W tab.
- 4 In the **Depth** text field, type H\_tab.
- 5 In the Height text field, type L neg cc/2.
- 6 Locate the **Position** section. In the y text field, type -H tab.
- 7 In the z text field, type L\_neg\_cc/2+L\_neg+L\_sep+L\_pos.
- 8 Click | Build Selected.

# Form Union (fin)

In the **Geometry** toolbar, click **Build All**.

#### DEFINITIONS

Scale the geometry in the z direction to make it easier to see the different layers in the model geometry.

# View 1

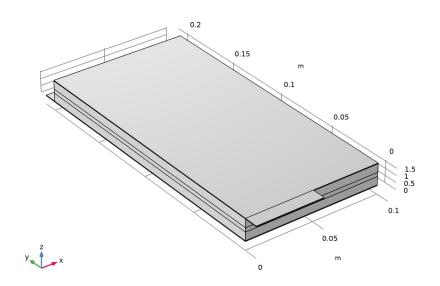
In the Model Builder window, expand the Component I (compl)>Definitions node.

### Camera

- I In the Model Builder window, expand the View I node, then click Camera.
- 2 In the Settings window for Camera, locate the Camera section.
- 3 From the View scale list, choose Manual.
- 4 In the z scale text field, type 100.
- 5 Click ( Update.

6 Click the Zoom Extents button in the Graphics toolbar.

The finalized geometry should now look like as follows.



#### **GEOMETRY I**

Create named selections of the different battery domains for ease of selection later in the model.

In the **Geometry** toolbar, click **Build All**.

# Positive Tab

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Positive Tab in the Label text field.
- **3** On the object **fin**, select Domain 1 only.

# Positive Current Collector

- I In the Geometry toolbar, click 🔓 Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Positive Current Collector in the Label text field.
- **3** On the object **fin**, select Domain 6 only.

#### Positive Electrode

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Positive Electrode in the Label text field.
- 3 On the object fin, select Domain 5 only.

# Negative Tab

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Negative Tab in the Label text field.
- **3** On the object **fin**, select Domain 7 only.

# Negative Current Collector

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Negative Current Collector in the Label text field.
- 3 On the object fin, select Domain 2 only.

# Negative Electrode

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Negative Electrode in the Label text field.
- **3** On the object **fin**, select Domain 3 only.

# Sebarator

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Separator in the Label text field.
- 3 On the object fin, select Domain 4 only.

#### Negative Tab End

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Negative Tab End in the Label text field.
- 3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.
- 4 Click the Paste Selection button for Entities to select.
- 5 In the Paste Selection dialog box, type 29 in the Selection text field.
- 6 Click OK.

#### Positive Tab End

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Positive Tab End in the Label text field.
- 3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.
- 4 Click the Paste Selection button for Entities to select.
- 5 In the Paste Selection dialog box, type 2 in the Selection text field.
- 6 Click OK.

# Negative Current Collector and Tab

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Union Selection.
- 2 In the Settings window for Union Selection, type Negative Current Collector and Tab in the Label text field.
- 3 Locate the **Input Entities** section. Click + Add.
- 4 In the Add dialog box, in the Selections to add list, choose Negative Tab and **Negative Current Collector.**
- 5 Click OK.

## Positive Current Collector and Tab

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Union Selection.
- 2 In the Settings window for Union Selection, type Positive Current Collector and Tab in the Label text field.
- 3 Locate the **Input Entities** section. Click Add.
- 4 In the Add dialog box, in the Selections to add list, choose Positive Tab and **Positive Current Collector.**
- 5 Click OK.

#### Metal Foil Domains

- I In the Geometry toolbar, click \( \frac{1}{2} \) Selections and choose Union Selection.
- 2 In the Settings window for Union Selection, type Metal Foil Domains in the Label text field.
- 3 Locate the Input Entities section. Click + Add.
- 4 In the Add dialog box, in the Selections to add list, choose Negative Current Collector and Tab and Positive Current Collector and Tab.
- 5 Click OK.