INTRODUCTION TO

Battery Design Module

6.3

COMSOL

Introduction to the Battery Design Module

Version: COMSOL 6.3

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Introduction

The Battery Design Module offers a wide range of functionality for modeling and simulation of batteries: from the fundamental processes in the electrodes and electrolytes of batteries to cell-to-cell temperature and current distributions in battery packs. These simulations may involve the transport of charged and neutral species, current conduction, fluid flow, heat transfer, and electrochemical reactions in porous electrodes.

You can use this module to investigate the performance of batteries at different operating conditions and for different electrode configurations, separators, current collectors and feeders, materials, and chemistry. The description of the involved processes and phenomena may be defined in a fairly detailed manner, whereby you can apply different hypotheses to gain an understanding of the investigated systems. With these detailed models you can study the influence of different electrode materials, pore distribution, electrolyte composition, and other fundamental parameters on various aspects such as battery performance, as well as capacity and power fade.

The module also allows for more lumped (“black-box”) modeling approaches where detailed knowledge of the battery chemistry is not required. Such lumped models can be used for investigating cell-to-cell dynamics in packs, thermal management, as well as battery dynamics in electrical circuit simulations. The small set of parameters used in lumped models are well suited for fitting to load-cycle experimental data, and parameter estimation tools, using optimization solvers, are also included in the Battery Design Module.

You can couple the battery models to other physics such as heat transfer, fluid flow, structural mechanics, and chemical species transport in order to study phenomena like aging, heat dissipation effects and stress-strain relationships.

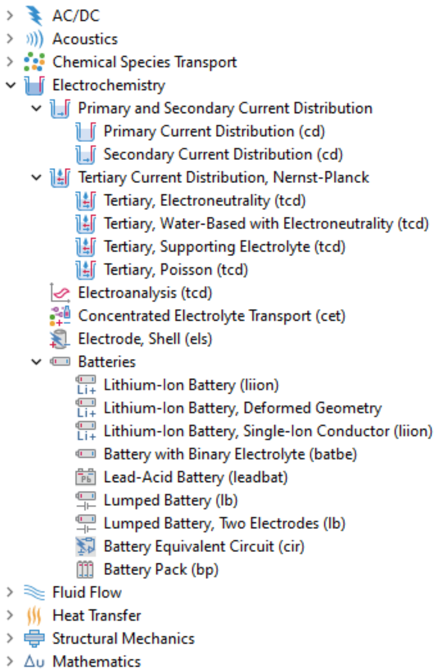


Figure 1: The 3D physics interfaces for the Battery Design Module, as shown in the Model Wizard, with the Electrochemistry branch fully expanded.

The figure above shows the available physics interface in the Battery Design Module under the Electrochemistry ( ) branch. These electrochemistry interfaces are based on the conservation of current, charge, chemical species, and energy. The Battery Interfaces form the basis for battery cell and pack modeling.

The Chemical Species Transport ( ), the Fluid Flow ( ) and the Heat Transfer ( ) interfaces are extended with functionality for battery modeling, for instance features for handling porous media. The different physics interfaces are further discussed below.

The Battery Design Module has a number of physics interfaces to model batteries. Choice of physics interface depends on the overall purpose of the model.

Detailed Cell Models

When studying the cell chemistry, aging, or high charge-discharge rates one typically resolves the different layers of the battery using space-dependent models on a micrometer scale, whereas coarser models for computing heat sources or predicting the voltage behavior for low or moderate charge-discharge rates may use a more lumped modeling approach.

Space-dependent battery models often model unit cells that consist of:

a) Current collectors and current feeders

b) Porous or solid metal electrodes

c) The electrolyte that separates the anode and cathode

To exemplify, we describe some of the charge and discharge processes in a rechargeable battery below.

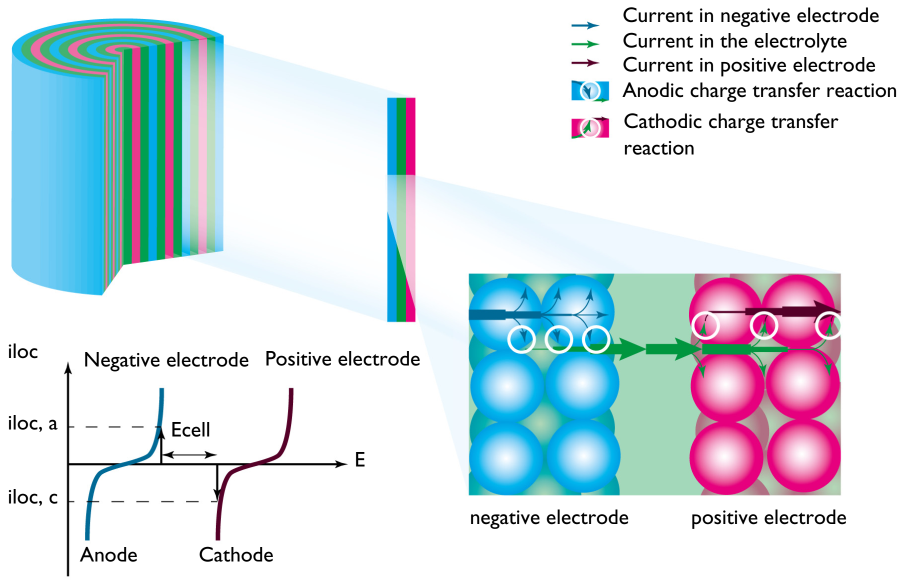


Figure 2: Direction of the current and charge transfer current during discharge in a battery with porous electrodes.

During discharge, chemical energy is transferred to electric energy in the charge transfer reactions at the anode and cathode. The conversion of chemical to electric energy during discharge may involve electrochemical reactions, transport of electric current, transport of ions and neutral species in the electrolyte, mass transport in the electrode particles, fluid flow, and the release of heat in irreversible losses, such as ohmic losses and losses due to activation energies.

Figure 2 shows a schematic picture of the discharge process. The current enters the cell from the current feeder at the negative electrode. The charge transfer reaction occurs at the interface between the electrode material and electrolyte contained in the porous electrode, also called the pore electrolyte. Here, an oxidation of the electrode material may take place through an anodic charge transfer reaction, denoted $i_{loc, a}$ in Figure 2. The shapes of the two curves in the graph are described by the electrode kinetics for the specific materials. The reaction may also involve the transport of chemical species from the pore electrolyte and also from the electrode particles.

From the pore electrolyte, the current is conducted by the transport of ions through the electrolyte that separates the positive and negative electrode (via separator or reservoir) to the pore electrolyte in the positive electrode.

At the interface between the pore electrolyte and the surface of the particles in the porous electrode, the charge transfer reaction transfers the electrolyte current to current conducted by electrons in the positive electrode. At this interface, a reduction of the electrode material takes place through a cathodic charge transfer reaction, denoted $i_{loc, c}$ in Figure 3. Also here, the charge transfer reaction may involve the transport of chemical species in the electrolyte and in the electrode particles.

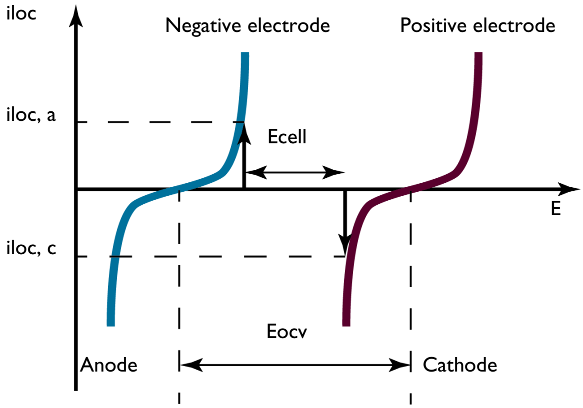


Figure 3: Electrode polarization during discharge. The figure is same as inset of Figure 2.

The current leaves the cell through the current collector. The conduction of current and the electrochemical charge transfer reactions also release heat due to ohmic losses, activation losses, and other irreversible processes.

The graph in Figure 3 plots the charge transfer current density, i_{loc}, as a function of the electrode potential, E. These curves describe the polarization of the electrodes during discharge.

The negative electrode is polarized anodically during discharge, a positive current as indicated by the arrow in Figure 3. The potential of the negative electrode increases. The positive electrode is polarized cathodically, a negative current as indicated by the arrow. The potential of the positive electrode decreases.

Consequently, Figure 3 also shows that the potential difference between the electrodes, here denoted E_{cell}, decreases during discharge compared to the open cell voltage, here denoted E_{ocv}. The value of E_{cell} is the cell voltage at a given current i_{loc}, if the ohmic losses in the cell are negligible. This is usually not the case in most batteries. This implies that the cell voltage in most cases is slightly smaller than that shown in Figure 3.

During charge, the processes are reversed; see Figure 4. Electric energy is transformed to chemical energy that is stored in the battery.

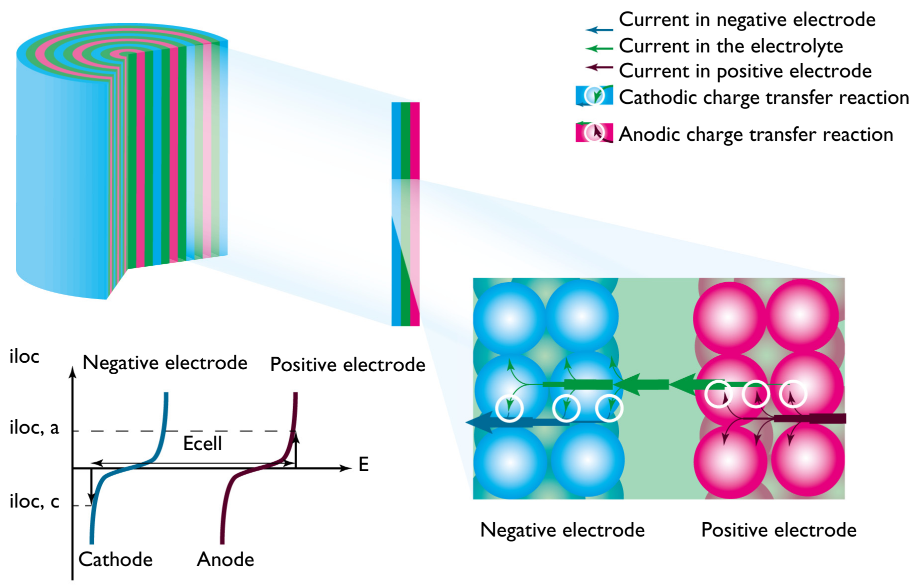


Figure 4: During charge, the positive electrode acts as the anode while the negative one acts as the cathode. The cell voltage increases (at a given current) compared to the open cell voltage. Note: direction of the currents is reversed here.

The current enters the cell at the positive electrode. Here, during charge, an oxidation of the products takes place through an anodic charge transfer reaction. The positive electrode is polarized anodically, with a positive current, and the electrode potential increases.

The current is then conducted via pore electrolyte, through the electrolyte in a separator (or a reservoir) that separates the electrodes, to the negative electrode.

In the negative electrode, a reduction of the products from the previous discharge reaction takes place through a cathodic charge transfer reaction. The negative electrode is polarized cathodically and the electrode potential decreases.

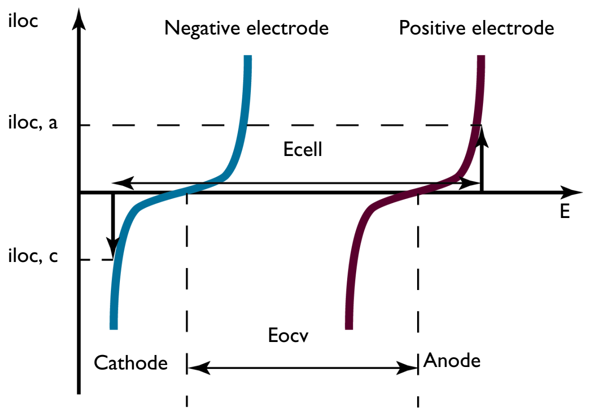


Figure 5: Electrode polarization during charge.

The difference in potential between the electrodes, here denoted E_{cell}, at a given i_{loc}, increases during charge, compared to the open cell voltage, here denoted E_{ocv}; see Figure 5. The value of E_{cell} is equal to the cell voltage when ohmic losses are neglected. In most cells, these losses are not negligible and they would add to the cell voltage.

The battery processes and phenomena described in the figures above can all be investigated using the Battery Design Module. The physics interfaces included in the module allow you to investigate the influence on battery performance and thermal management of parameters such as the:

- Choice of materials and chemistry
- Dimensions and geometry of the current collectors and feeders
- Dimension and geometry of the electrodes
- Size of the particles that the porous electrodes are made of
- Porosity and specific surface area of the porous electrode
- Configuration of the battery components

- The kinetics of interfacial and bulk reactions
- Potential or applied current dependent load cycles
- Aging of electrochemical cells

Lumped Models

When modeling larger systems such as a battery pack, including detailed geometrical details of the individual battery layers, electrode structures and chemistry may not be practical from a modeling point of view. Many details about the battery cell may not be known to the modeler, and numerical constraints (memory and computational time) may favor less complex models. For these cases one often replaces the detailed cell model by simpler zero-dimensional cell elements, forming an equivalent circuit, lumped battery or single particle model. For instance, instead of a detailed mass and charge balance of charge-carrying ions in the electrolyte phase along the length of the negative electrode, the separator, and the positive electrode, all voltage contributions from these phenomena are lumped into a single resistor.

In a battery pack model a number of these zero-dimensional models for each battery cell are then combined to define the cell-to-cell current distribution of the pack.

The Battery Modeling Physics Interfaces

The Lithium-Ion Battery interface ( ) is tailored detailed modeling of lithium-ion batteries using liquid electrolytes and includes functionality that describes the transport of charged species in porous electrodes, electrolyte, intercalation reactions in electrodes, binders, charge transfer reactions, internal particle diffusion, temperature dependence of transport quantities, aging mechanism, and the solid electrolyte interface (SEI).

The Lithium-Ion Battery, Single-Ion Conductor interface ( ) is similar to the above interface, but uses a different default for charge-balance equation in the electrolyte, typically suitable for solid electrolytes.

The Battery with Binary Electrolyte interface ( ) describes the conduction of electric current in the electrodes, the charge transfer reactions in the porous electrodes, the mass transport of ions in the pore electrolyte and in the electrolyte that separates the electrodes, and the intercalation of species in the particles that form the porous electrodes. The descriptions are available for cells with basic aqueous binary electrolytes, which for instance covers nickel-metal hydride and nickel-cadmium batteries.

The Lumped Battery interface ( ) defines a battery model based on a small set of lumped parameters, requiring no knowledge of the internal structure or design of the battery electrodes, or choice of materials. Models created with the Lumped Battery interface can typically be used to monitor the state-of-charge and the voltage response of a battery during a load cycle. The interface also defines a battery heat source that may be coupled to a Heat Transfer interface for modeling battery cooling and thermal management.

The Lumped Battery, Two Electrodes interface ( ) offers a slightly more advanced definition of the battery model where each electrode material is handled individually, but still in a lumped context. It accounts for solid diffusion in the electrode particles, the intercalation electrode reaction kinetics and ohmic potential drop in the separator using a lumped solution resistance term. Models defined in this way are also known as single-particle models in literature.

The Battery Equivalent Circuit ( ) can be used to define a battery model based on an arbitrary number of electrical circuit elements. Models created with the Battery Equivalent Circuit can typically be used to monitor the state-of-charge and the voltage response of a battery during a load cycle. When selecting the Battery Equivalent Circuit in the Model Wizard, this adds an Electrical Circuit ( ) interface to the model, including a number of predefined circuit elements that are used to define the open circuit voltage, the load current and an internal resistance. You can add additional circuit elements such as resistors, capacitors, and inductors.

The Lead-Acid Battery interface ( ) is tailored for this type of battery and includes functionality that describes the transport of charged species, charge transfer reactions, the variation of porosity due to charge and discharge, and the average superficial velocity of the electrolyte caused by the change in porosity.

The Battery Pack interface ( ) features a one-to-many approach for setting up multiple lumped battery models and for connecting them in a 3D geometry. The Battery Pack interface is typically used together with a heat transfer interface for modeling of thermal pack management. The interface also includes thermal events, which can be used to study thermal runaway propagation problems.

The current distribution interfaces are generic electrochemical cell interfaces. The Tertiary Current Distribution, Nernst-Planck interface ( ) describes the transport of charged species in diluted electrolytes through diffusion, migration, and convection. In addition, it also includes ready-made formulations for porous and nonporous electrodes, including charge transfer reactions and current conduction in the electronic conductors.

The Concentrated Electrolyte Transport interface ( ) is a generic interface for defining electrolyte transport. The electrolyte transport model is based on concentrated solution theory and can be applied to any type of electrochemical cell for an arbitrary number of electrolyte species, for instance cells based on molten-salt or ionic-liquid electrolytes. The Lithium-Ion, Battery with Binary Electrolyte and Lead-Acid interfaces mentioned above all make use of variants of concentrated solution theory for specific ternary (anion/cation/solvent) electrolyte systems.

The Chemical Species Transport interfaces ( ) can be used to describe for instance the transport of trace ions in the pore electrolyte and in the electrolyte that separates the anode and cathode. Reactions other than pure electrochemical reactions can be added to, for example, describe the degradation of materials.

The Chemistry interface ( ), found within the Chemical Species Transport branch, can be used to define systems of reacting species, electrode reactions and ordinary chemical reactions. As such, it serves as a reaction kinetics and material property provider to the space-dependent transport interfaces, such as the Tertiary Current Distribution, Nernst–Planck interface, or Transport of Diluted Species interface.

The Fluid Flow interfaces ( ) describe the fluid flow in the porous electrodes and in free media if this is relevant for a specific type of battery, for example, certain types of lead-acid batteries.

The Heat Transfer in Porous Media interface ( ) describes heat transfer in the cells. This includes the effects of Joule heating in the electrode material and in the electrolyte, heating due to activation losses in the electrochemical reactions, and of the net change of entropy. The heat from reactions other than the electrochemical reactions can also be described by these physics interfaces. The heat transfer interfaces are also extended with tailor-made functionality for homogenization of layered battery materials, which are typically used in thermal simulations of battery packs.

The Solid Mechanics interface ( ) is extended with functionality for modeling electrode strain due to, for instance, lithium intercalation in graphite electrodes.

Physics Interface Guide by Space Dimension and Study Type

The table lists the physics interfaces available in the Battery Design Module in addition to those included with the COMSOL basic license.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Chemical Species Transport				
Transport of Diluted Species		tds	all dimensions	stationary; time dependent
Transport of Concentrated Species		tcs	all dimensions	stationary; time dependent
Chemistry		chem	all dimensions	stationary; time dependent
Nernst–Planck–Poisson Equations		tds+es	all dimensions	stationary; time dependent; stationary source sweep; small-signal analysis, frequency domain
Electrophoretic Transport		el	all dimensions	stationary; stationary with initialization; time dependent; time dependent with initialization
Transport of Diluted Species in Porous Media		tds	all dimensions	stationary; time dependent
Transport of Concentrated Species in Porous Media		tcs	all dimensions	stationary; time dependent
Surface Reactions		sr	all dimensions	stationary (3D, 2D, and 2D axisymmetric models only); time dependent
Transport of Diluted Species in Fractures		dsf	3D, 2D, 2D axisymmetric	stationary; time dependent
Reacting Flow				
Laminar Flow, Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Laminar Flow, Concentrated Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Reacting Flow in Porous Media				
Transport of Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Reacting Flow				
Brinkman Equations		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Electrochemistry				
Primary Current Distribution Secondary Current Distribution		cd	all dimensions	stationary; stationary with initialization; time dependent; time dependent with initialization; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
Tertiary Current Distribution, Nernst–Planck (Electroneutrality, Water-Based with Electroneutrality, Supporting Electrolyte, Poisson)		tcd	all dimensions	stationary; stationary with initialization; time dependent; time dependent with initialization; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
Concentrated Electrolyte Transport		cet	all dimensions	stationary; stationary with initialization; time dependent; time dependent with initialization;

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Electroanalysis		tcd	all dimensions	stationary; time dependent; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent; cyclic voltammetry
Electrode, Shell		els	3D, 2D, 2D axisymmetric	stationary; time dependent
Battery Interfaces				
Lithium-Ion Battery (Binary 1:1 Liquid Electrolyte, Single-Ion Conductor)		liion	all dimensions	stationary; time dependent; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
Battery with Binary Electrolyte		batbe	all dimensions	stationary; time dependent; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
Lead–Acid Battery		leadbat	all dimensions	stationary; time dependent; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
Lumped Battery		lb	all dimensions	time dependent; AC impedance, initial values;
Battery Equivalent Circuit		ec	Not space dependent	stationary; time dependent; frequency domain
Battery Pack		bp	3D	time dependent
Fluid Flow				
Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Darcy's Law		dl	all dimensions	stationary; time dependent
Free and Porous Media Flow, Brinkman		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Darcy		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Flow				
Brinkman Equations		—	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF
Heat Transfer				
Heat Transfer in Porous Media		ht	all dimensions	stationary; time dependent

Tutorial of a Lithium-Ion Battery

The following tutorial defines a three-dimensional model of a lithium-ion battery pouch cell. In the 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.

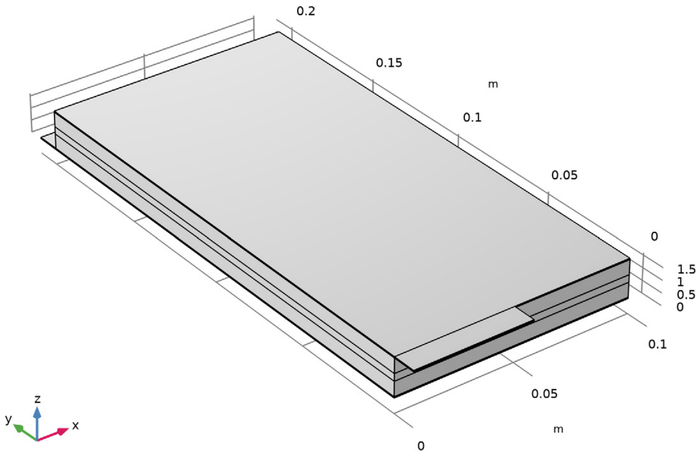
The aim of the tutorial is to get acquainted to the most common features in the Lithium-Ion Battery interface for battery modeling, and to investigate the current distribution and electrode utilization in a large format lithium-ion battery pouch cell.

(A more common, and computationally more favorable, approach for battery modeling is often to define the model geometry in 1D, and as we will see in this tutorial, this is often a valid approximation. Tutorials featuring more conventional geometries are available in the *Battery Design Module Application Library*.)

The model defines and solves the current and material balances in the lithium-ion battery. The intercalation of lithium inside the particles in the porous electrodes is solved using a fourth independent variable r for the particle radius (x, y, and t are the other three). The reaction kinetics and the intercalation are coupled to the material and current balances at the surface of the particles. The model equations are found in the *Battery Design Module User's Guide*. The model was originally formulated for 1D simulations by John Newman and his coworkers at the University of California at Berkeley. The original 1D model is popularly known as pseudo-2D model (or P2D model) in literature, for our 3D case the corresponding popular name would be P4D.

Model Definition

The cell geometry is shown in the figure below. Note that all plots are scaled 100 times in the *z* direction due to the high aspect ratio of the geometric features.



Model geometry, scaled 100 times in the z direction.

The geometry defines one foil-to-foil unit cell, stacking five layers in the z direction:

- Negative metal current collector foil: 10 mm, Cu (due to symmetry, half of this thickness is used in the model geometry)
- Negative electrode: 60 mm, graphite
- Separator: 30 mm
- Positive electrode: 60 mm, LMO
- Positive metal current collector foil: 10 mm, Al (due to symmetry, half of this thickness is used in the model geometry)

The electrolyte is $LiPF_6$ dissolved in the organic solvents EC and EMC at a 3:7 ratio.

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).

The Lithium-Ion Battery interface is used to set up the physics, using Material data from the Battery Material Library. After finishing the modeling instructions later the part of the model tree defining the materials and physics will look as below.

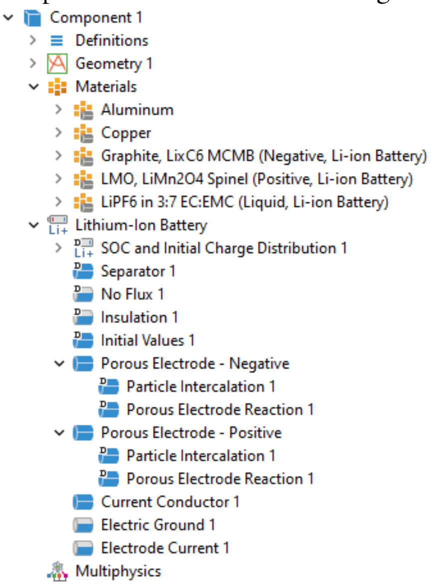


Figure 6: Part of the model tree defining the materials and physics.

The Particle Intercalation subnodes to the Porous Electrode nodes model the solid lithium concentration in an additional particle dimension (extra dimension).

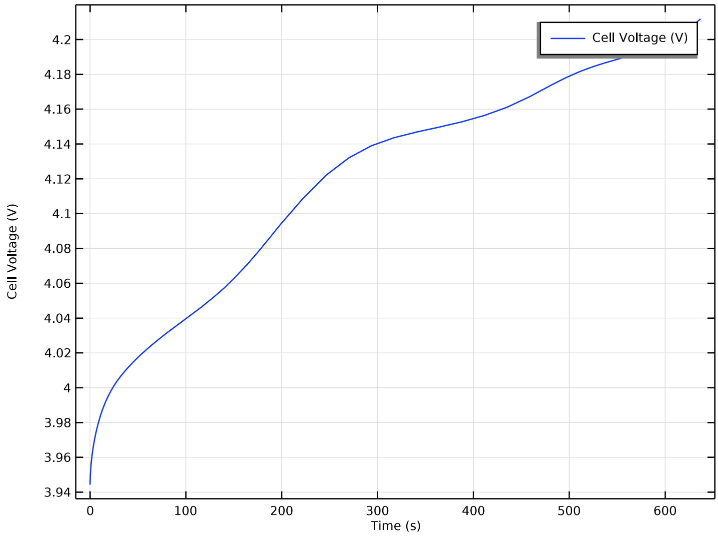
The SOC and Initial Cell Charge Distribution node is used to set the initial cell state of charge.

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 time-dependent solver is used to simulate the charging from a 20% to 90% cell state of charge at a rate of 4 C. (A 1 C rate corresponds to the charge or discharge current required to fully charge or discharge the battery in 1 h).

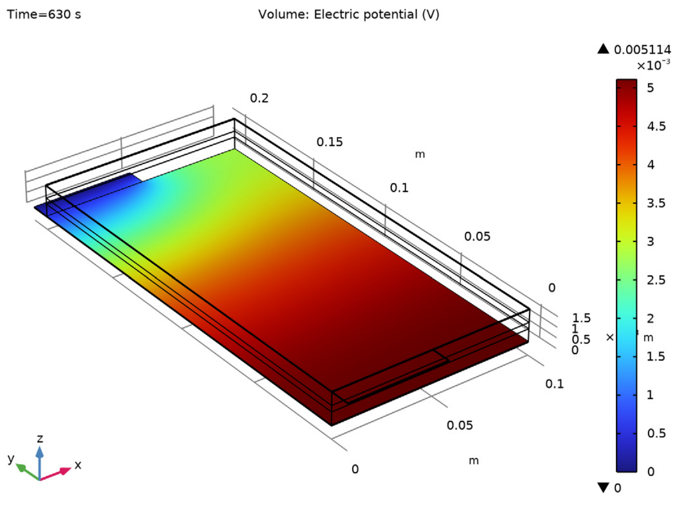
Results and Discussion

The figure below shows the simulated cell voltage vs time.

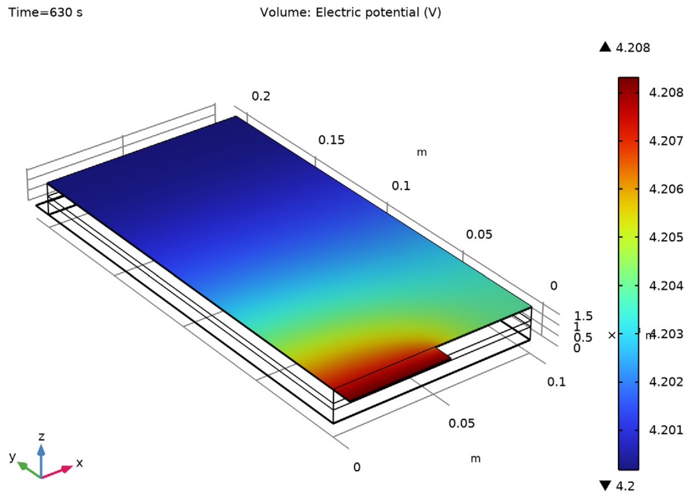


Cell voltage vs time.

The two following figures show the potential distribution in the negative and positive metal foils (current collector and tab) at the end of the 4C charge.



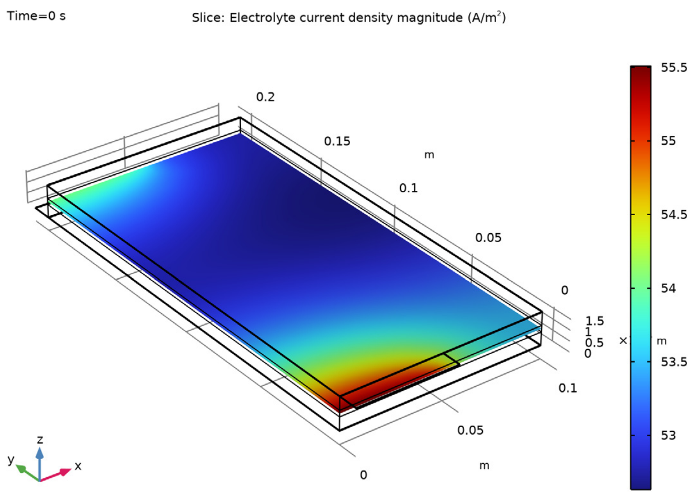
Potential distribution in the negative metal foil at the end of the 4C charge.



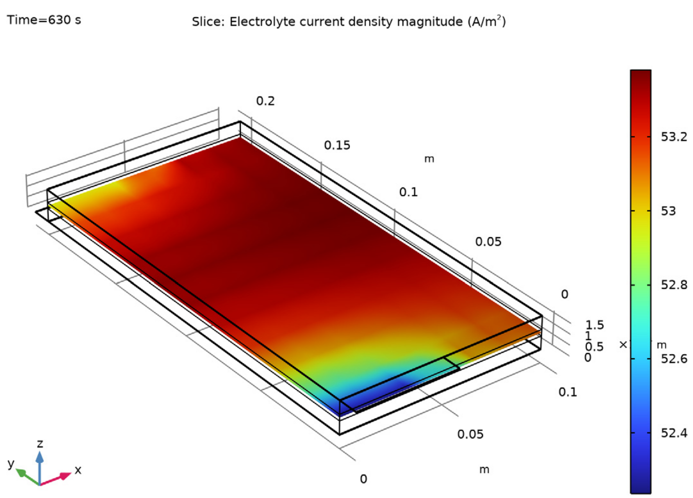
Potential distribution in the positive metal foil at the end of the 4C charge.

The potential variation is about 5 mV in the negative current collector and 9 mV in the positive current collector at the 4C charge current. For a 1C charge current the corresponding potential variation would be below 2 mV (results not shown here).

The two figures below show the electrolyte current magnitude 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 would be 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.



Current density magnitude in the middle of the separator at the beginning of the 4C charge.



Current density magnitude in the middle of the separator at the end of the 4C charge.

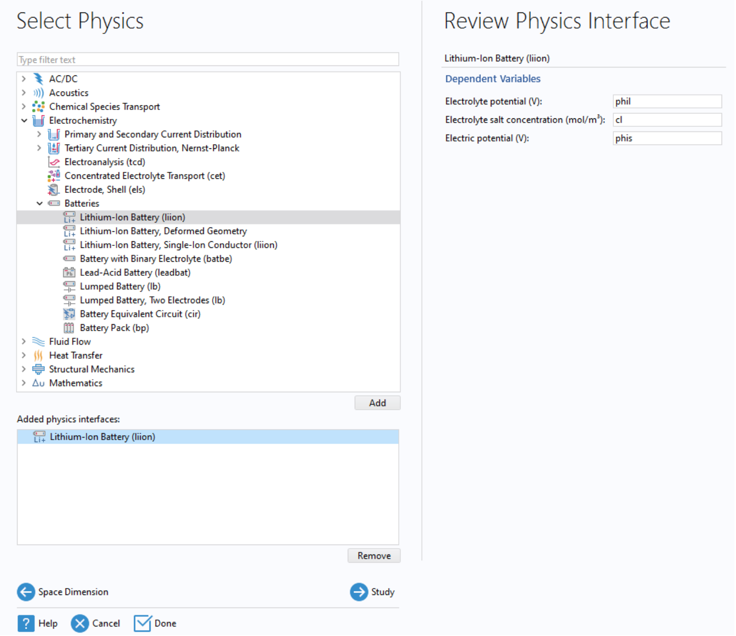
The following instructions show how to formulate, solve, and reproduce this model.

Model Wizard

1. To start the software, double-click the COMSOL Multiphysics icon on the desktop. When the software opens, you can choose to use the Model Wizard to create a new COMSOL Multiphysics model or Blank Model to create one manually. For this tutorial, click the Model Wizard button.

   If COMSOL Multiphysics is already open, you can start the Model Wizard by selecting New from the File menu and then click Model Wizard.

2. From the File menu, choose New.
3. In the New window, click Model Wizard.
4. In the Model Wizard window, click 3D.
5. In the Select Physics tree, select Electrochemistry > Batteries > Lithium-Ion Battery (liion) and click Add.

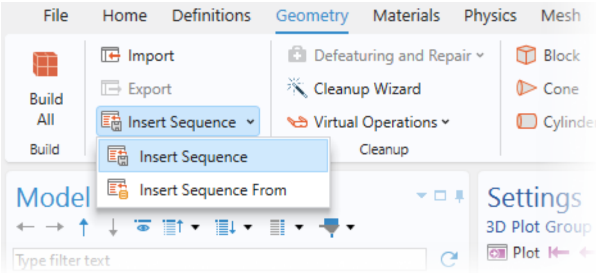


6. Click Study.
7. In the Select Study tree, select Preset Studies for Selected Physics Interfaces > Time Dependent with Initialization.
8. Click Done.

Geometry 1

The model geometry is available as a parameterized geometry sequence in a separate MPH-file. Load it from file with the following steps.

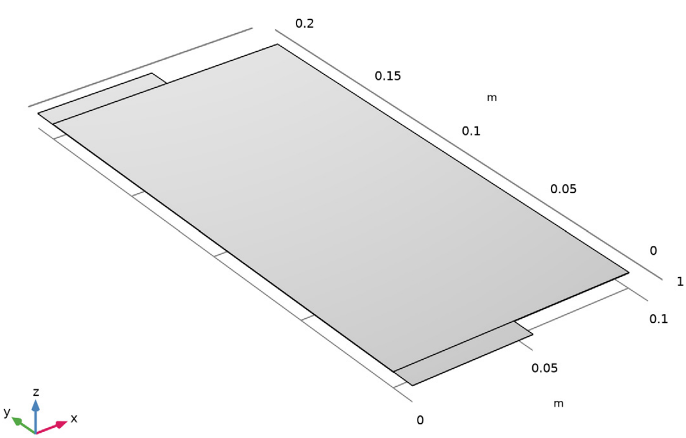
1 In the Geometry toolbar, click Insert Sequence and choose Insert Sequence.



2 Browse to the model's Application Libraries folder and double-click the file `pouch_cell_utilization_geom_sequence.mph`. Note that the location of the files used in this exercise may vary depending on the installation. For example, if the installation is on your hard drive, the file path might be similar to `C:\Program Files\COMSOL\COMSOL63\Multiphysics\applications\Battery_Design_Module\Lithium-Ion_Batteries,_Performance\`.

3 In the Geometry toolbar, click Build All.

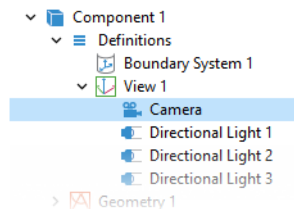
4 In the Model Builder window, under Component 1 click Geometry 1.



5 Since the geometry has now been finalized, you may now collapse the Geometry 1 node in the Model Builder window.

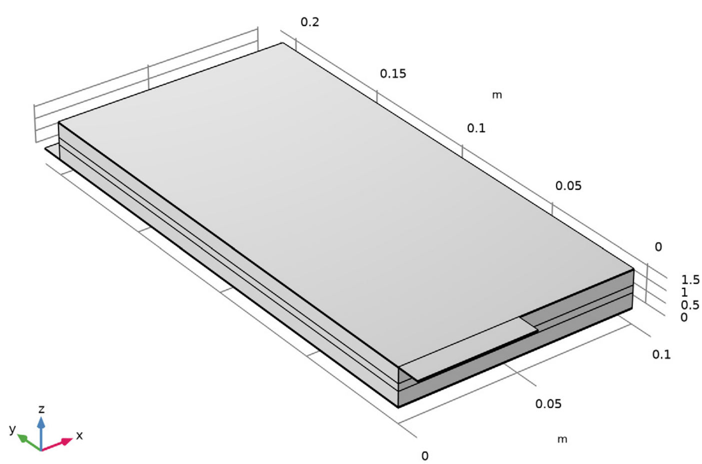
Change the Scaling of the Graphics Window

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:



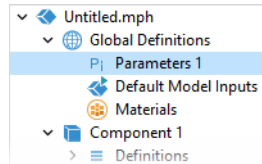
Camera

1 In the Model Builder window, expand the Component 1 > Definitions node, expand the View 1 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.



Parameters

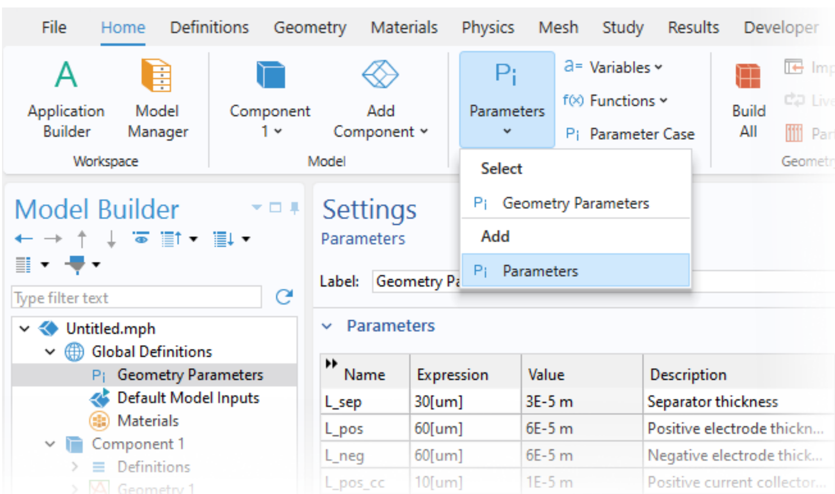
Some parameters were loaded with the geometry sequence into the Parameters 1 node.



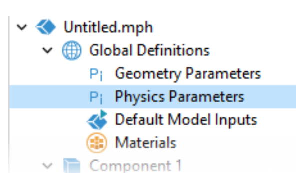
1 In the Model Builder window, under Global Definitions click Parameters 1.
2 In the Settings window for Parameters, type `Geometry Parameters` in the Label text field to rename it.

Add some more parameters from a text file.

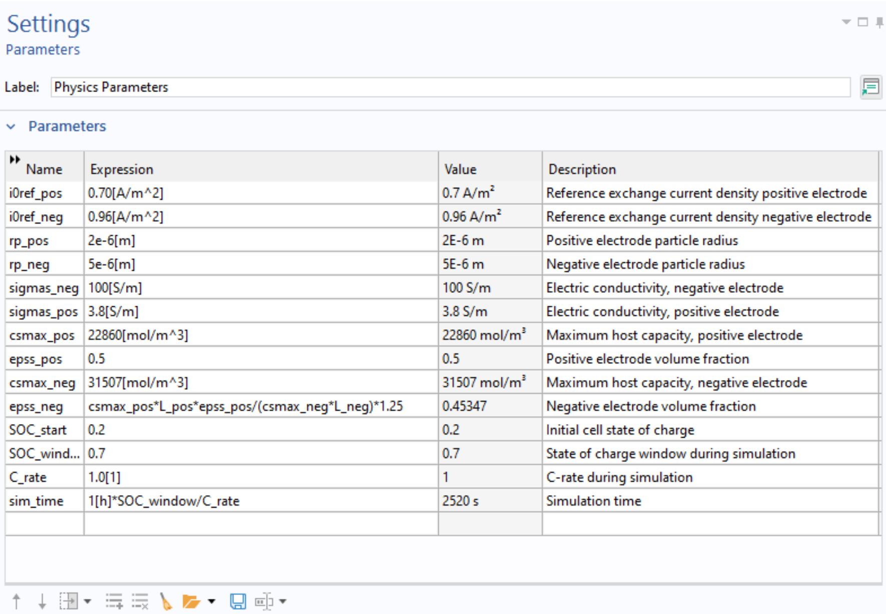
1 In the Home toolbar, click Pi Parameters and choose Add > Parameters.



2 In the Settings window for the new Parameters node, type `Physics Parameters` in the Label text field.
3 Locate the Parameters section. Click Load from File.



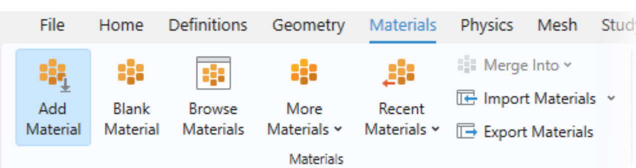
4 Browse to the model's Application Libraries folder and double-click the file `pouch_cell_utilization_physics_parameters.txt`.



Name	Expression	Value	Description
i0ref_pos	0.70[A/m^2]	0.7 A/m²	Reference exchange current density positive electrode
i0ref_neg	0.96[A/m^2]	0.96 A/m²	Reference exchange current density negative electrode
rp_pos	2e-6[m]	2E-6 m	Positive electrode particle radius
rp_neg	5e-6[m]	5E-6 m	Negative electrode particle radius
sigmas_neg	100[S/m]	100 S/m	Electric conductivity, negative electrode
sigmas_pos	3.8[S/m]	3.8 S/m	Electric conductivity, positive electrode
csmax_pos	22860[mol/m^3]	22860 mol/m³	Maximum host capacity, positive electrode
epss_pos	0.5	0.5	Positive electrode volume fraction
csmax_neg	31507[mol/m^3]	31507 mol/m³	Maximum host capacity, negative electrode
epss_neg	csmax_pos*L_pos*epss_pos/(csmax_neg*L_neg)*1.25	0.45347	Negative electrode volume fraction
SOC_start	0.2	0.2	Initial cell state of charge
SOC_wind...	0.7	0.7	State of charge window during simulation
C_rate	1.0[1]	1	C-rate during simulation
sim_time	1[h]*SOC_window/C_rate	2520 s	Simulation time

Add Materials

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

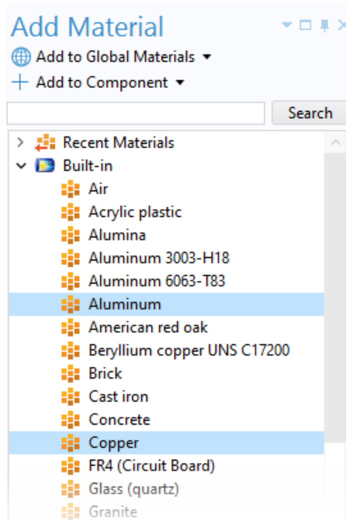


1 In the Materials toolbar, click Add Material to open the Add Material window.

2 Go to the Add Material window.

3 In the tree, select both Built-in > Aluminum and Built-in > Copper.

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

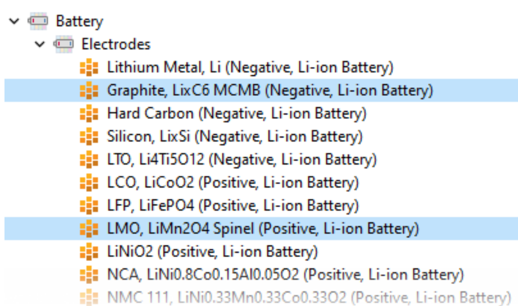


Next add the material properties for the electrolyte and electrode materials.

1 Go to the Add Material window.

2 In the tree, select both Battery > Electrodes > Graphite, LixC6 MCMB (Negative, Li-ion Battery) and Battery > Electrodes > LMO, LiMn2O4 Spinel (Positive, Li-ion Battery).

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



4 Similarly, in the tree, select Battery > Electrolytes > LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) and click the Add to Component button in the window toolbar.

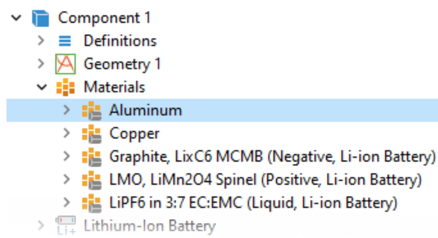
5 In the Materials toolbar, click Add Material to close the Add Material window.

A red cross may show at the Aluminum node at this point, indicating missing material properties.This is expected and will be fixed later when setting up the physics. Also, no selection warnings may be seen at the other material nodes.

Assign the Materials to the Domains of the Geometry

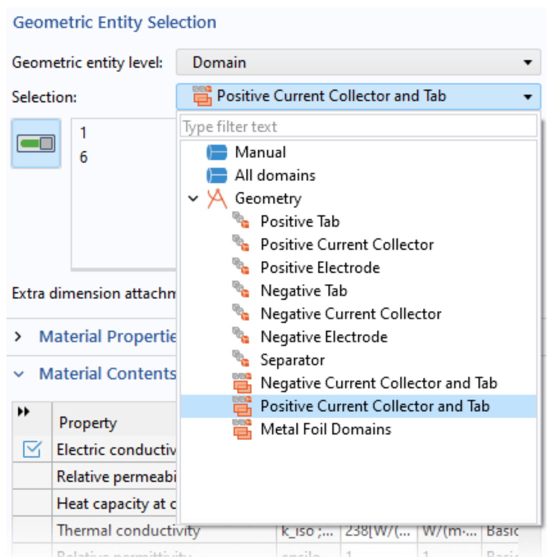
Assign the materials to the corresponding battery domains.

1 In the Model Builder window, click Aluminum.



2 In the Settings window for the Materials>Aluminum node, locate the Geometric Entity Selection section.

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



The named selections that appear in the list are created under the Geometry node, and were automatically included in the geometry sequence file you imported earlier.

Proceed similarly for the other materials:

1 Click Copper, and in the corresponding Geometric Entity Selection section, choose Negative Current Collector and Tab.

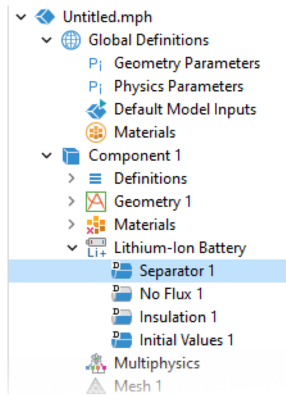
2 Click Graphite, LixC6 MCMB (Negative, Li-ion Battery) and choose Negative Electrode.

3 Click LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) and choose Positive Electrode.

4 Click LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) and choose Separator.

The geometry has now been defined, and we have imported the needed parameters. We are now ready to start defining the actual physics of the problem.

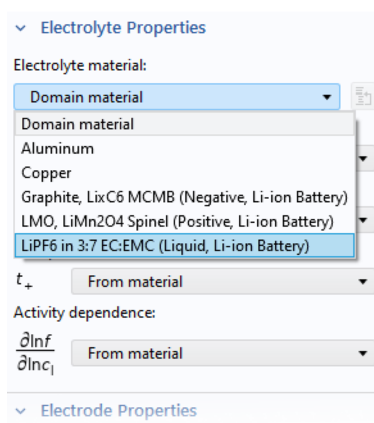
The Separator node was added to the interface by default.



Add and Define the Negative Electrode

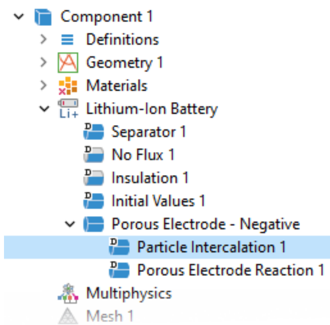
Keep the default settings for the Separator, and proceed to add and set up the physics in the porous electrodes and current collectors.

1. In the Physics toolbar, click Domains 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) .
5. Locate the Electrode Properties section. In the σ_s text field, type `sigmas_neg`.
6. Locate the Porous Matrix Properties section. In the ε_s text field, type `epss_neg`.
7. In the ε_l text field, type `1-epss_neg`.



Particle Intercalation 1

1 In the Model Builder window, click Particle Intercalation 1.
2 In the Settings window for Particle Intercalation, locate the Particle Transport Properties section.
3 In the r_p text field, type `rp_neg`.



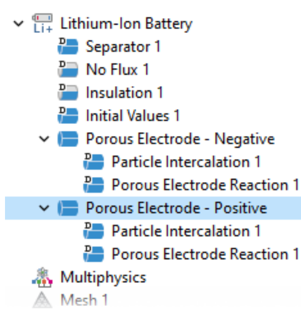
Leave the settings of the Species Settings section as is for now. The initial species concentration setting will be made inactive later when we define the cell state of charge on a different node.

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 $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_neg`.

Add and Define the Positive Electrode

Proceed similarly to define the positive electrode.



1 In the Physics toolbar, click Domains and choose Porous Electrode and rename the node by typing `Porous Electrode - Positive` in the Label text field.
2 Locate the Domain Selection section. From the Selection list, choose Positive Electrode.
3 Locate the Electrolyte Properties section. From the Electrolyte material list, choose LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery.
4 Locate the Electrode Properties section. In the σ_s text field, type `sigmas_pos`.
5 Locate the Porous Matrix Properties section. In the ε_s text field, type `epss_pos`.
6 In the ε_l text field, type `1-epss_pos`.

Particle Intercalation 1

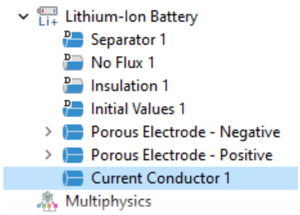
1 Click Particle Intercalation 1 child node and in the Particle Transport Properties section, in the r_p text field, type `rp_pos`.

Porous Electrode Reaction 1

1. Click Porous Electrode Reaction 1 and in the Electrode Kinetics section, type `i0ref_pos`.

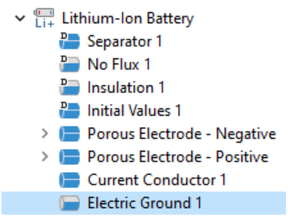
Current Conductor 1

1. 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.



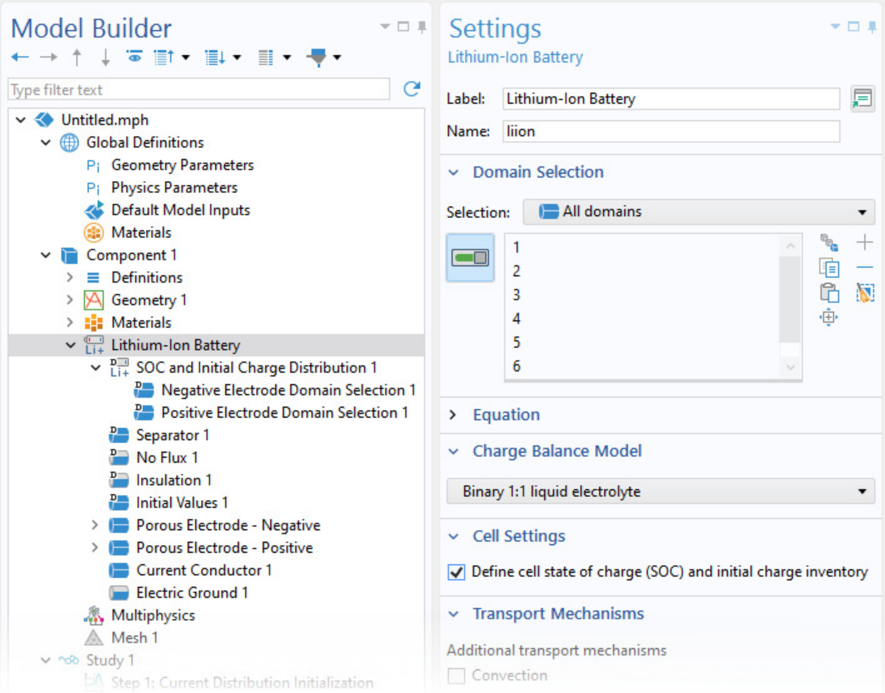
Electric Ground 1

1. 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 SOC and Initial Charge Distribution

1 Enable the Define cell state of charge (SOC) and initial charge inventory on the Lithium-Ion Battery interface top node. This will allow us to set the initial SOC of the battery cell.

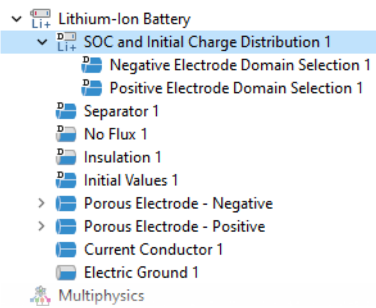


Then set the initial state of charge of the cell as follows:

2 In the Model Builder window, click SOC and Initial Charge Distribution 1.

3 In the Settings window for SOC and Initial Charge Distribution, locate the Initial Cell Charge Distribution section.

4 In the SOC_0 text field, type `SOC_start`.



Set the Electrode Domain Selections

1 In the Model Builder window, click Negative Electrode Domain Selection 1.

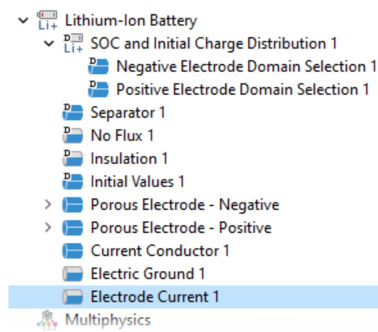
2 In the Settings window for Negative Electrode Domain Selection, locate the Domain Selection section. From the Selection list, choose Negative Electrode.

Proceed similarly for the positive selection:

3 Click Positive Electrode Domain Selection 1, choose Positive Electrode.

Electrode Current 1

Enabling the SOC and Initial Charge Distribution node means that the capacity of the cell can be defined. Add the final current boundary condition current based on a C-rate multiple as follows:



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

2 In the Settings window for Electrode Current, locate the Boundary Selection section.

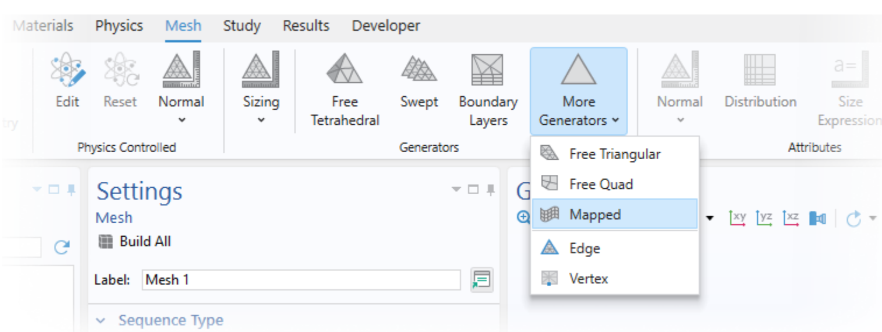
3 From the Selection list, choose Positive Tab End.

4 Locate the Electrode Current section. From the list, choose C-rate multiple.

5 In the C_{rate} text field, type `C_rate`.

Mesh 1

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

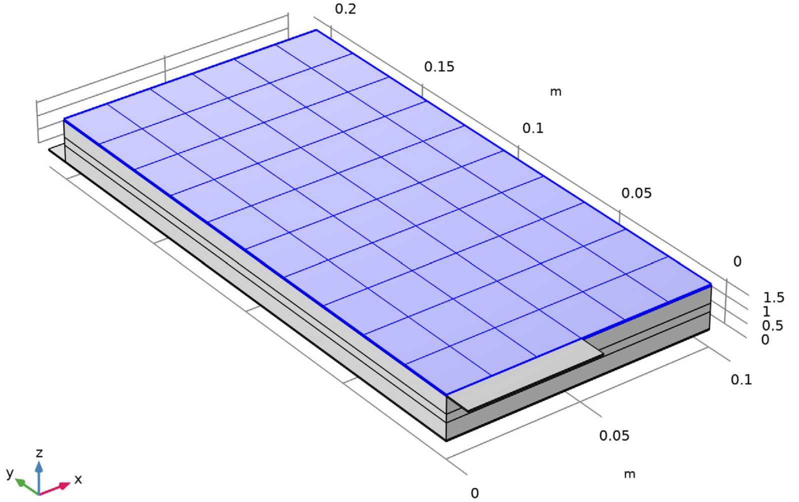


Add a Mapped on the Topmost Boundary

1 In the Mesh toolbar, click More Generators and choose Mapped.

2 Select Boundary 20 only. (This is the topmost boundary of the geometry.)

3 Click Build Mesh.

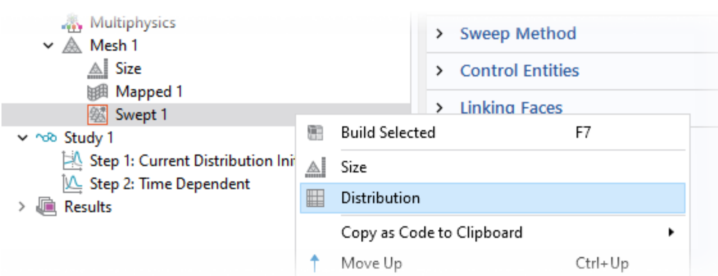


Add a Swept Mesh

1 In the Mesh toolbar, click Swept.

Distribution of Mesh Elements in the Negative Electrode

1 Right-click Swept 1 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`.

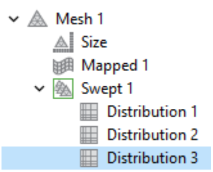
Proceed similarly for the other domains, with different number of element and ratio settings as follows:

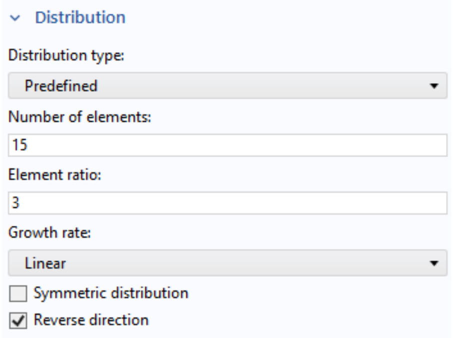
Distribution of Mesh Elements in the Separator

1 In the Model Builder window, right-click Swept 1 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`. Keep the other default settings.

Distribution of Mesh Elements in the Positive Electrode

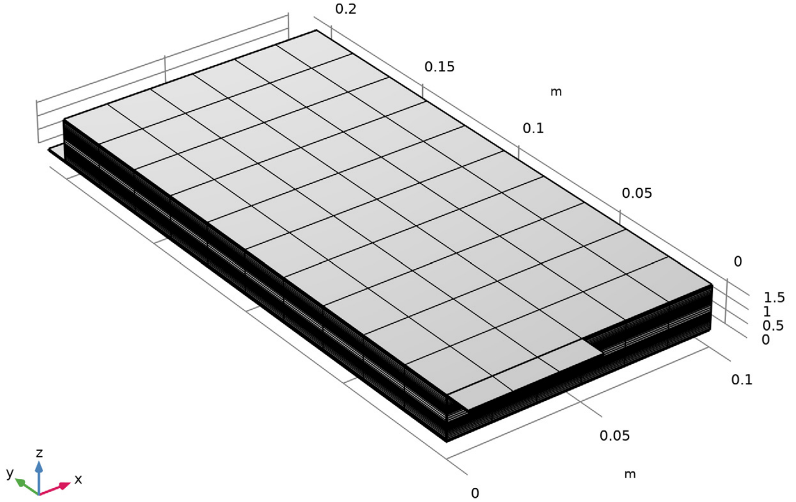
1 Right-click Swept 1 and choose Distribution.
2 In the Settings window for Distribution, locate the Domain Selection section.
3 From the Selection list, choose Positive Electrode.
4 Locate the Distribution section. From the Distribution type list, choose Predefined.
5 In the Number of elements text field, type `15`.
6 In the Element ratio text field, type `3`.
7 Select the Reverse direction checkbox.





8 Click Build Mesh.

The finalized mesh should now look as follows.



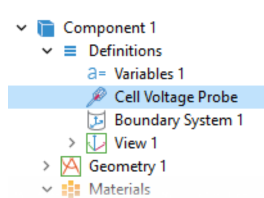
Definitions

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.

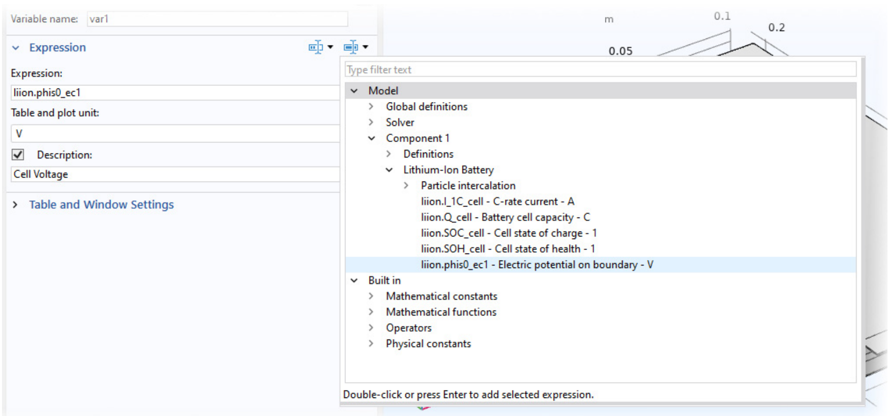
Cell Voltage Probe

1 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 1 (comp1) > Lithium-Ion Battery > liion.phis0_ec1 - Electric potential on boundary - V.

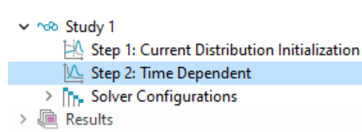


4 Select the Description checkbox. In the associated text field, type `Cell Voltage`.

Study 1

The physics is now fully defined and ready for solving. Change the output times based on the `sim_time` parameter to store the solution at the beginning of, half way into, and at the end of the charge 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 sim_time/2 sim_time`.

4 In the Study toolbar, click Compute.

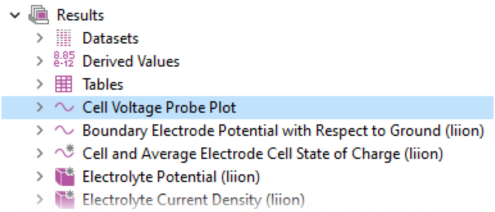
The model takes approximately 2-3 minutes to solve.

Results

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

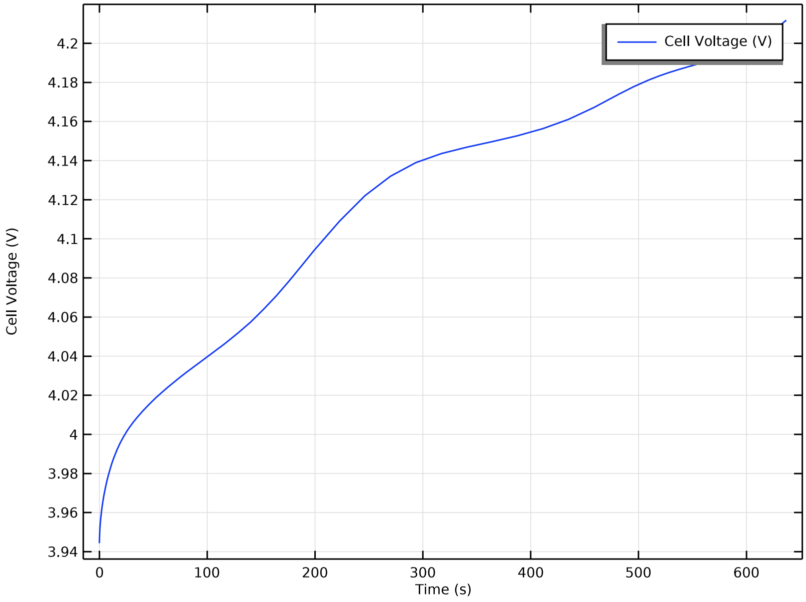
Rename the Default Probe Plot

1 In the Model Builder window, under Results click Probe Plot Group 1.



2 In the Settings window for 1D Plot Group, type `Cell Voltage Probe Plot` in the Label text field.

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



Add a Plot Group for the Potential in Negative Current Collector and Tab

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

1 In the Results toolbar, click 3D Plot Group to create a new plot group.

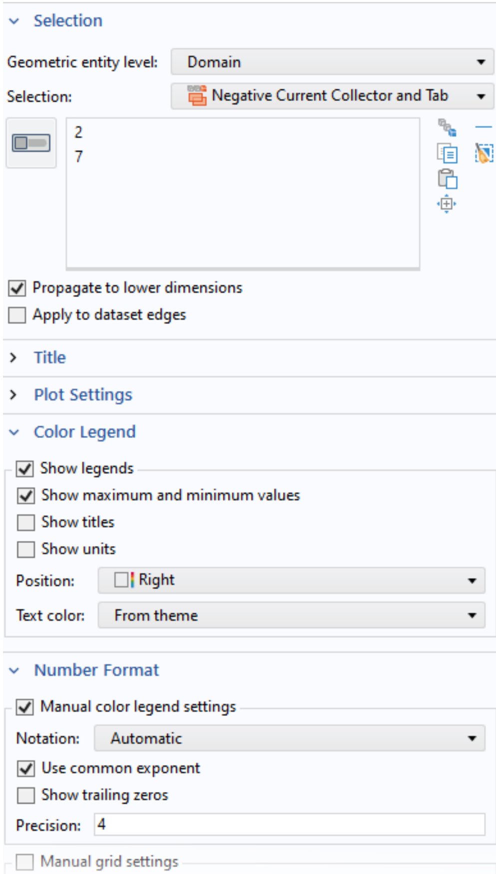
2 In the Settings window for 3D Plot Group, type `Potential in Negative Current Collector and Tab` in the Label text field.

3 Click to expand the Selection section. Select Domain as Geometric entity level and thereafter Negative Current Collector and Tab as Selection.

4 Locate the Color Legend section. Select the Show maximum and minim um values checkbox.

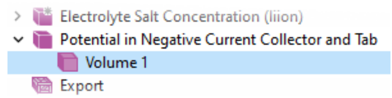
5 Click to expand the Number Format section. Select the Manual color legend setting s checkbox.

6 In the Precision text field, type 4.



Add Volume Plot to Plot the Potential

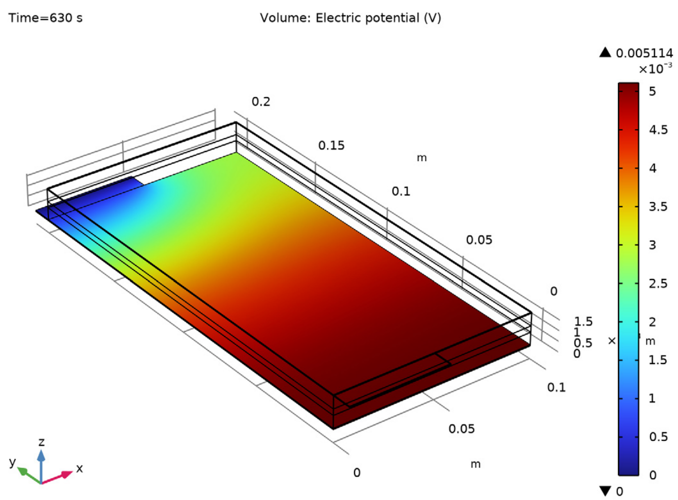
1 Right-click
Potential in Negative Current Collector and Tab and choose Volume.



2 In the Settings window for Volume, locate the Expression section.

3 Click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component 1 (comp1) > Lithium-Ion Battery > phis - Electric potential - V.

4 In the Potential in Negative Current Collector and Tab toolbar, click Plot.



Potential in Positive Current Collector and Tab

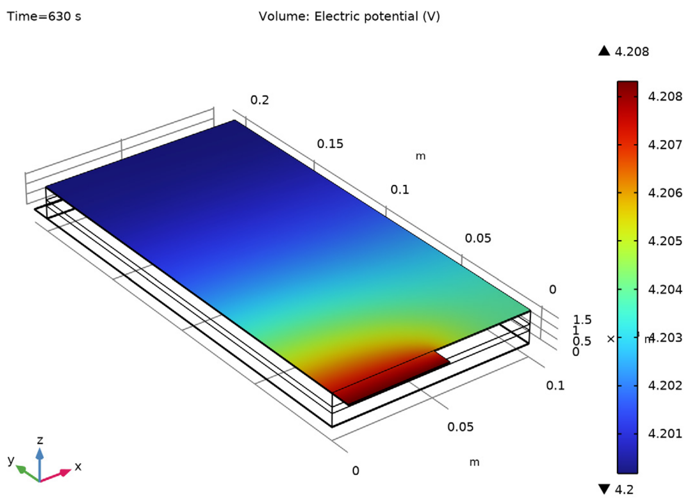
Duplicate the plot and modify the copy in order to view the potential at the positive current collector and tab.

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

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.

4 Locate the Selection section. Select Positive Current Collector and Tab as Selection and click Plot.



Current Density Across Separator at t=0 s

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

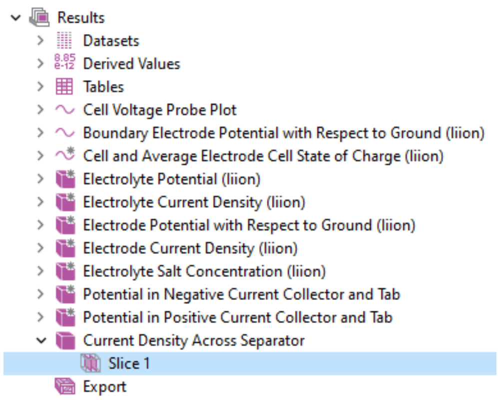
1 In the Results toolbar, click 3D Plot Group.

2 In the Settings window for 3D Plot Group, type `Current Density Across Separator` in the Label text field.

3 From the Time (s) list, choose 0.

Slice 1

1 Right-click Current Density Across Separator and choose Slice.



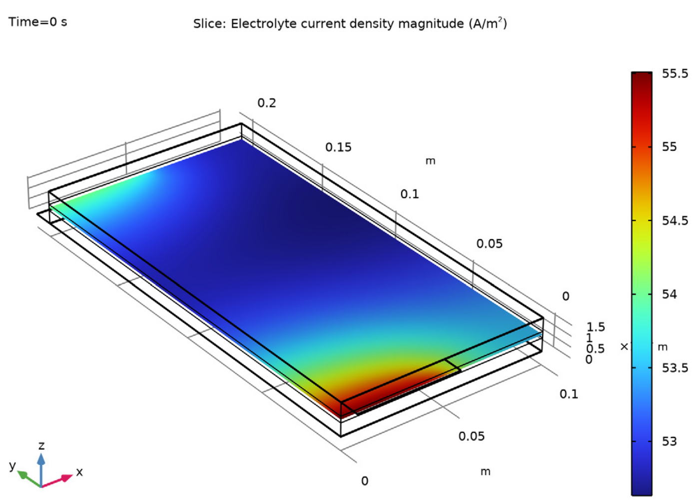
2 In the Settings window for Slice, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component 1 (comp1) > Lithium-Ion Battery > liion.IlMag - Electrolyte current density magnitude - A/m².

3 Locate the Plane Data section. From the Plane list, choose XY-planes.

4 From the Entry method list, choose Coordinates.

5 In the Z-coordinates text field, type `L_neg_cc/2+L_neg+L_sep/2`.

6 In the Current Density Across Separator toolbar, click Plot.



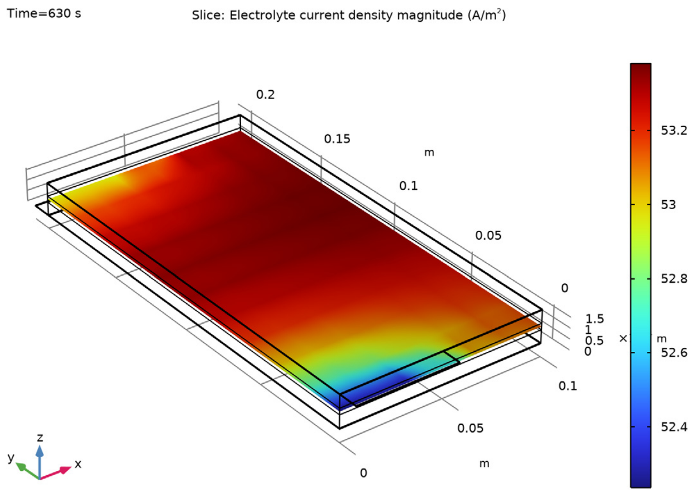
Current Density Across Separator at t=630 s

1 In the Model Builder window, click 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 Current Density Across Separator toolbar, click Plot.



Additional instructions for how to plot integrated measures of the electrode utilization over the whole charge cycles, using general projection operators, can be found toward the end of the modeling instructions for the *Electrode Utilization in a Large-Format Lithium-Ion Battery Pouch Cell* tutorial found in the *Battery Design Application Library*. There you also find a number of other tutorials covering a multitude of cell chemistries and application areas.