INTRODUCTION TO

Battery Design Module

COMSOL

Introduction to the Battery Design Module

Version: COMSOL 6.0

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Introduction

The Battery Design Module models and simulates the fundamental processes in the electrodes and electrolytes of batteries. 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 for different electrode configurations, separators, current collectors and feeders, materials, and chemistry. The description of the involved processes and phenomena is rather detailed, and you can therefore apply different hypotheses to gain an understanding of the investigated systems. You can study the influence of different electrocatalysts, pore distribution, electrolyte composition, and other fundamental parameters directly in the physics interface.

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

The figure below shows the Battery Design Module interfaces and other physics interfaces in COMSOL Multiphysics that are modified by the module, for example the Chemical Species Transport branch interfaces.
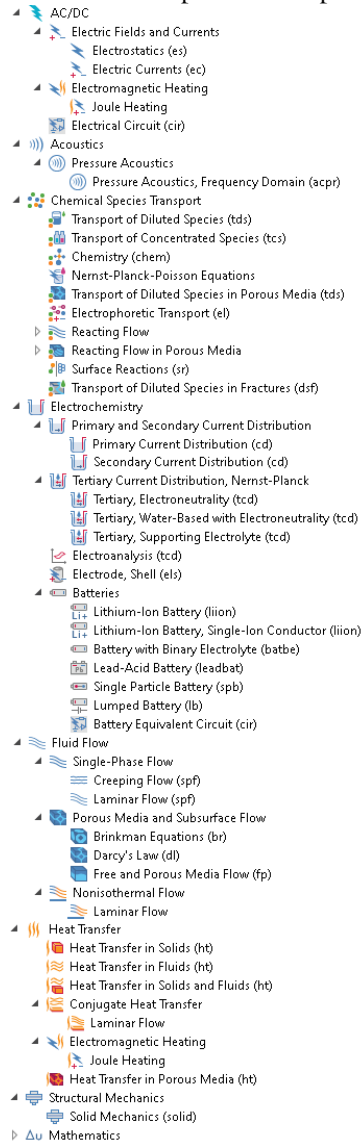
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Figure 1: The 3D physics interfaces for the Battery Design Module as shown in the Model Wizard.

The Electrochemistry (⊔) interfaces are based on the conservation of current, charge, chemical species, and energy. The Battery Interfaces form the basis for battery modeling whereas the Current Distribution interfaces typically are the starting point for fuel cell models.

The Chemical Species Transport (⠿), the Fluid Flow (≋) and the Heat Transfer (⧘) interfaces are extended with functionality for battery fuel cell modeling, for instance features for handling porous media, gas phase mass transport and coupling of fluxes, sources and sinks to electrode reactions. The different physics interfaces are further discussed below.

Battery Modeling

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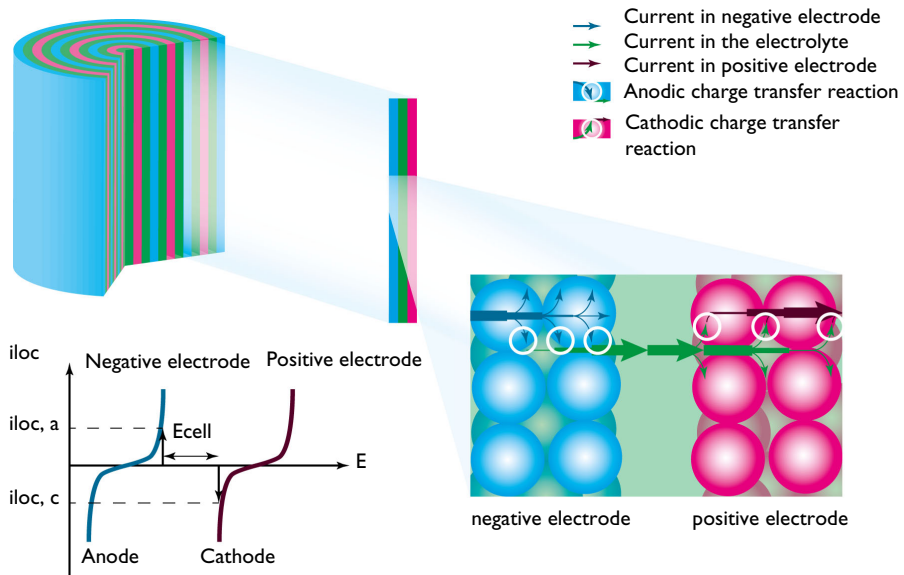
Figure 2: Direction of the current and charge transfer current during discharge in a battery with porous electrodes.

During discharge, chemical energy is transferred to electrical energy in the charge transfer reactions at the anode and cathode. The conversion of chemical to electrical 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.
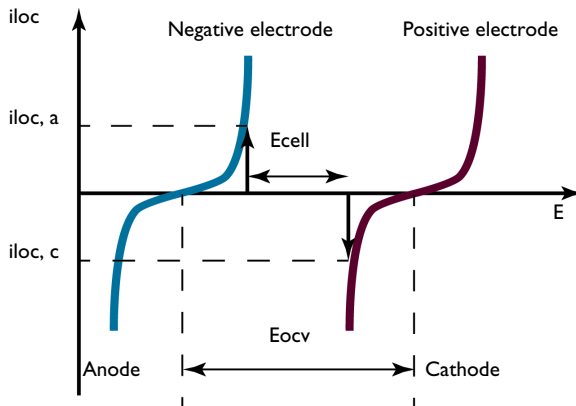

Figure 3: Electrode polarization during discharge. The figure is same as inset of Figure 2.

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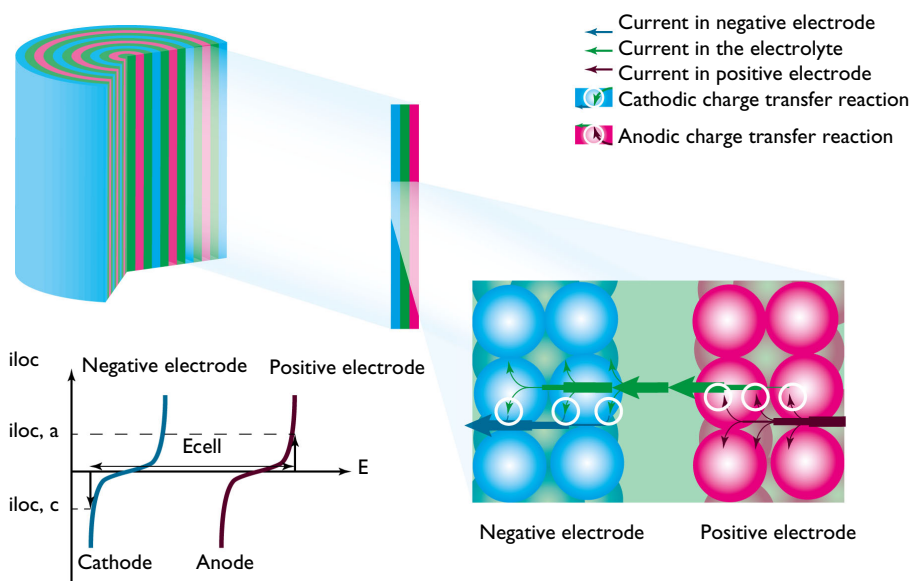
Figure 4: During charge, the positive electrode acts as the anode while the negative one acts as the cathode. The cell voltage increases (at a given current) compared to the open cell voltage. Note: direction of the currents is reversed here.

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.
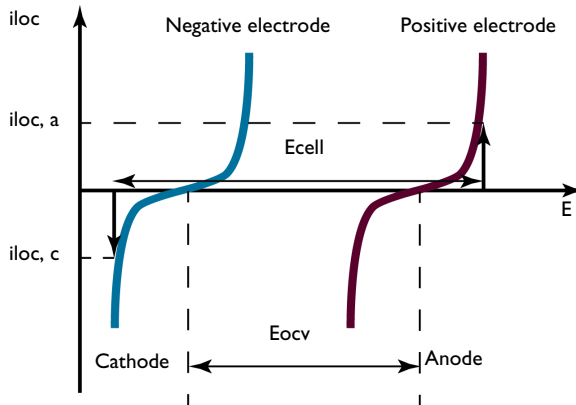
Figure 5: Electrode polarization during charge.

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

The Battery Modeling Physics Interfaces

The Lithium-Ion Battery interface (⊡) is tailored for 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 Single Particle Battery interface (⊟) offers a simplified (compared to for instance the Lithium-Ion Battery interface) approach to battery modeling. This interface models the charge distribution in a battery using one separate single particle model each for the positive and negative electrodes of the battery. It accounts for solid diffusion in the electrode particles, the intercalation reaction kinetics and ohmic potential drop in the separator using a lumped solution resistance term.

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 binary electrolyte, which covers the nickel-metal hydride and the 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 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. Additional circuit elements such as resistors, capacitors, and inductors may be added by the user.

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 Tertiary Current Distribution, Nernst-Planck interface (🔋) describes the transport of charged species in electrolytes through diffusion, migration, and convection. In addition, it also includes ready-made formulations for porous and non-porous electrodes, including charge transfer reactions and current conduction in the electronic conductors.

The Chemical Species Transport interfaces (⚬⚬) describe the transport of ions in the pore electrolyte and in the electrolyte that separates the anode and cathode. Other reactions can be added other than pure electrochemical reactions to, for example, describe the degradation of materials. In combination with the Secondary Current Distribution interface (🔋), the Transport of Concentrated Species interface (🧪), and the Transport of Diluted Species in Porous Media interface (🔵) can be used to model the transport of charged species and the electrochemical reactions in most battery systems.

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.

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

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Laminar Flow, Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Reacting Flow				
Laminar Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Reacting Flow in Porous Media				
Transport of Diluted Species		rfds	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species		rfcs	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)		tcd	all dimensions	stationary; stationary with initialization; time dependent; time dependent with initialization; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
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

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
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
Single Particle Battery		spb	all dimensions	time dependent; time dependent with initialization
Lumped Battery		lb	all dimensions	time dependent; AC impedance, initial values;
Battery Equivalent Circuit		ec	Not space dependent	stationary; time dependent; frequency domain
Fluid Flow				
Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent
Free and Porous Media Flow		fp	3D, 2D, 2D axisymmetric	stationary; time dependent

| PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
≋ **Nonisothermal Flow**				
Brinkman Equations	🔷	—	3D, 2D, 2D axissymmetric	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF
🏄 **Fluid-Structure Interaction**				
))) **Heat Transfer**				
Heat Transfer in Porous Media	🔴	ht	all dimensions	stationary; time dependent

Tutorial of a Lithium-Ion Battery

The following is a two-dimensional model of a lithium-ion battery. The cell geometry could be a small part of an experimental cell but here it is only meant to demonstrate a 2D model setup. The battery contains a positive porous electrode, electrolyte, a negative lithium metal electrode and a current collector. This cell configuration is sometimes called a "half-cell", since the lithium metal electrode is usually considered to have negligible impact on cell voltage and polarization. A realistic 2D geometry is shown in the model Edge Effects in a Spirally Wound Li-Ion Battery available in the Battery Design Module application library.

Model Definition
The cell geometry is shown in the figure below. Due to symmetry along the height of the battery, the 3D geometry can be modeled using a 2D cross section. The figure shows the positioning of the positive and negative electrodes, and the

current collector attached to the positive electrode. The positive electrode is porous and the negative electrode consists of lithium metal.

Positive electrode | Electrolyte | Negative electrode | Current collector | Lithium metal negative electrode | Cross-section
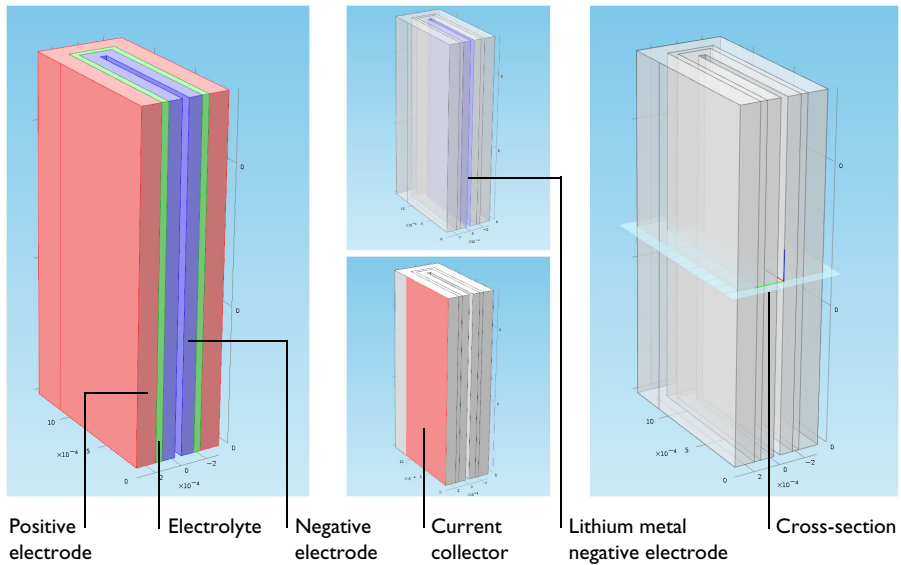
The modeled 2D cross section is shown in light blue (right).

Since the electrochemical reaction only takes place at the surface of the lithium metal which is in contact with electrolyte in the separator, and the electronic conductivity is very high compared to the porous positive electrode, the thickness of the metal can be neglected in the model geometry. The modeled 2D cell geometry is shown in the figure below. During discharge, the positive electrode

acts as the cathode and the contact of the metallic tab acts as a current collector. The lithium metal electrode acts as the anode and current feeder.
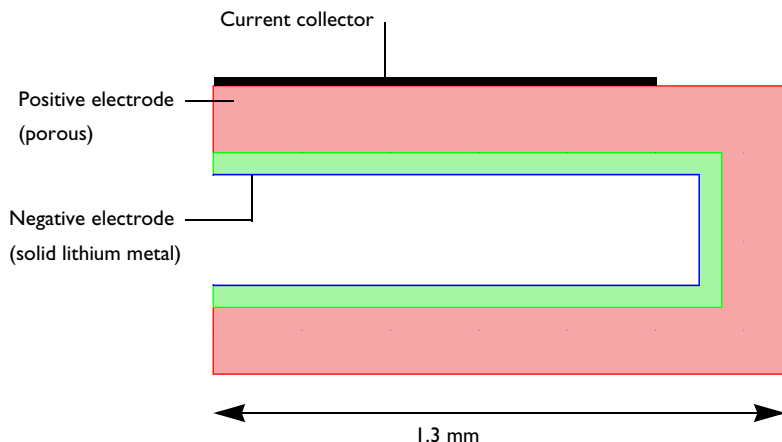
The model defines and solves the current and material balances in the lithium-ion battery. The intercalation of lithium inside the particles in the positive electrode is solved using a fourth independent variable r for the particle radius (x, y, and t are the other three). The reaction kinetics and the 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 Nobel Laureate John Newman and his co-workers at the University of California at Berkeley. The model is popularly known as pseudo-2D model (or P2D model) in the literature.

Results and Discussion

The purpose of the 2D simulation is to reveal the depth of discharge in the positive electrode, as a function of discharge time. The corresponding current distribution depends on the positioning of the current collector and the thickness of the positive electrode and electrolyte layer, in combination with the electrode kinetics and transport properties.

The figure below shows the concentration of lithium at the surface of the positive electrode particles in the electrodes after 2700 s of discharge at 0.05 A.

The high concentration at the positive electrodes is proportional to the local depth of discharge of these parts of the electrode. The figure shows that the back side of the electrode, with respect to the position of the current collector, is less utilized during discharge. As the discharge process continues, these parts will subsequently discharge. However, for repeated cycling of the cell (charge and discharge), the

different parts of the electrodes will age in a nonuniform way if the electrodes are only discharged to a moderate degree during cycling.
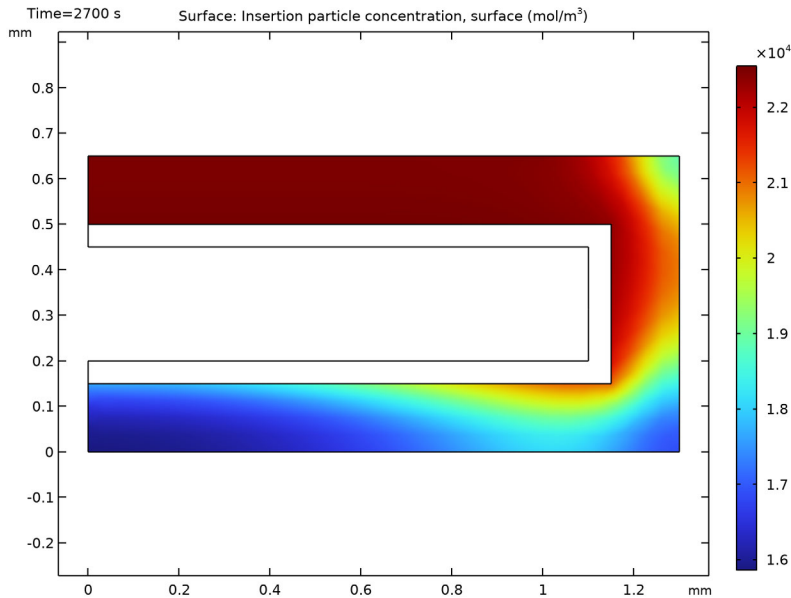
Despite the simplicity of this model, it shows a problem that may arise in realistic battery geometry if the shape and configuration of the electrodes, current collectors, and current feeders are not investigated thoroughly using modeling and simulations.

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

Model Wizard

Note: These instructions are for the user interface on Windows but apply, with minor differences, also to Linux and macOS.

I To start the software, double-click the COMSOL icon on the desktop or Start menu of the computer. When the software opens, you can choose to use the

Model Wizard to create a new COMSOL model or Blank Model to create one manually. For this tutorial, click the Model Wizard button.

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

The Model Wizard guides you through the first steps of setting up a model. First you select the dimension of the modeling space.

2 In the Space Dimension window click the 2D button ◉ .

3 On the Select Physics tree under Electrochemistry>Battery, double-click Lithium-Ion Battery (liion) ⃞ to add it to the Added physics interfaces list.

4 Click Study ➜ .

5 On the Studies window under Preset Studies, click Time Dependent with Initialization ⃞ . This study type simplifies the modeling, since it reduces the number of initial values that need to be set by computing the initial potentials in the battery interface.

6 Click Done ☑ .

Geometry I

Insert a prepared geometry sequence from a file. After insertion you can study each geometry step in the sequence.

1 On the Geometry toolbar, click Insert Sequence.

2 Browse to the file `li_battery_tutorial_2d_geom_sequence.mph` in the application library folder Battery_Design_Module\Batteries,_Lithium-Ion on your computer. Double-click to add or click Open.

3 On the Geometry toolbar, click Build All.

4 Click zoom extents ⃞ button.

Note: The location of the file used in this exercise varies based on the installation of COMSOL Multiphysics. For example, if the installation is on your hard drive, the file path might be similar to `C:\Program Files\COMSOL56\applications\`.
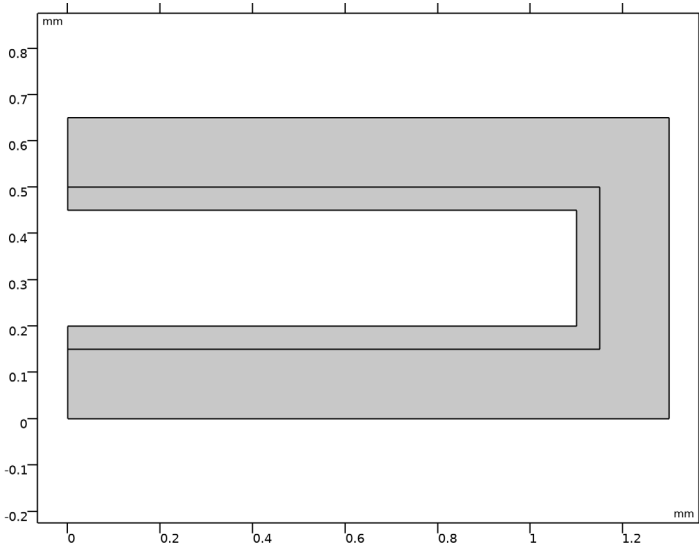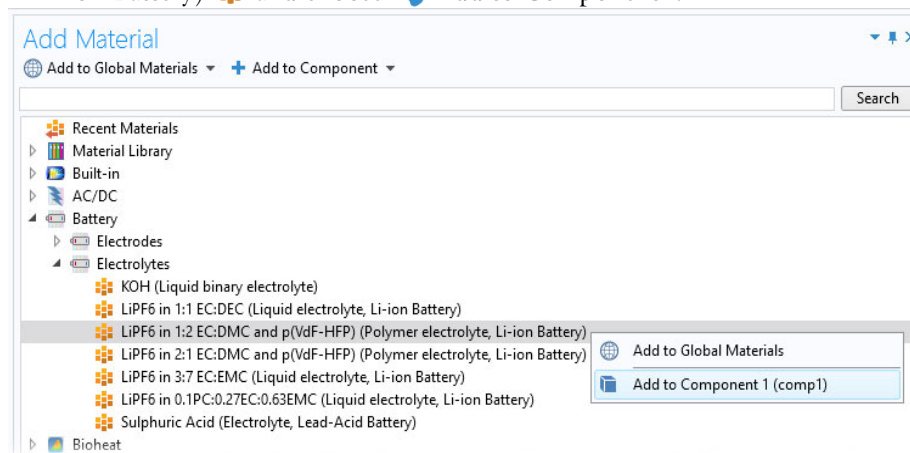

Materials

Use the Battery material library to set up the material properties for the electrolyte and electrode (anode and cathode) materials. By adding the electrolyte material to the model first, this material becomes the default material for all domains.

Add Material

I On the Home toolbar, click Add Material ⚏ .

2 Go to the Add Material window. In the tree under Battery, under Electrolytes right-click LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer electrolyte, Li-ion Battery) ⬛ and choose ⊙ Add to Component1.

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

1 In the tree under Battery under Electrodes click LMO Electrode, LiMn2O4 Spinel (Positive, Li-ion Battery). ⬛ . In the Add Material window click ➕ Add to Component.

The node sequence in the Model Builder under the Materials node should match this figure.
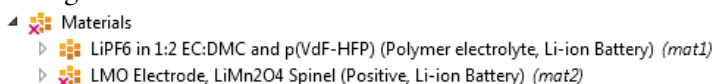
The first material (LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer electrolyte, Li-ion Battery)) was assigned by default to all domains. Override this default selection by assigning the electrode material to domain 1.

2 On the LMO Electrode, LiMn2SO4 Spinel (Positive, Li-ion Battery), select Domain 1.

The LMO material node will now be marked with a small red cross in the model tree, indicating missing material properties. This is expected at this point and will be resolved when setting up the physics for the porous electrode node.

If you want you may now click, expand and inspect the various properties present in the nodes you under Materials (cEeqref denotes the maximum Li concentration in the active material). Most of these properties will be used by the physical model you will now proceed to define.

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An Electrolyte domain node has already been added to the model by default. The electrolyte parameters, which depend on the electrolyte concentration, are set by default to be taken from the Materials node so no further settings are needed for this node.

Now set up the physics in the positive electrode, using a porous electrode domain node.

Porous Electrode 1

1 On the Physics toolbar click Domains ⬤. Choose Porous Electrode to add it to the model.
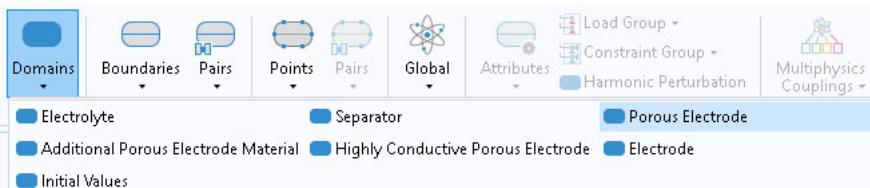
2 Locate the Domain Selection section of the Porous Electrode node and select Domain 1 only.

Note: There are many ways to select geometric entities. When you know the geometric entity to add, such as in these exercises, you can click the Paste Selection button 📋 and enter the information in the Selection text field. For more information about selecting geometric entities in the Graphics window, see the *COMSOL Multiphysics Reference Manual.*

The porous electrode node defines a domain to consist of a homogeneous mix of both an electrode (solid) and electrolyte (liquid) phase. You therefore need to assign different materials to the different phases. By default, the material properties for each phase will be taken from the material assigned to the domain under Materials, which in this case is LMO electrode material. You hence need to set the electrolyte phase material selection manually.

3 In the same window under Electrolyte
  Properties, select LiPF6 in 1:2
  EC:DMC and p(VdF-HFP) (Polymer
  electrolyte, Li-ion Battery) from the
  Electrolyte material list.

In this model we will assume that the
porous electrode consists of a mix of 40%
electrode and 15% inert binder material.
The remaining volume is filled up with
electrolyte.

4 Within the Electrolyte volume fraction
  text field, located in the Volume
  Fractions section, enter 1-0.4-0.15.

The small red cross on the LMO material
node should now have disappeared in the
model tree.

Particle Intercalation l

The Porous Electrode has two child nodes
added by default. The Particle
Intercalation node adds an extra
dimension to the selected domain, and
solves for the diffusion of solid lithium in
this extra dimension, assuming spherical particles. Keep the default settings for this
node.

Porous Electrode Reaction l

The Porous Electrode Reaction node sets up
the equilibrium potential, kinetics and
stoichiometry of the lithium insertion
reaction occurring at the interface between
the electrolyte and electrode phases within
the porous matrix. Keep the default settings
also for this node.

Electrode Current l

Now define the battery average discharge current density.

**1** On the Physics toolbar click Boundaries ⊜ and choose Electrode Current ⊜.

2 Select boundary 10 only.

3 In the Electrode Current section, select Average current density in the list and enter -50[A/m2] in the average current density text field.

Electrode Surface 1

Finish the model by defining the negative electrode. Due to the high conductivity of the lithium metal it suffices to define the electrode surface between the lithium metal domain (not included in the model geometry) and the electrolyte domain (included in the model geometry).

1 On the Physics toolbar click Boundaries ⊜ and choose Electrode Surface ⊜.
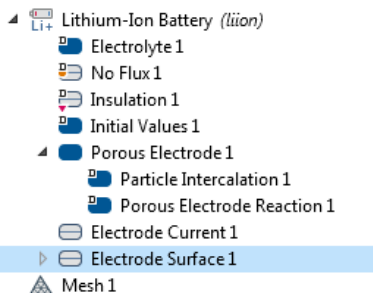
2 Select Boundary 5, 7, and 12 only.

The metal potential of the electrode is grounded (set to 0 V) by default so no further settings are needed for this node.
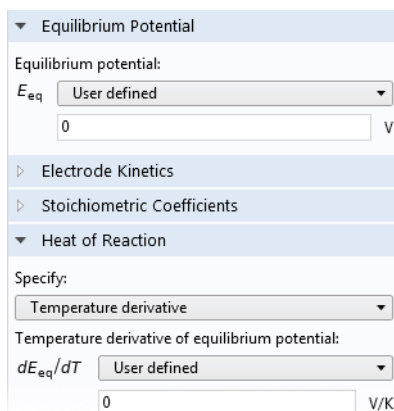
Electrode Reaction 1

Similar to the Porous Electrode node, the Electrode Surface node comes with a default Electrode Reaction subnode. Expand the Electrode Surface node and inspect the various settings of the subnode. The equilibrium potential inputs need to be set to values that are applicable for a lithium metal surface.

Electrode Reaction1

1 In the Model Builder, expand the Electrode Surface 1 node and click the Electrode Reaction 1 node ⊖.

2 Under Equilibrium Potential select User defined for the Equilibrium potential. Enter 0 in the V text field.

3 In the same window under Heat of Reaction, select User defined for the Temperature derivative of equilibrium potential. Enter 0 in the V/K text field.

The values of 0 V and 0 V/K for the two inputs, respectively, are applicable for a lithium metal surface.

▼ Equilibrium Potential

Equilibrium potential:

E_{eq} | User defined ▼

0 | V

▷ Electrode Kinetics

▷ Stoichiometric Coefficients

▼ Heat of Reaction

Specify:

Temperature derivative ▼

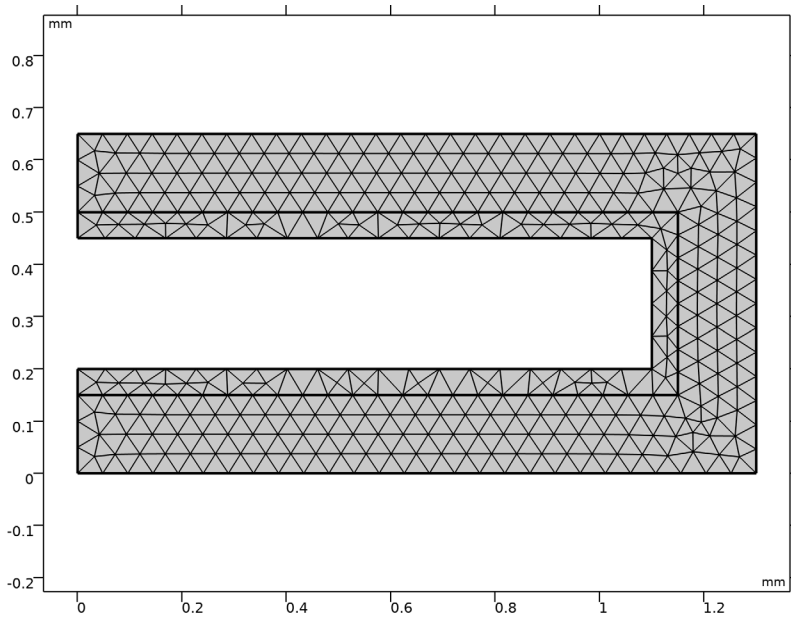Temperature derivative of equilibrium potential:

dE_{eq}/dT | User defined ▼

0 | V/K

Mesh 1

In this example the automatically generated mesh is used so no manual mesh settings are required. You may inspect the automatically generated mesh as follows:

I In the Model Builder window, under Component 1 (comp1) right-click Mesh 1 and choose Build All.
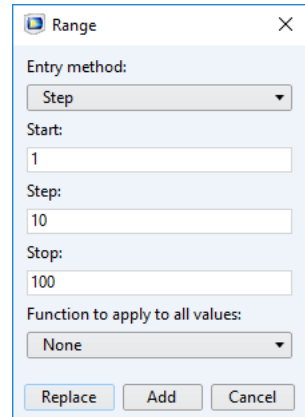

Study 1

Set up a 2700 second time-dependent solver to store the solution at 10 second intervals during the first 100 seconds, and 100 second intervals during the last 2600 seconds. Then solve the problem.

Step 2: Time Dependent

I In the Model Builder expand the Study 1 node and click Step 2: Time Dependent ⬓.

2 In the Settings window for Time Dependent, locate the Study Settings section.
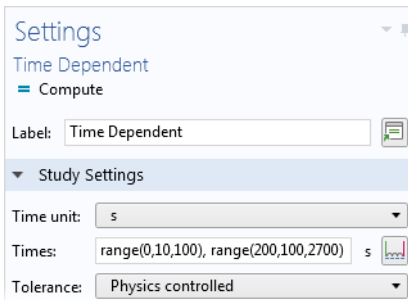
3 Click Range (▨ icon to the right of the Times text field).

4 In the Range dialog box, type 10 in the Step text field.

5 In the Stop text field, type 100.

6 Click Replace.

7 Click Range again and type 200 in the Start text field.

8 In the Step text field, type 100.

9 In the Stop text field, type 2700.

10 Click Add.

(Alternatively, you may also type in the expression range(0,10,100) range(200,100,2700) directly in the Times text field.)

**11** On the Home toolbar click Compute ═ .

Results

Boundary Electrode Potential vs Ground (liion)

A plot of the electrode voltage where you set the Electrode Current condition is created by default. Since you grounded the other electrode this equals the battery voltage during the simulation.

1 In the Model Builder window, under Results click Boundary Electrode Potential vs Ground (liion).

2 Rename the plot group by typing `Battery Voltage` in the Label text field available in the Settings window, click Plot ⊡ .

Global: Electric potential on boundary (V)
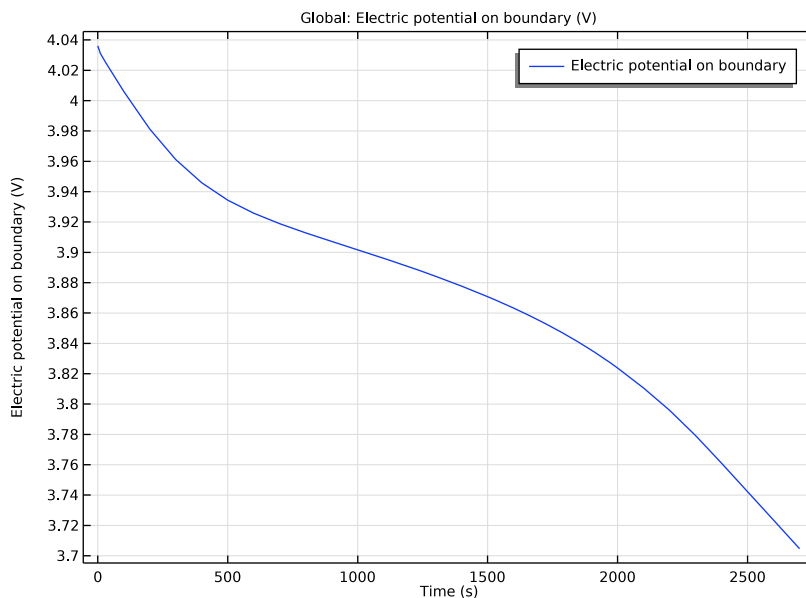
Also browse through the other default plots created. For the 2D plots you can select the time to plot for in the Data section.

2D Plot Group 8

The following steps create a plot of the solid lithium concentration at the surface of the electrode particles at 2700 seconds.

1 On the Home toolbar, click Add Plot Group ⊡ and choose 2D Plot Group ■ .

2 Rename the plot group by typing `Lithium concentration on Particle Surface` in the Label text field available in the Settings window.

3 On the `Lithium concentration on Particle Surface` toolbar click Surface ■ .

4 In the Settings window for Surface click Replace Expression ▶ ▾ (it is in the upper-right corner of the Expression section). Go to Component 1, Lithium-Ion Battery menu. Choose Insertion particle concentration, surface (liion.cs_surface) from the list under the Particle Intercalation menu.

5 On the `Lithium concentration on Particle Surface` toolbar click Plot ⊡ .

6 On the Graphics toolbar click the Zoom Extents button ⊕.

Time=2700 s   Surface: Insertion particle concentration, surface (mol/m³)
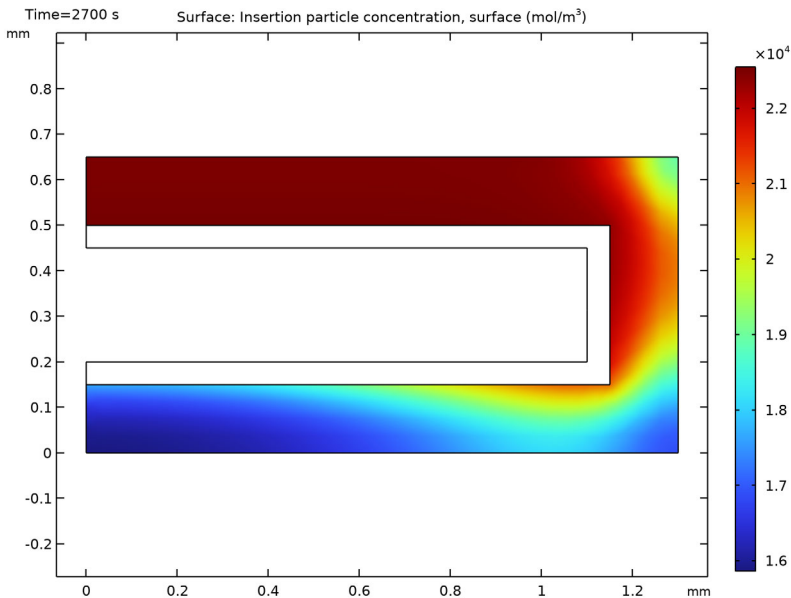
Datasets

As mentioned before, the Particle Intercalation node adds an extra dimension to the porous electrode domain, and solves for the concentration of solid lithium in this extra dimension. To create a plot of the lithium concentration in the particles in the positive electrode you need to first create a Solution dataset that refers to the extra dimension.

1 On the Results toolbar, click More Datasets ▦ and choose Solution ▥.

2 In the Solution Settings window, choose Extra Dimension from Porous Electrode 1 (`liion_pce1_pin1_xdim`) in the Component list displayed within the Solution section.

1D Plot Group 9

Start with the settings to plot the solid lithium concentration in the negative electrode.

1 On the Results toolbar, click 1D Plot Group ⊞.

2 Rename the plot group by typing `Lithium Concentration in Positive Electrode Particles` in the Label text field available in the Settings window.

3 In the Settings window for 1D Plot Group, choose None from the Dataset list located in the Data section.

4 On the Lithium Concentration in Particle toolbar, click Line Graph 〰.

5 In the Settings window for Line Graph, find the Dataset list in the Data section and choose Study 1/Solution 1 (3).

6 From the Time selection list, choose Last to plot only the last time step of the solution.

7 From the Selection list in the Selection section, choose All domains.

8 The atxd2( ) operator is used to specify the x and y coordinates in the battery geometry and the variable that is plotted. In the Expression text field of the y-Axis Data section, type `comp1.atxd2(5e-4,1e-4,liion.cs_pce1)`.

9 Create Legends in the plot:

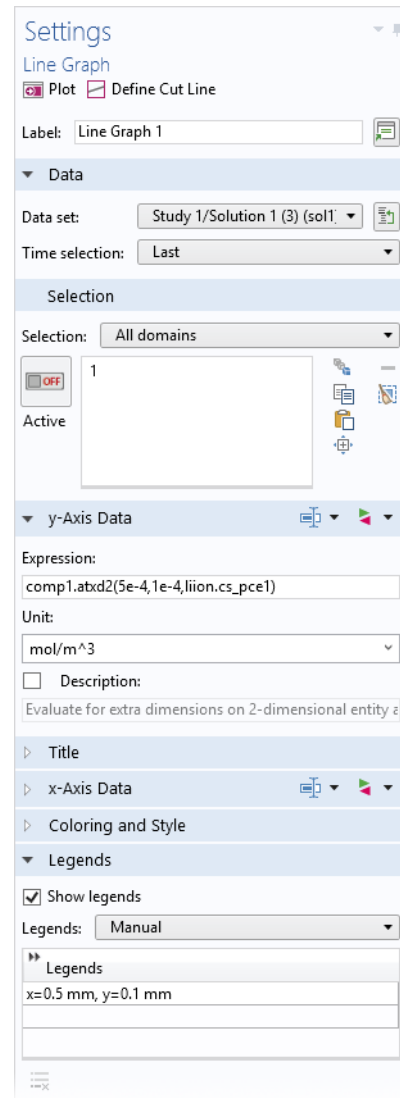**10** Click to expand the Legends section. Select the Show legends check box.

11 From the Legends list, choose Manual and enter `x=0.5 mm, y=0.1 mm` in the table.

12 Right-click Line Graph 1 and choose Duplicate to plot the concentration in an additional location within the positive electrode.

13 In the Settings window for Line Graph, locate the y-Axis Data section.

14 In the Expression text field of the y-Axis Data section, type `comp1.atxd2(5e-4,5.5e-4,liion.cs_pce1)`.

15 Click to expand the Legends section and replace the text in the table with `x=0.5 mm, y=0.55 mm`.

Settings panel:

Settings

Line Graph

▣ Plot ⊟ Define Cut Line

Label: Line Graph 1

▼ Data

Data set: Study 1/Solution 1 (3) (sol1)

Time selection: Last

Selection

Selection: All domains

□OFF 1
Active

▼ y-Axis Data

Expression:
comp1.atxd2(5e-4,1e-4,liion.cs_pce1)

Unit:
mol/m^3

☐ Description:
Evaluate for extra dimensions on 2-dimensional entity a

▷ Title

▷ x-Axis Data

▷ Coloring and Style

▼ Legends

☑ Show legends

Legends: Manual

Legends
x=0.5 mm, y=0.1 mm

16 To finalize the plot group, return to the Lithium Concentration in Particle toolbar ▥ node by clicking it in the Model Builder.

```
▲ ■ Lithium concentration on Particle Surface
      ■ Surface 1
▲ ∿ Lithium Concentration in Positive Electrode Particles
      ∿ Line Graph 1
      ∿ Line Graph 2
    ▤ Export
    ▤ Reports
```
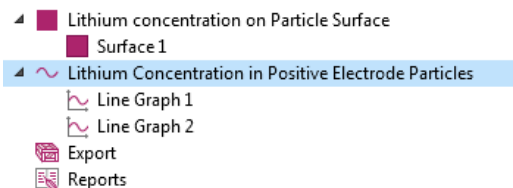
17 In the Settings window for 1D Plot Group, click to expand the Title section, where you choose Manual from the Title type list.

18 In the Title text area, enter

Lithium Concentration Positive Electrode Particles, t=2700 s.

19 In the Plot Settings section:

- Select the x-axis label check box and type in the associated text field Normalized Particle Dimension.

- Select the y-axis label check box and type Lithium Concentration (mol/m³).

20 Click to expand the Legend section, choose Upper left from the Position list.

21 Click the Zoom Extents ⊹ button on the Graphics toolbar and click Plot ▣ on the Lithium Concentration in Particle toolbar.

Lithium Concentration Positive Electrode Particles, t=2700 s

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