



INTRODUCTION TO

Batteries & Fuel Cells Module

Introduction to the Batteries & Fuel Cells Module

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Introduction

The Batteries & Fuel Cells Module models and simulates the fundamental processes in the electrodes and electrolytes of batteries and fuel cells. 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 and fuel cells 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 Batteries & Fuel Cells Module interfaces and other physics interfaces in COMSOL Multiphysics that are modified by the module, for example the Chemical Species Transport branch interfaces.

- Chemical Species Transport
 - Transport of Diluted Species (tds)
 - Transport of Concentrated Species (tcs)
 - Chemistry (chem)
 - Nernst-Planck-Poisson Equations
 - Transport of Diluted Species in Porous Media (tds)
 - Electrophoretic Transport (el)
 - Reacting Flow
 - Laminar Flow
 - Laminar Flow, Diluted Species
 - Reacting Flow in Porous Media
 - Transport of Diluted Species
 - Transport of Concentrated Species
 - Surface Reactions (sr)
 - Transport of Diluted Species in Fractures (dsf)
 - Electrochemistry
 - Primary and Secondary Current Distribution
 - Primary Current Distribution (cd)
 - Secondary Current Distribution (cd)
 - Tertiary Current Distribution, Nernst-Planck
 - Tertiary, Electroneutrality (tcd)
 - Tertiary, Water-Based with Electroneutrality (tcd)
 - Tertiary, Supporting Electrolyte (tcd)
 - Electroanalysis (tcd)
 - Electrode, Shell (els)
 - Battery Interfaces
 - Lithium-Ion Battery (liion)
 - Lithium-Ion Battery, Single-Ion Conductor (liion)
 - Battery with Binary Electrolyte (batbe)
 - Lead-Acid Battery (leadbat)
 - Single Particle Battery (spb)
 - Lumped Battery (lb)
 - Battery Equivalent Circuit (cir)
 - Fluid Flow
 - Single-Phase Flow
 - Creeping Flow (spf)
 - Laminar Flow (spf)
 - Porous Media and Subsurface Flow
 - Brinkman Equations (br)
 - Darcy's Law (dl)
 - Free and Porous Media Flow (fp)
 - Nonisothermal Flow
 - Laminar Flow
 - Heat Transfer
 - Heat Transfer in Solids (ht)
 - Heat Transfer in Fluids (ht)
 - Heat Transfer in Solids and Fluids (ht)
 - Conjugate Heat Transfer
 - Laminar Flow
 - Electromagnetic Heating
 - Joule Heating
 - Heat Transfer in Porous Media (ht)

Figure 1: The 3D physics interfaces for the Batteries & Fuel Cells 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 under [Battery Modeling](#) and [Fuel Cell Modeling](#).

Battery Modeling

The Batteries & Fuel Cells Module has a number of physics interfaces to model batteries. Which physics interface to choose 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.

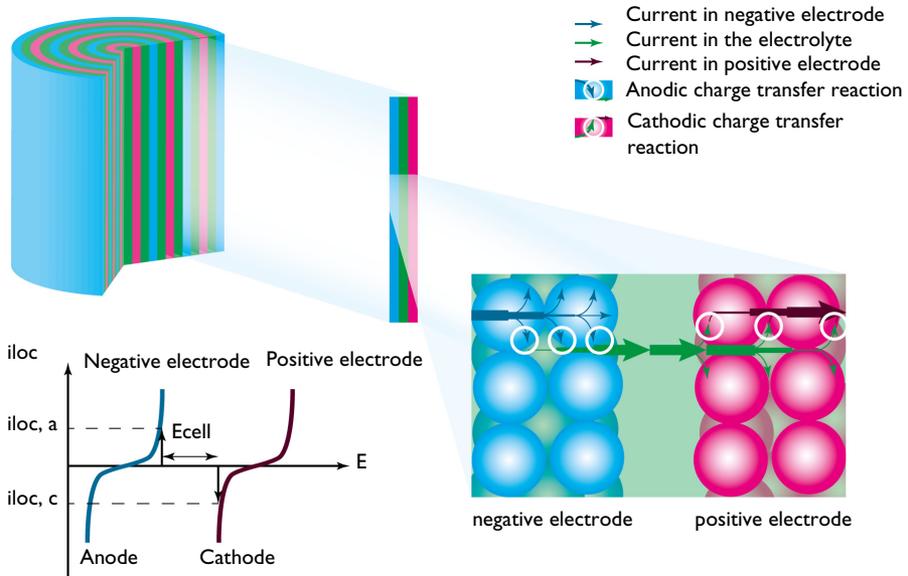


Figure 2: Direction of the current and charge transfer current during discharge in a battery with porous electrodes.

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.

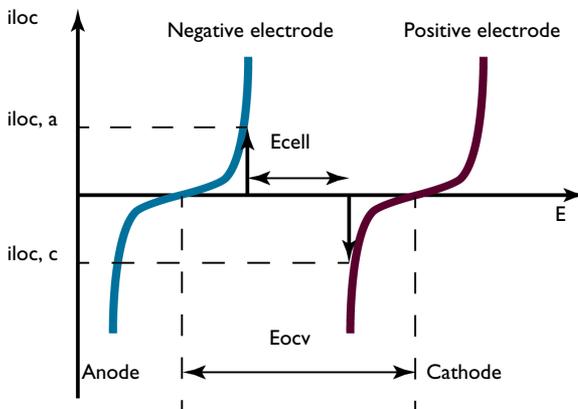


Figure 3: Electrode polarization during discharge. The figure is same as inset of Figure 2.

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.

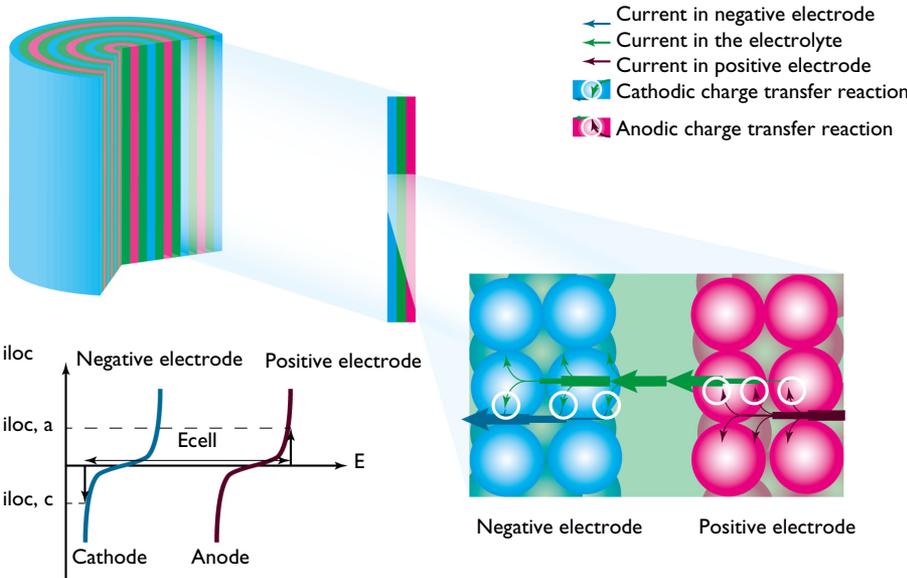


Figure 4: During charge, the positive electrode acts as the anode while the negative one acts as the cathode. The cell voltage increases (at a given current) compared to the open cell voltage. Note: direction of the currents is reversed here.

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 from the 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.

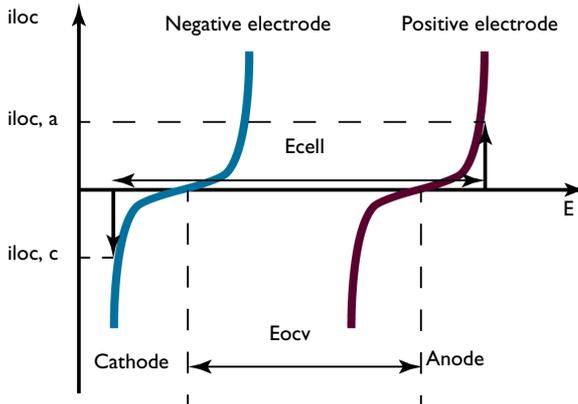


Figure 5: Electrode polarization during charge.

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 Batteries & Fuel Cells 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.

Fuel Cell Modeling

This module includes functionality to model fuel cell unit cells that consist of:

- Current collectors and current feeders
- Gas channels usually formed by grooves in the current collectors and feeders
- Porous gas diffusion electrodes (GDEs)
- An electrolyte that separates the anode and cathode

Figure 6 shows a schematic drawing of a fuel cell unit cell and the structure of one of the GDEs. It represents a fuel cell unit cell and a magnified section of the cathode GDE and its contact with the electrolyte.

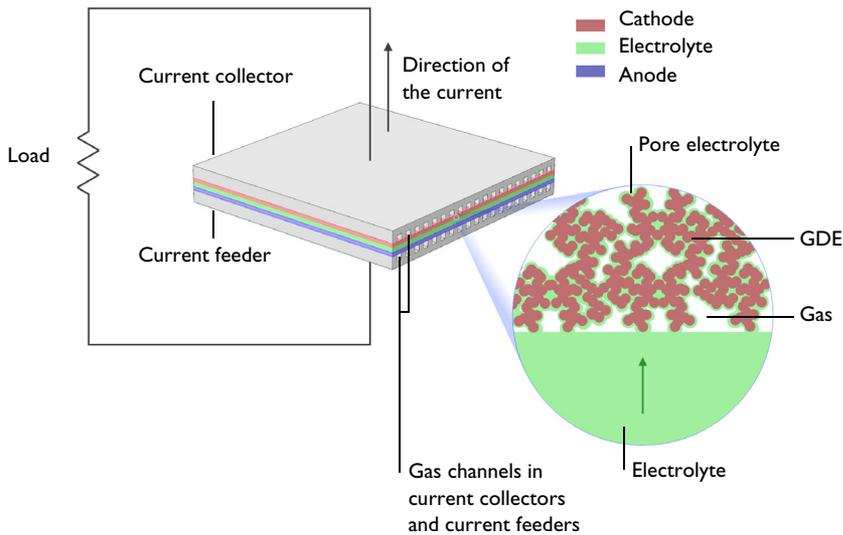


Figure 6: Fuel cell unit cell and a magnified section of the cathode GDE and its contact with the electrolyte.

Oxygen and hydrogen are supplied to the cell through the gas channels in the current collector and current feeder, respectively. The current collector and the current feeder are made of electrically conductive materials and are equipped with grooves that form the gas channels. These grooves are open channels with the open side facing the surface of the GDEs.

The current collectors and feeders also conduct the current to the wires connected to the load. They can also supply cooling required during operation and heating required during start-up of the cell.

The GDE magnified in Figure 6 is an oxygen-reducing cathode in a fuel cell with acidic electrolyte, for example the PEMFC. In the PEMFC, the active GDE is confined to a thin active layer supported by a pure gas diffusion layer (GDL).

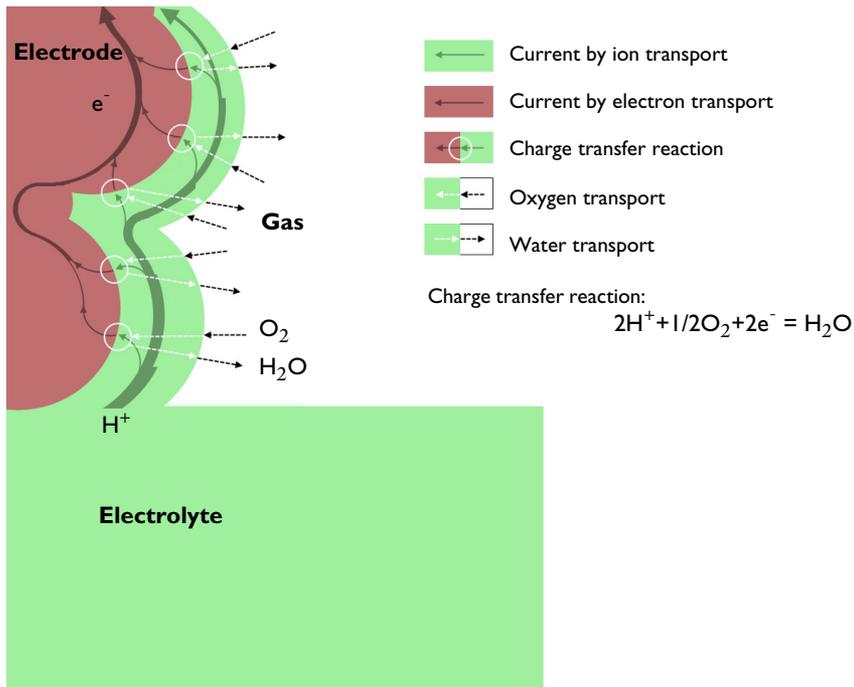


Figure 7: Transport of oxygen, water, protons, and electrons to and from the reaction site in an oxygen reducing GDE.

Figure 7 shows the principle of the oxygen reduction process in the electrode. From the free electrolyte, current enters the electrolyte contained in the GDE (also called pore electrolyte) as protons and is transferred to electron current in the charge transfer reaction at the reaction sites. These reaction sites are situated at the interface between the electrocatalyst in the electrode material and the pore electrolyte.

Figure 7 also describes the schematic path of the current in the electrode. The current in the pore electrolyte decreases as a function of the distance from the free electrolyte as it is transferred to electron current in the electrode. The direction of the current in the electrode is opposite to that of the electrons, by definition.

The supply of oxygen takes place in conjunction with the charge transfer reaction and can be subject to mass transport resistance both in the gas phase and in the thin layer of pore electrolyte that covers the reaction site.

The water balance in the electrode is maintained through evaporation and transport through the gas pores.

The pore electrolyte has to form a continuous path from the free electrolyte, between the anode and the cathode, to the reaction site. Also, the electrode material and the gas pores must each form a continuous path to the reaction site or to the pore electrolyte covering the reaction site.

The processes described above include fluid flow, chemical species transport, heat transfer, current conduction in the collectors, feeders, electrodes and electrolytes, and the electrochemical reactions. These are all coupled together, and determine the characteristics of a unit cell.

Several important design parameters can be investigated by modeling these processes. Among these parameters are:

- Porosity, active surface area, and pore electrolyte content of the GDEs
- Geometry of the GDEs (active layer and GDL for the PEMFC) and electrolyte in relation to the gas channels, the current collectors, and feeders
- Geometry of the grooves that form the gas channels and dimensions of the current collectors and feeders

The Fuel Cell Modeling Physics Interfaces

The fluid flow in the gas channels and in the GDEs is addressed by the Fluid Flow interfaces — the Laminar Flow (🌀), Free and Porous Media Flow (🏠), and Darcy's Law (🏠) interfaces.

The transport of gaseous species and the mass transport resistance in the pore electrolyte are handled by the Chemical Species Transport interfaces (🌈), which all have nodes that couple the transport in the gas phase to the electrochemical reactions. The Chemical Species Transport interfaces are also coupled to the Fluid Flow interfaces (🌀) through the gas density, which is influenced by the gas composition. A convenient way of coupling chemical species transport to fluid flow is by using one of the Reacting Flow interfaces (Fluid Flow (🌀), Reacting Flow (🌀) and Reacting Flow in Porous Media (🏠)), which contain predefined multiphysics couplings.

The Heat Transfer interfaces (🔥) handle the effects of Joule heating in the electrolyte, in the pore electrolyte, and in the electrodes. They include the contribution to the thermal balance from the electrochemical reactions due to the activation overpotential and the net change of entropy.

The current transport by ions in the free electrolyte and in the pore electrolyte, the current transport by electrons, and the charge transfer reactions are all treated in the Primary Current Distribution (🔌), Secondary Current Distribution (🔌), and the Tertiary Current Distribution, Nernst-Planck (🔌) interfaces.

The Primary Current Distribution interface neglects the variations in composition in the electrolyte and the activation losses for the charge transfer reactions. It should typically be used for electrolytes with fixed charge carriers or well mixed electrolytes, and in the cases where the activation losses are substantially smaller than the conductivity losses. In the Secondary Current Distribution interface, the variations in composition in the electrolyte are also neglected, while the activation losses for the charge transfer reactions are taken into account. In the Tertiary Current Distribution, Nernst-Planck interface, also the contribution of diffusion to the transport of ions, and thus the contribution to the current in the electrolyte, is taken into account.

The Electrode, Shell interface () models electric current conduction in the tangential direction on a boundary. The physics interface is suitable to use for thin electrodes where the potential variation in the normal direction to the electrode is negligible. This assumption allows for the thin electrode domain to be replaced by a partial differential equation formulation on the boundary. In this way the problem size can be reduced, and potential problems with mesh anisotropy in the thin layer can be avoided.

Physics Interface Guide by Space Dimension and Study Type

The table lists the physics interfaces available in the Batteries & Fuel Cells 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
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
Laminar Flow, Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
 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		cd	all dimensions	stationary; stationary with initialization; time dependent; time dependent with initialization; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
Secondary Current Distribution				
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
 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

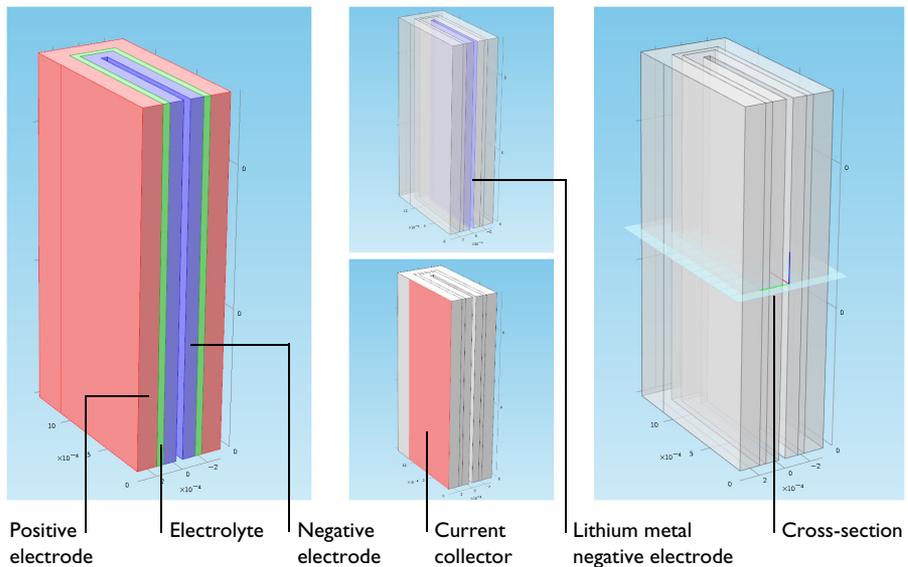
PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Battery with Binary Electrolyte		batbe	all dimensions	stationary; time dependent; AC impedance, initial values; AC impedance, stationary; AC impedance, time dependent
Lead Acid Battery		leadbat	all dimensions	stationary; time dependent; 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
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 Batteries & Fuel Cells Module application library.

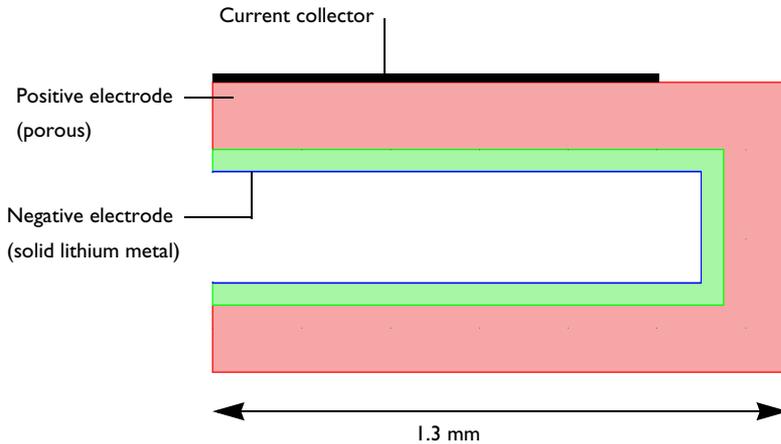
Model Definition

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.



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 negative lithium metal electrode acts as the anode and current feeder.



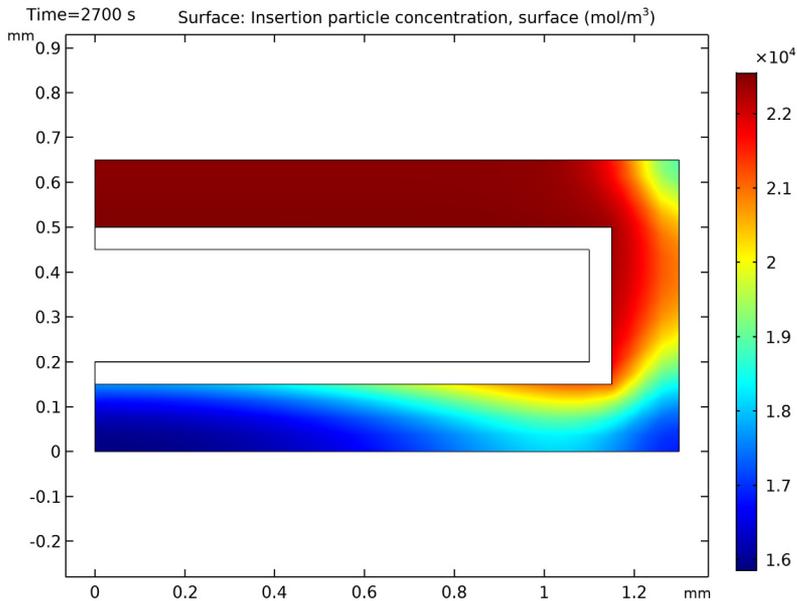
The model defines and solves the current and material balances in the lithium-ion battery. The intercalation of lithium inside the particles in the positive electrode is solved using a fourth independent variable r for the particle radius (x , y , and t are the other three). The reaction kinetics and the intercalation are coupled to the material and current balances at the surface of the particles. The model equations are found in the *Batteries & Fuel Cells Module User's Guide*. The model was originally formulated for 1D simulations by John Newman and his co-workers at the University of California at Berkeley.

Results and Discussion

The purpose of the 2D simulation is to reveal the distribution of the depth of discharge in the positive electrode, as a function of discharge time. This 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 Mac.

1 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 Interfaces, 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

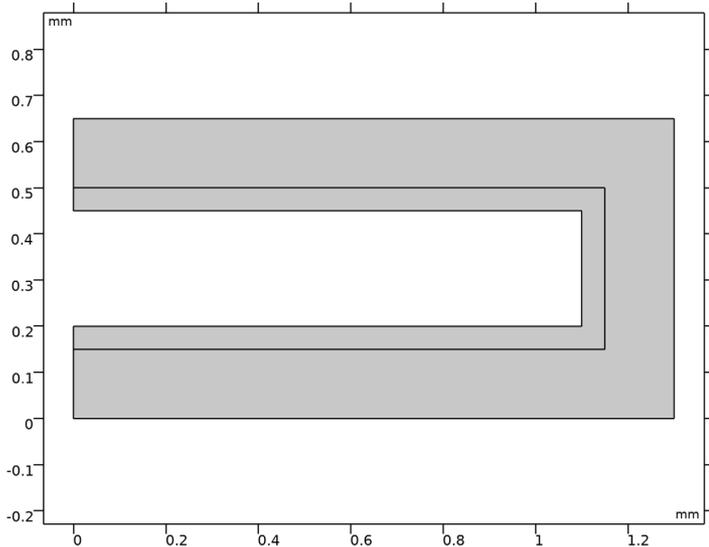
Insert a prepared geometry sequence from a file. After insertion you can study each geometry step in the sequence.

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 on your computer, `Batteries_and_Fuel_Cells_Module\Batteries,_Lithium-Ion`. Double-click to add or click Open.

3 On the Geometry toolbar, click Build All.

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\COMSOL55\applications\.



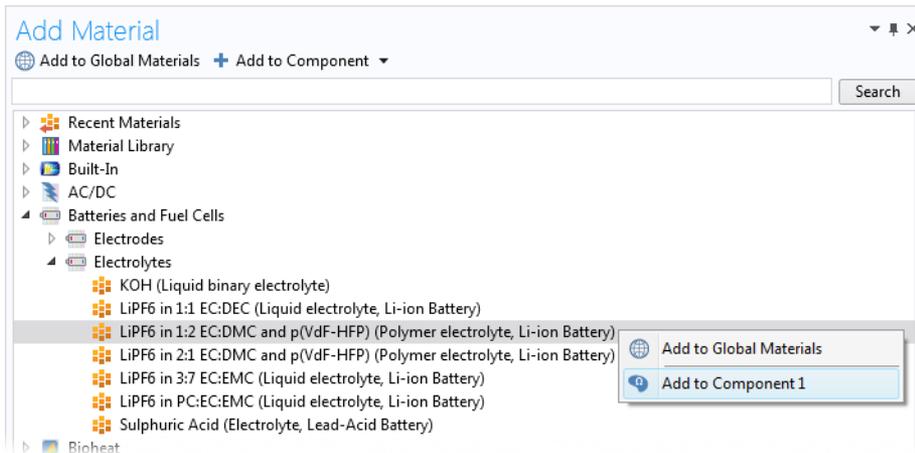
Materials

Use the Batteries and Fuel Cells 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.

1:2 EC:DMC and p(VdF-HFP) (Polymer electrolyte, Li-ion Battery)

I On the Home toolbar, click Add Material .

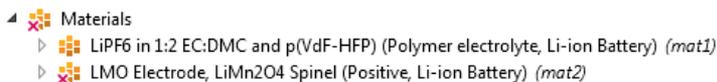
- Go to the Add Material window. In the tree under Batteries and Fuel Cells, under Electrolytes right-click LiPF₆ in 1:2 EC:DMC and p(VdF-HFP) (Polymer electrolyte, Li-ion Battery)  and choose  Add to Component 1.



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

- Go to the Add Material window.
- In the tree under Batteries and Fuel Cells 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...) was assigned by default to all domains. Override this default selection by assigning the electrode material to domain 1.

- 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 (cEqref 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.

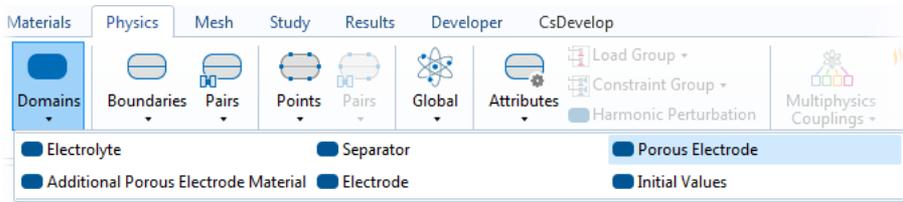
Lithium-Ion Battery Interface

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 I

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 I

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 I

Now define the battery average discharge current density.

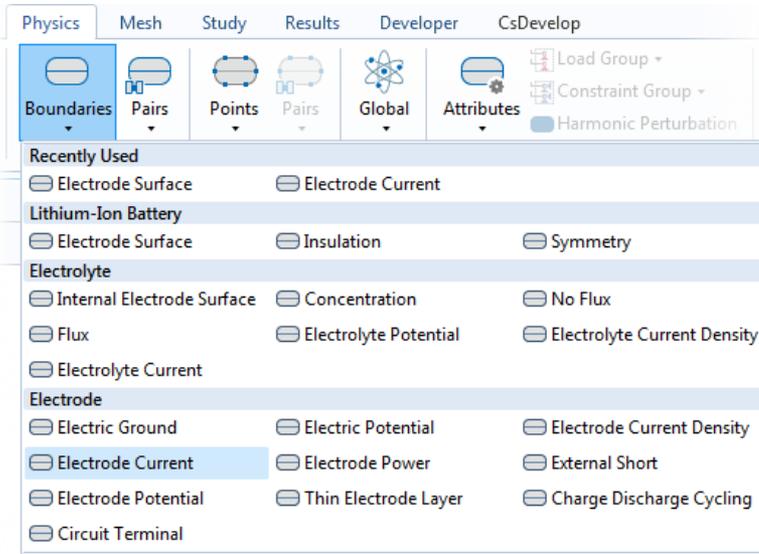
The screenshot shows the following settings in the software interface:

- Electrolyte Properties:**
 - Electrolyte material: LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer ele)
 - Electrolyte conductivity: σ_1 From material
 - Electrolyte salt diffusivity: D_1 From material
 - Transport number: t_+ From material
 - Activity dependence: $\frac{\partial \ln f}{\partial \ln c_1}$ From material
- Electrode Properties:**
 - Electrode material: Domain material
 - Electrical conductivity: σ_s From material
- Particle Properties:** (Expanded)
- Porous Matrix Properties:**
 - Electrode volume fraction: ϵ_s 0.4
 - Electrolyte volume fraction: ϵ_l 1-0.4-0.15

The model tree shows the following structure:

- Lithium-Ion Battery (liion)
 - Electrolyte 1
 - No Flux 1
 - Insulation 1
 - Initial Values 1
 - Porous Electrode 1
 - Particle Intercalation 1
 - Porous Electrode Reaction 1
 - Mesh 1

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

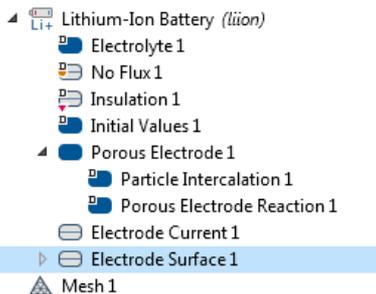


- 2 Select boundary 10 only.
- 3 In the Electrode Current section, select Average current density in the list and enter $-50[\text{A}/\text{m}^2]$ in the average current density text field.

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.

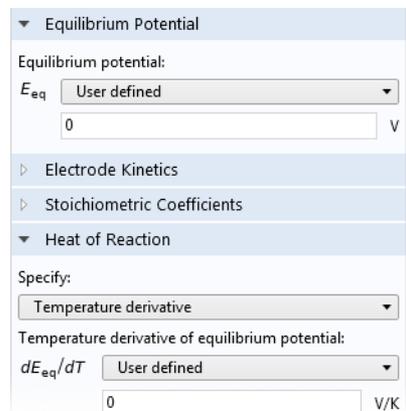
Electrode Reaction 1

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 Reaction 1

- 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:

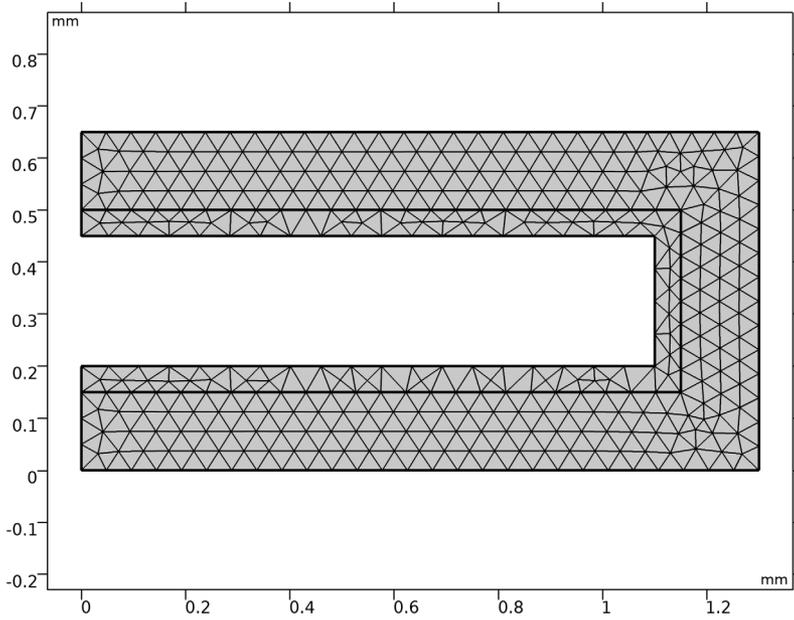
dE_{eq}/dT User defined

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:

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



Study 1

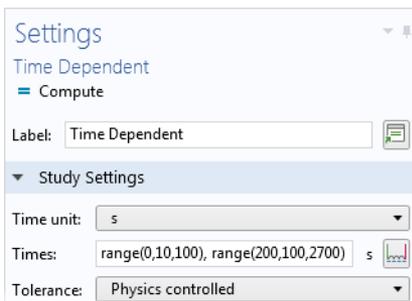
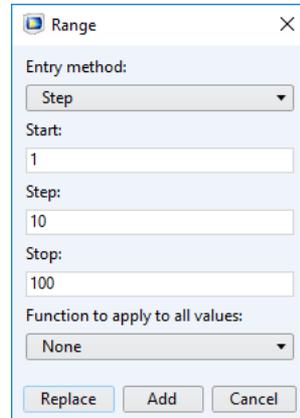
Set up a 2700 second time-dependent solver to store the solution at 10 second intervals during the first 100 seconds, and 100 second intervals during the last 2600 seconds. Then solve the problem.

Step 2: Time Dependent

- 1 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 (the small 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  .

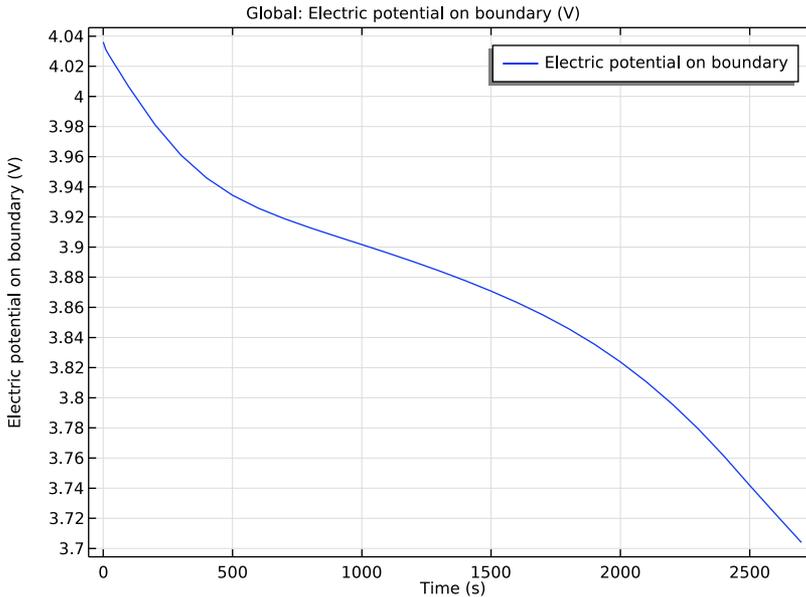
Results

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 .



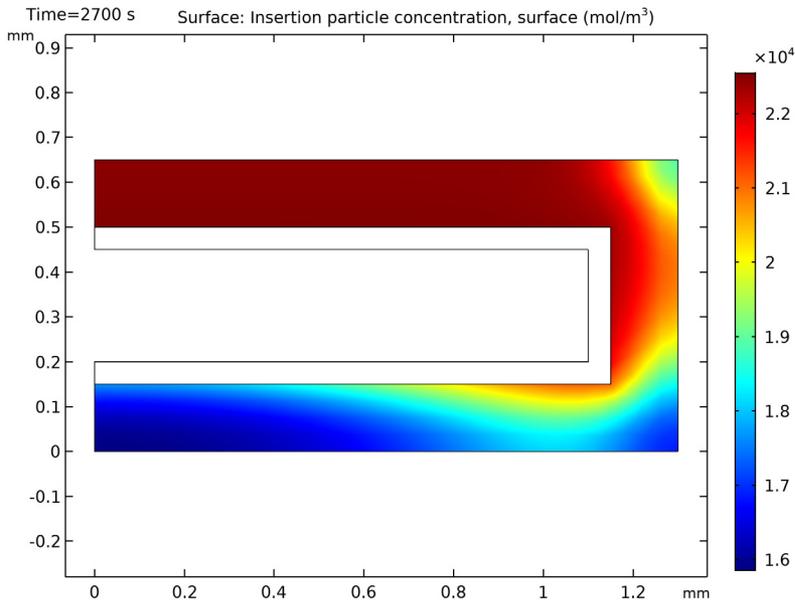
Also browse through the other default plots created. For the 2D plots you can select the time to plot for in the Data section.

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). Choose Insertion particle concentration, surface (liion.cs_surface), 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 .



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.

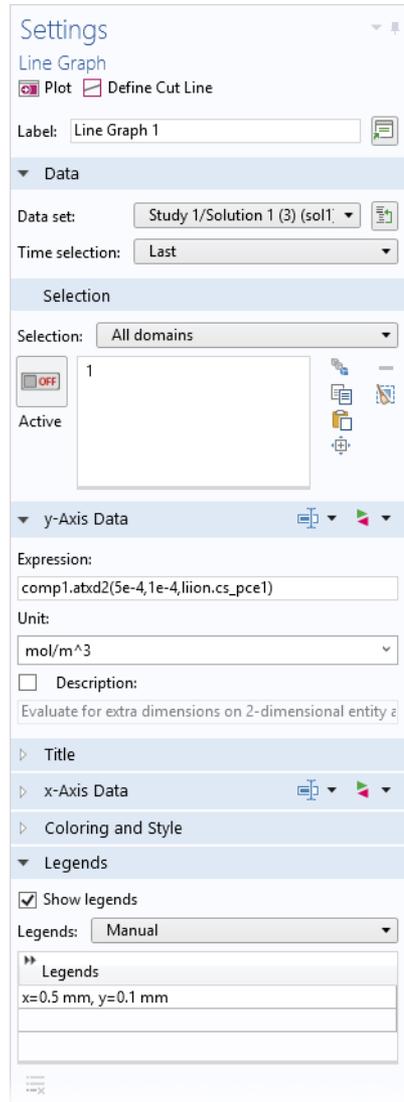
- 1 On the Results toolbar, click More Datasets  and choose Solution .
- 2 In the Solution Settings window, choose Extra Dimension from Porous Electrode I (liion_pce1_pin1_xdim) in the Component list displayed within the Solution section.

1D Plot Group 9

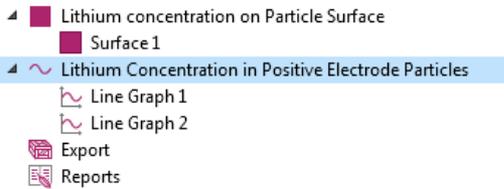
Start with the settings to plot the solid lithium concentration in the negative electrode.

- 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.



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



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

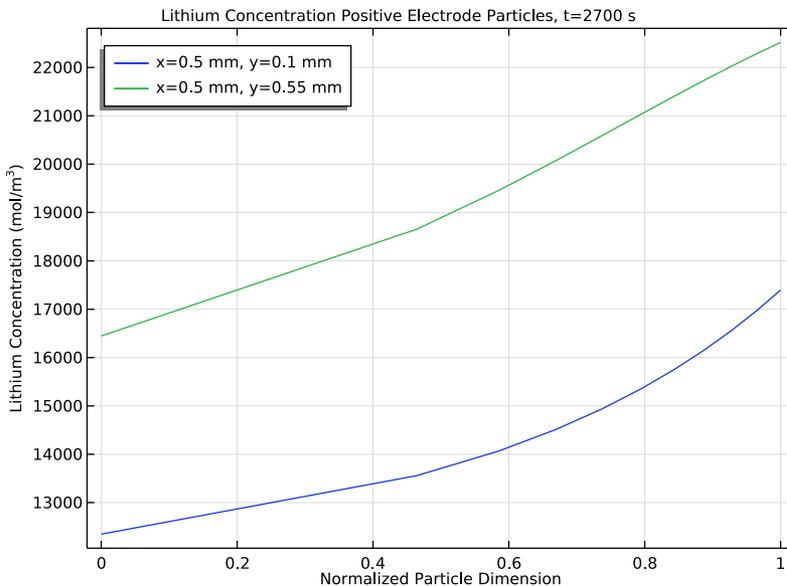
Lithium Concentration Positive Electrode Particles, $t=2700$ s.

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/m^3).

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.



Tutorial of a Fuel Cell Cathode

One of the most important—and most difficult—parameters to model in a fuel cell is the mass transport through gas diffusion and reactive layers. Gas concentration gradients may often be quite large and are significantly affected by the reactions that take place. In addition, their molar fractions of reactants and products are typically large (>10%), which makes Fickian diffusion an inappropriate assumption for modeling the diffusive mass transport.

Figure 8 shows an example 3D geometry of a cathode from a fuel cell with perforated current collectors. It is often seen in self-breathing cathodes or in small experimental cells. Due to the perforation layout, a 3D model is needed in the study of the mass transport, current, and reaction distributions.

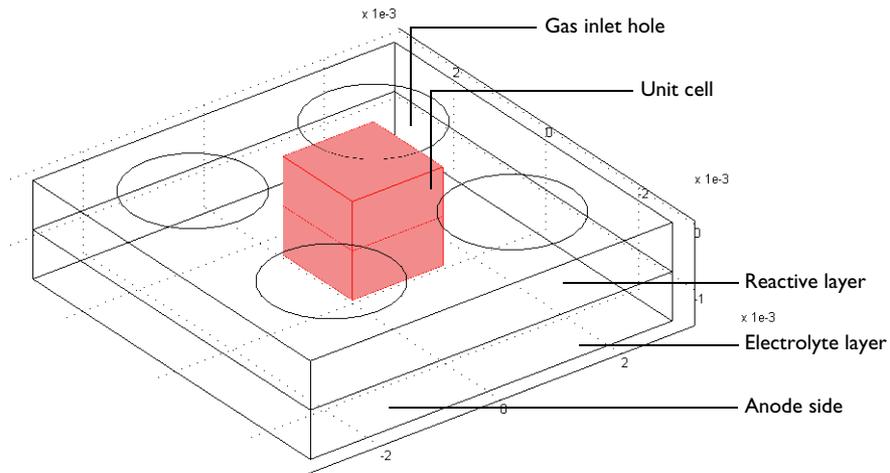
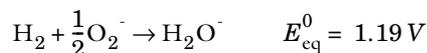


Figure 8: A fuel cell cathode with a perforated current collector.

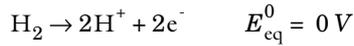
This example investigates such a geometry and the mass transport that occurs through Maxwell-Stefan diffusion. It couples this mass transport to a concentration-dependent Butler-Volmer electrochemical kinetic expression in a porous cathode. Darcy's law is used to define the convective velocity in the porous electrode.

The electrochemical reaction for a PEM fuel cell to produce electrical energy is given by:

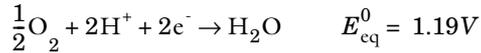


where E_{cq}^0 denotes the standard equilibrium potential of the cell reaction, assuming all reactants reacting in the gas phase at atmospheric pressure.

At the anode Hydrogen Oxidation Reaction (HOR) yield protons:



whereas on the cathode, water is produced via Oxygen Reduction Reaction (ORR):



Model Definition

Figure 9 shows details for a unit cell from Figure 8. The circular hole in the collector is where the gas enters the modeling domain, where the composition is known. The upper rectangular domain is the reaction-zone electrode. It is a three phase porous structure that contains the feed-gas mixture, an electronically conducting material covered with an electrocatalyst, and an ionically conducting electrolyte. The lower domain corresponds to a solid electrolyte ionically interconnecting the two electrodes of the fuel cell. No reaction takes place in this domain and the current is conducted ionically. In addition, there are no pores present to allow gas to flow, nor any material present for electronic current conduction.

The reaction zone is 0.075 mm thick, as is the electrolyte layer. The unit cell is 1.5-by-1.5 mm in surface, and the gas inlet hole has a radius of 1.0 mm.

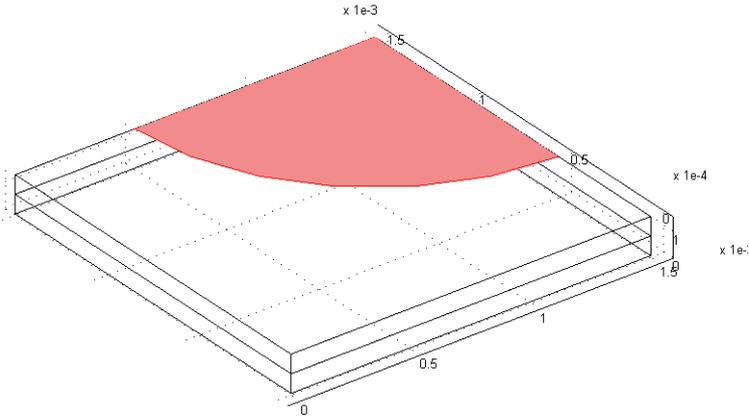


Figure 9: The modeled fuel cell cathode unit cell. The marked zone is the surface of the cathode that is open to the feed gas inlet, while the rest of the top surface sits flush against the current collector. In the unit cell the top domain is the porous cathode, while the bottom domain is the solid electrolyte.

The electronic and ionic current balances are modeled using a Secondary Current Distribution interface, solving for the potentials ϕ_s and ϕ_l in the electrode and electrolyte phases, respectively. The anode side of the cell is grounded, whereas the current collector boundary at the cathode is set to a cell potential value.

The species (mass) transport is modeled by the Maxwell-Stefan equations for the mass fractions of oxygen, water and nitrogen in the gas phase using a Transport of Concentrated Species interface. Mass transport is solved for in the electrode domain only. As boundary conditions, inlet molar fractions are set for the three gas species corresponding to a humidified air mixture at 90% relative humidity at atmospheric pressure.

The pressure and the resulting velocity vector is solved for using a Darcy's law interface.

The cell operates at 80°C. Reference equilibrium potentials for the higher temperature, the reference state, for each reaction are calculated from the standard free energies of formation and reaction entropies according to

$$E_{\text{cq, ref}}(T) = -\frac{(\Delta G^0 - (T - T^0)\Delta S^0)}{nF}$$

where $T^0=25^\circ\text{C}$ denotes the temperature of the standard state.

Generally, the equilibrium potentials of the electrode reactions will depend on the local partial pressures of the reacting species according to the Nernst Equation:

$$E_{\text{eq}} = E_{\text{eq, ref}}(T) - \frac{RT}{nF} \ln \prod_i \left(\frac{p_i}{p_{\text{ref}}} \right)^{\nu_i}$$

where ν_i are the stoichiometric coefficients of the reacting species.

The cathode electrode kinetics of the cathode are defined using a Butler-Volmer type of expression according to

$$i_{\text{loc, O}_2} = i_{0, \text{ref, O}_2} \left(\left(\frac{p_{\text{H}_2\text{O}}}{p_{\text{ref}}} \right)^2 \exp\left(\frac{\alpha_{a, \text{O}_2} F \eta_{\text{ref, O}_2}}{RT}\right) - \frac{p_{\text{O}_2}}{p_{\text{ref}}} \exp\left(-\frac{\alpha_{c, \text{O}_2} F \eta_{\text{ref, O}_2}}{RT}\right) \right)$$

where p_i is the partial pressure of the reacting species, $p_{\text{ref}}=1$ atm is the reference pressure and η_{ref} , the overpotential with respect to the reference state, is defined as

$$\eta_{\text{ref, O}_2} = \phi_s - \phi_l - E_{\text{eq, ref, O}_2} \cdot$$

The local current density expression in the cathode is multiplied by a specific area of $10^9 \text{ m}^2/\text{m}^3$ to create a volumetric current source term in the electrode domain. Assuming ideal kinetics according to the mass action law, $\alpha_{a, \text{O}_2} + \alpha_{c, \text{O}_2} = n$.

For the anode, the kinetics is assumed to be so fast that a linearized Butler-Volmer expression may be used on the anode boundary.

$$i_{\text{loc, H}_2} = i_{0, \text{ref, H}_2} \left(\frac{p_{\text{H}_2}}{p_{\text{ref}}} \exp\left(\frac{\alpha_{a, \text{H}_2} F \eta_{\text{ref, H}_2}}{RT}\right) - \exp\left(-\frac{\alpha_{c, \text{H}_2} F \eta_{\text{ref, H}_2}}{RT}\right) \right)$$

$$i_{\text{loc, H}_2} \approx i_{0, \text{ref, H}_2} \left(\frac{p_{\text{H}_2}}{p_{\text{ref}}} \right)^{\frac{\alpha_{c, \text{H}_2}}{n}} \left(\frac{nF\eta}{RT} \right)$$

assuming $\alpha_{a, \text{H}_2} + \alpha_{c, \text{H}_2} = n$ and where, since the anode boundary is grounded, the overpotential is defined as

$$\eta = 0 - \phi_l - E_{\text{eq, H}_2} \cdot$$

The partial pressure of hydrogen is assumed to be constant on the anode boundary. No mass transport effects nor any current distribution along the depth of the anode electrode are hence considered.

Results and Discussion

Figure 10 shows the oxygen concentration. The figure shows that concentration variations are small along the thickness of the cathode for this relatively small current density, while they are substantially larger along the electrode's width.

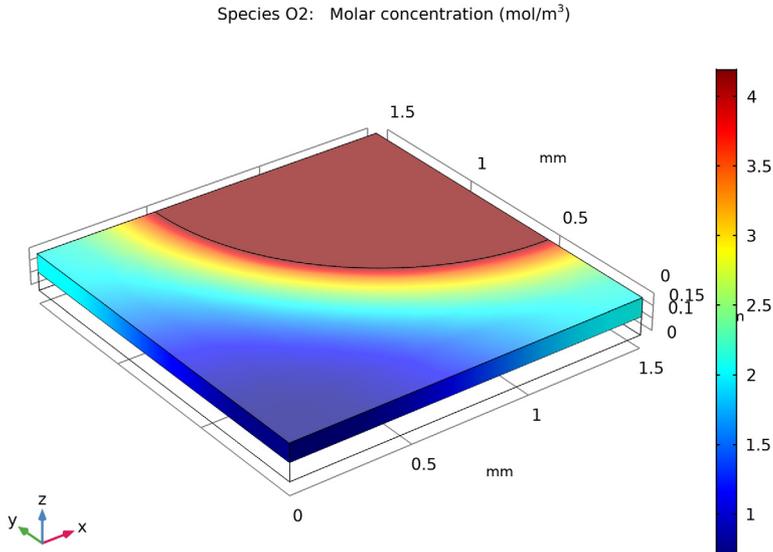


Figure 10: Molar concentration of oxygen.

Figure 11 shows the gas velocity in the porous cathode. There is a significant velocity peak at the edge of the inlet orifice. This is caused by the contributions of the reactive layer underneath the current collector because in this region the convective flux dominates the mass transport. Thus it is important to model the velocity field properly. In this case, the combination of a circular orifice and square unit cell eliminates the possibility to approximate the geometry with a rotationally symmetric model.

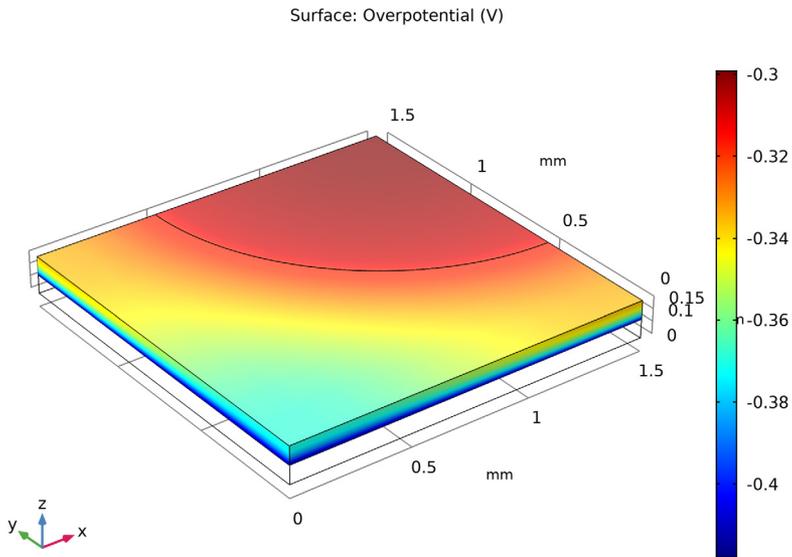


Figure 12: Local overpotential in the cathode reactive layer.

The combination of the overpotential and oxygen concentration distributions will result in a highly uneven reaction rate in the reactive layer. One way to study the

distribution of the reaction rate is to plot the ionic current density at the bottom boundary of the electrolyte. Figure 13 shows such a plot.

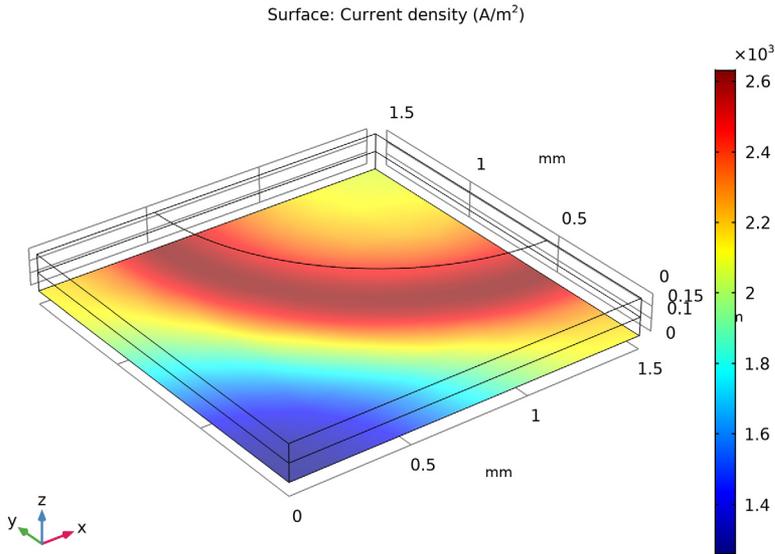


Figure 13: Current density perpendicular to the lower, electrolyte boundary.

The current-density distribution shows that the variations are rather large. The reaction rate and the current production are higher beneath the orifice and decrease as the distance to the gas inlet increases. This means that the mass transport of reactant dictates the electrode's efficiency for this design at these particular conditions.

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

Model Wizard

Start by adding a Secondary Current Distribution interface and a Stationary study to set up and solve for a current distribution model of the cell. Later you will add more physics features for modeling mass transport and convection.

- 1 If COMSOL is already open, you can start the Model Wizard by selecting New  from the File menu and then click Model Wizard .
- 2 In the Space Dimension window click the 3D button .

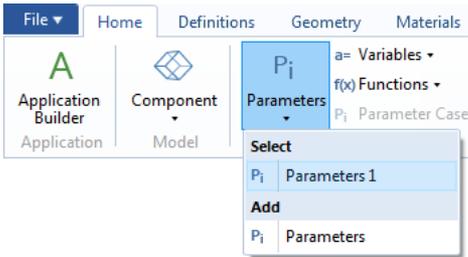
- 3 In the Select Physics tree under Electrochemistry>Primary and Secondary Current Distribution, click Secondary Current Distribution (cd) .
- 4 Click Add and then click the Study  button.
- 5 Under Preset Studies for Selected Physics Interfaces, click Stationary with Initialization .
- 6 Click Done .

Global Definitions

Load the model parameters from a text file.

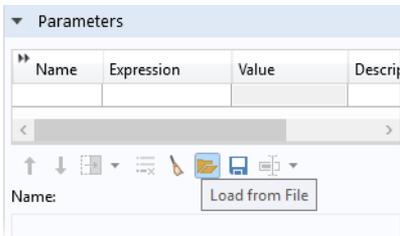
Parameters

- 1 On the Home toolbar click Parameters  and select Parameters 1 .



Note: On Linux and Mac, the Home toolbar refers to the specific set of controls near the top of the Desktop.

- 2 In the Settings window for Parameters locate the Parameters section. Click Load from File .



- 3 In the application library folder on your computer, applications\Batteries_and_Fuel_Cells_Module\Fuel_Cells, double-click the file fuel_cell_cathode_parameters.txt to import it to the Parameters table. 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\COMSOL55\applications\.

Geometry I

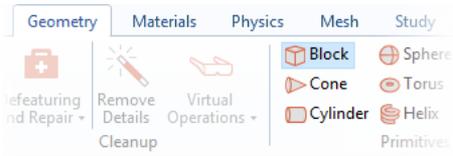
Now draw the model geometry. Use blocks to define the electrolyte and the porous electrode domains. Then use a workplane to draw the inlet hole at the top of the porous electrode. Facilitate geometry selection later (when setting up the physics interfaces) by enabling Resulting objects selection and renaming the geometry objects.

Begin by setting the default length unit to millimeters.

- 1 In the Model Builder under Component 1, click Geometry 1 .
- 2 In the Settings window for Geometry locate the Units section. From the Length unit list, choose mm.

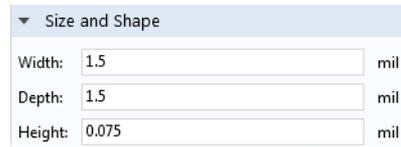
Create the First Block

- 1 On the Geometry toolbar click Block .



- 2 In the Model Builder under Geometry 1, click Block 1 .
- 3 In the Settings window for Block, type Electrolyte in the Label text field.
- 4 In the Settings window for Block locate the Size section.

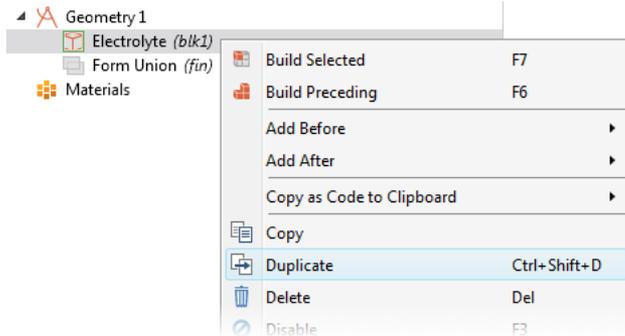
- In the Width text field, type 1.5.
- In the Depth text field, type 1.5.
- In the Height text field, type 0.075.



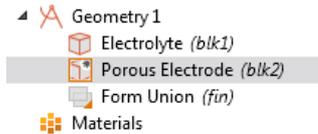
- 5 Locate the Selections of Resulting Entities section. Enable the Resulting objects selections check box. By enabling Resulting objects selection here, the domain created by this rectangular block will also be available as a named domain option later on when setting up the physics.
- 6 Click the Build Selected button .

Duplicate the Block and Change z Position

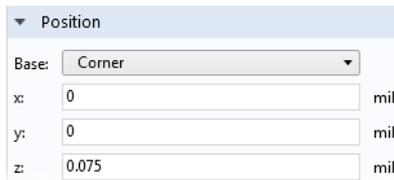
7 Right-click Electrolyte  and choose Duplicate .



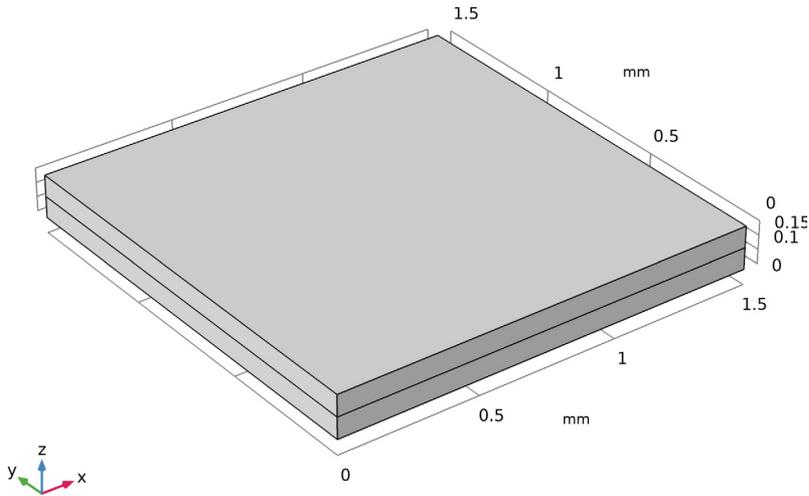
8 In the Label text field, type Porous Electrode.



9 In the Settings window for Block locate the Position section. In the z text field, type 0.075.



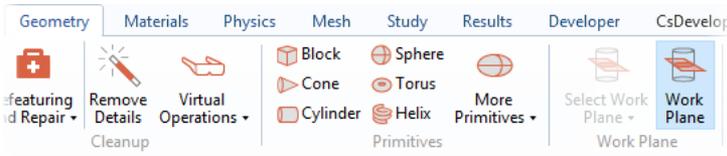
10 Click Build Selected. Your geometry should now look like this:



Create a Work Plane for Drawing the Inlet Hole

Proceed to draw the inlet hole, placed at the top of the porous electrode block.

1 On the Geometry toolbar click Work Plane .



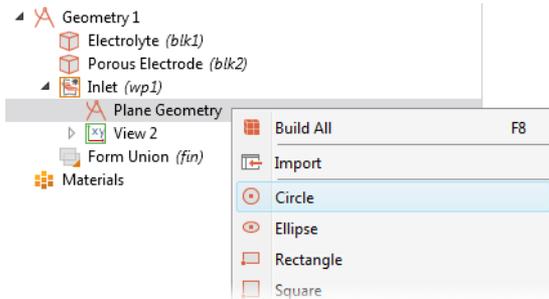
2 In the Label text field, type Inlet.

3 In the Settings window for Work Plane locate the Plane Definition section. In the z-coordinate field, type 0.15.

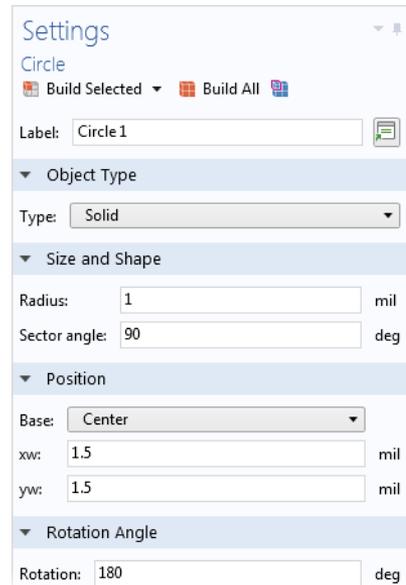
4 Locate the Selections of Resulting Entities section. Enable the Resulting objects selections check box.

Draw the Inlet Hole

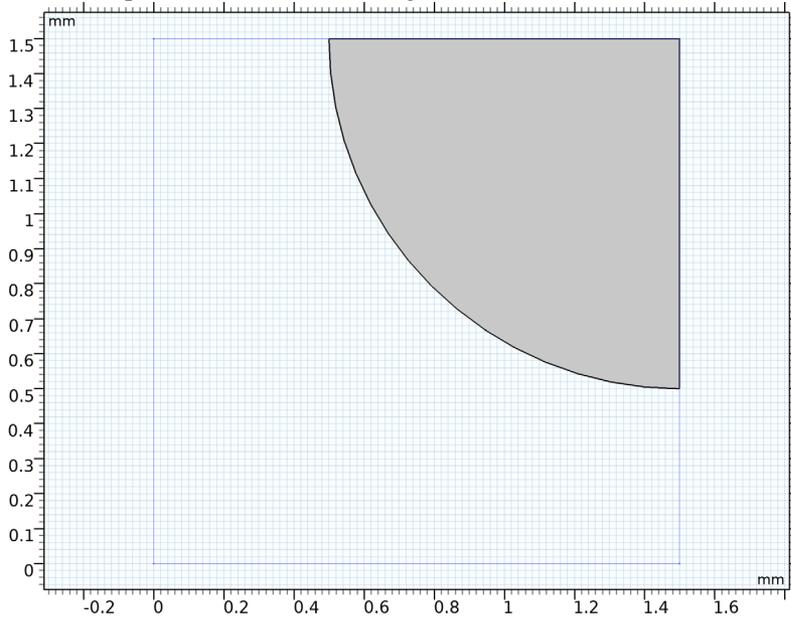
- 1 In the Model Builder under Geometry 1>Inlet, right-click Plane Geometry and choose Circle .



- 2 In the Settings window for Circle locate the Size and Shape section.
 - In the Radius text field, type 1.
 - In the Sector angle text field, type 90.
- 3 Locate the Position section.
 - In the xw text field, type 1.5.
 - In the yw text field, type 1.5.
- 4 Locate the Rotation Angle section. In the Rotation text field, type 180.



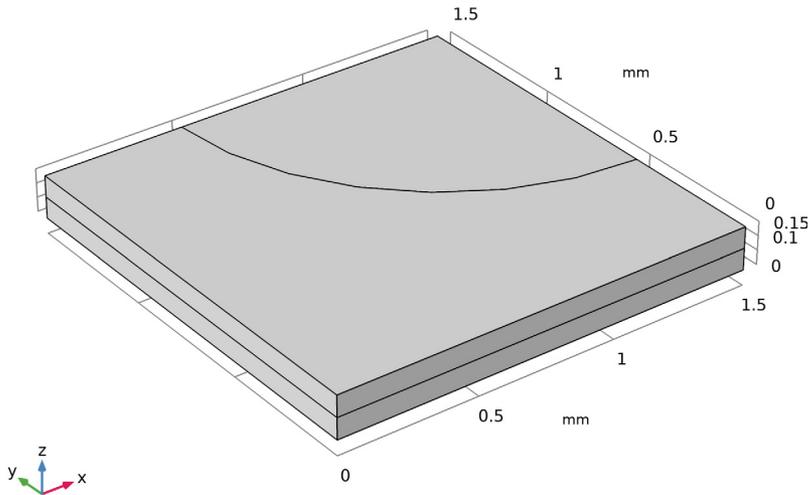
- 5 Click the Build Selected button  . Your work plane 2D geometry should now contain a quarter of a circle, looking as follows:



Form a Union to Finalize the Geometry

- 1 In the Model Builder click the Form Union node  and then click the Build Selected button  .

- 2 Click the Zoom Extents button  on the Graphics toolbar. The final 3D geometry should now look like this:



Secondary Current Distribution

An Electrolyte node was added by default in the Secondary Current Distribution interface. Keep the default settings for this node.

We will not be including the anode as a domain in this model. Instead we will set up the (very fast) electrode kinetics on the anode boundary using an Electrode Surface node.

Electrode Surface 1 - The Anode

- 1 In the Physics toolbar, click Boundaries and choose Electrode Surface.
- 2 In the Settings window for Electrode Surface, type **Electrode Surface - Anode** in the Label text field.
- 3 Select Boundary 3 only.
- 4 You can also create named selections directly here as follows: Locate the Boundary Selection section. Click Create Selection. (The small icon to the right in the Boundary Selection section.) In the Create Selection dialog box, type **Anode Boundary** in the Selection name text field, and click OK.

Keep the default voltage setting of 0[V] for this node, but use the Electrode Reaction child node that was added by default to set up the thermodynamics and kinetics of the hydrogen oxidation reaction.

Electrode Reaction 1 - Hydrogen Kinetics

- 1 In the Model Builder window, expand the Component 1>Secondary Current Distribution>Electrode Surface - Anode node, then click Electrode Reaction 1.
- 2 In the Settings window for Electrode Reaction, locate the Equilibrium Potential section.
- 3 From the E_{eq} list, choose Nernst equation, and in the $E_{\text{eq,ref}}(T)$ text field, type Eeq_ref_H2.
- 4 In the C_R text field, type x_H2.
- 5 Locate the Stoichiometric Coefficients section. In the n text field, type 2.
- 6 Locate the Electrode Kinetics section. From the Exchange current density type list, choose From Nernst Equation.
- 7 In the $i_{0,\text{ref}}(T)$ text field, type i0_ref_H2.
- 8 In the α_a text field, type alpha_a_H2.

▼ Stoichiometric Coefficients

Number of participating electrons:
 n 1

▼ Equilibrium Potential

Equilibrium potential:
 E_{eq} ▼

Reference equilibrium potential:
 $E_{\text{eq,ref}}(T)$ V

Reduced species expression:
 C_R 1

Oxidized species expression:
 C_O 1

$$E_{\text{eq}} = E_{\text{eq,ref}}(T) - \frac{RT}{nF} \ln \frac{C_R}{C_O}$$

▼ Electrode Kinetics

Kinetics expression type:
 ▼

Exchange current density type:
 ▼

Reference exchange current density:
 $i_{0,\text{ref}}(T)$ A/m²

Anodic transfer coefficient:
 α_a 1

$$i_{\text{loc}} = i_0 \left(\frac{(\alpha_a + \alpha_c)F}{RT} \eta \right)$$

$$i_0 = i_{0,\text{ref}}(T) C_R^{\alpha_c/n} C_O^{\alpha_a/n}$$

$$\alpha_c = n - \alpha_a$$

Limiting current density

Porous Electrode 1 - The Cathode

Use a Porous Electrode node to model the cathode gas diffusion electrode.

- 1 On the Physics toolbar click Domains  and choose Porous Electrode .
- 2 In the Settings window for Porous Electrode, type Porous Electrode - Cathode in the Label text field.
- 3 Locate the Domain Selection section. From the Selection list, choose Porous Electrode.
- 4 Set the volume fractions for the electrolyte and electrode phases of the porous cathode. Locate the Electrolyte Current Conduction section. In the ϵ_1 text field,

type ϵ_{s1} . Similarly, locate the Electrode Current Conduction section. In the ϵ_s text field, type ϵ_{s2} .

The volume fractions you just specified will be used to calculate effective conductivities, based on the bulk conductivity values for each phase, which we will now define in the Materials node.

Materials

Note that the Materials node in the model tree now is marked with a small red x, indicating that there are some material properties needing to be specified.

Material 1 - Set the Conductivities

- 1 In the Model Builder, under Component 1, right click on Materials  and click Blank Material .
- 2 Locate the Material Contents section. In the table enter the following settings:

PROPERTY	VALUE
Electrolyte conductivity	5[S/m]
Electrical conductivity	1000[S/m]

The red cross should now have vanished.

Secondary Current Distribution

Porous Electrode Reaction 1 - Oxygen Kinetics

Use the Porous Electrode Reaction child node that was added by default to set up the thermodynamics and kinetics of the oxygen reduction reaction.

- 1 In the Model Builder window, expand the Secondary Current Distribution >Porous Electrode - Cathode node, then click Porous Electrode Reaction 1.
- 2 In the Settings window for Porous Electrode Reaction, locate the Equilibrium Potential section.
- 3 From the E_{eq} list, choose Nernst equation, and in the $E_{eq,ref}(T)$ text field, type E_{eq,ref_O2} .
- 4 In the C_R text field, type $x_{H2O_in}^2$.
- 5 In the C_O text field, type x_{O2_in} .

For now we will use constant values for all parameters defined in this node. Later on, when we include mass transport, we will make the equilibrium potential and exchange current density concentration dependent.

- 6 Locate the Stoichiometric Coefficients section. In the n text field, type 4.
- 7 Locate the Electrode Kinetics section. From the Kinetics expression type list, choose Butler-Volmer.
- 8 From the Exchange current density type list, choose From Nernst Equation.
- 9 In the $i_{0,\text{ref}}(T)$ text field, type i0_ref_02.
- 10 In the α_a text field, type alpha_a_02.
- 11 Locate the Active Specific Surface Area section. In the av text field, type Av.

The Nernst and Butler-Volmer equations make use of a temperature variable. Since we will be using the same temperature everywhere in the model, we will define the temperature only once in the Default Model Inputs node.

- 1 In the Settings window for the Porous Electrode Reaction node, locate the Model Input section. In the T text field, the Common model input value is set by default. Click the Go to Source button on the right to go to the Default Model Inputs node.

Model Input

Temperature:
 T Common model input

Equilibrium Potential

Electrode Kinetics

Kinetics expression type:
 Butler-Volmer

Exchange current density type:
 From Nernst Equation

Reference exchange current density:
 $i_{0,\text{ref}}(T)$ i0_ref_02 A/m²

Anodic transfer coefficient:
 α_a alpha_a_02 1

$$i_{\text{loc}} = i_0 \left(\exp\left(\frac{\alpha_a F \eta}{RT}\right) - \exp\left(\frac{-\alpha_c F \eta}{RT}\right) \right) = i_{0,\text{ref}}(T) \left(C_R \exp\left(\frac{\alpha_a F \eta_{\text{ref}}}{RT}\right) - C_O \exp\left(\frac{-\alpha_c F \eta_{\text{ref}}}{RT}\right) \right)$$

$$i_0 = i_{0,\text{ref}}(T) C_R^{\alpha_c/n} C_O^{\alpha_a/n}$$

$$\alpha_c = n - \alpha_a$$

Limiting current density

- 2 In the Default Model Inputs node's Settings window, locate the Browse Model Inputs section. In the tree, select Temperature (K) - minput.T under General.

Then find the Expression for remaining selection subsection, and enter T for the Temperature text field.

Electric Potential 1 - Specify the Cell Potential

Finalize the secondary current distribution model by setting the cell potential on the current collector boundary as follows:

- 1 On the Physics toolbar click Boundaries  and choose Electric Potential .
- 2 In the Settings window for Electric Potential, locate the Boundary Selection section. Select Boundary 7.
- 3 In the Settings window for Electric Potential, locate the Boundary Selection section. Click Create Selection and in the Create Selection dialog box, type Current Collector in the Selection name text field. Click OK.
- 4 Locate the Electric Potential section. In the $\phi_{s,bnd}$ text field, type E_cell.

Solve the Secondary Current Distribution and Evaluate the Results

The physics settings for the secondary current distribution model are now complete.

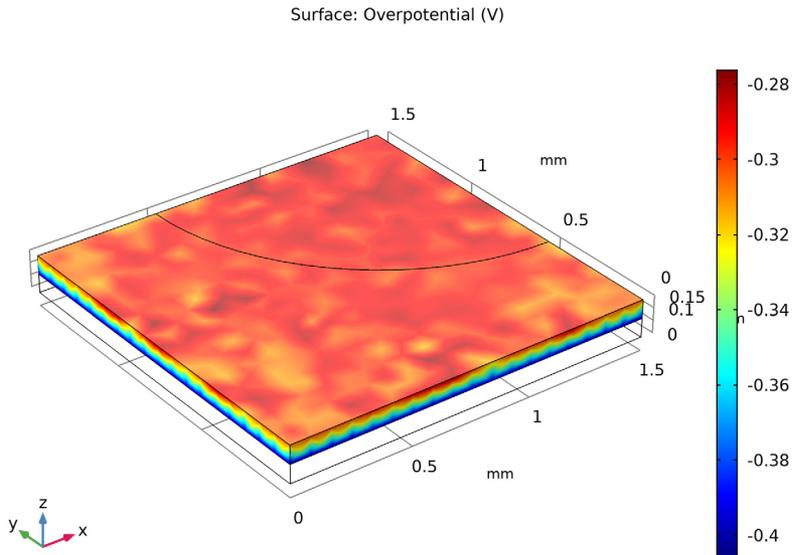
- 1 In the Home toolbar, click Compute.

A number of default plots are created by default. You may also create additional plots manually. We will analyze the solution by creating additional plots for the activation overpotential, the local volumetric current density and the current density at the anode boundary.

Overpotential Plot

- 1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Overpotential in the **Label** text field.
- 3 Right-click Overpotential and choose Surface.
- 4 In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component 1>Secondary Current Distribution>Electrode kinetics>cd.eta_per 1 - Overpotential - V.

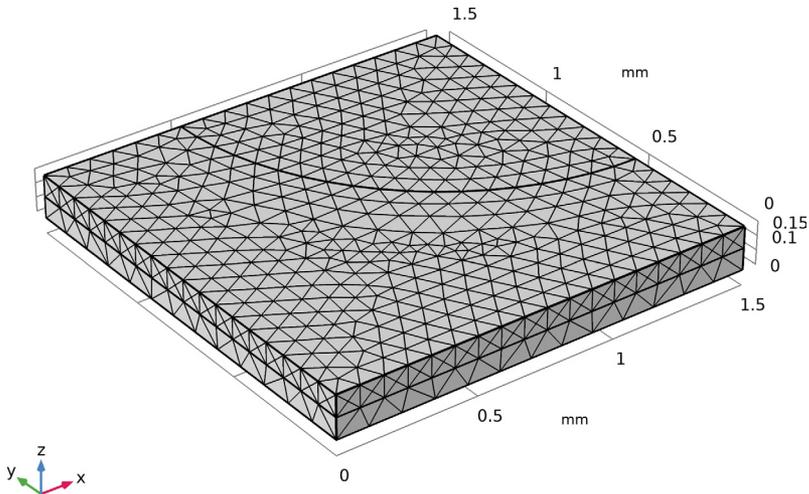
5 In the Overpotential toolbar, click Plot. The overpotential plot should look as follows:



Generally the highest overpotentials (in magnitude) are found in the region facing the Electrolyte domain. Since the overpotential is the driving force for the electrochemical reactions, this is the region where we can expect higher reaction rates. Also note that the overpotential plot looks a bit unregular and “noisy”. To improve the resolution of the solution we will now create a user-defined mesh.

Improve the Mesh

- 1 Select the Mesh 1 and inspect the mesh.



The default mesh that was created automatically is fairly coarse, featuring only one or two mesh elements in the z direction. To improve accuracy of the results, the mesh needs to be refined. For this geometry a swept mesh can be used to get accurate control of the number of elements in the z direction.

Swept 1

- 1 In the Model Builder window, under Component 1 (comp1) right-click Mesh 1 and choose Swept.
- 2 In the Settings window for Swept, click to expand the Source Faces section.
- 3 Select Boundaries 7 and 10 only.

Distribution 1

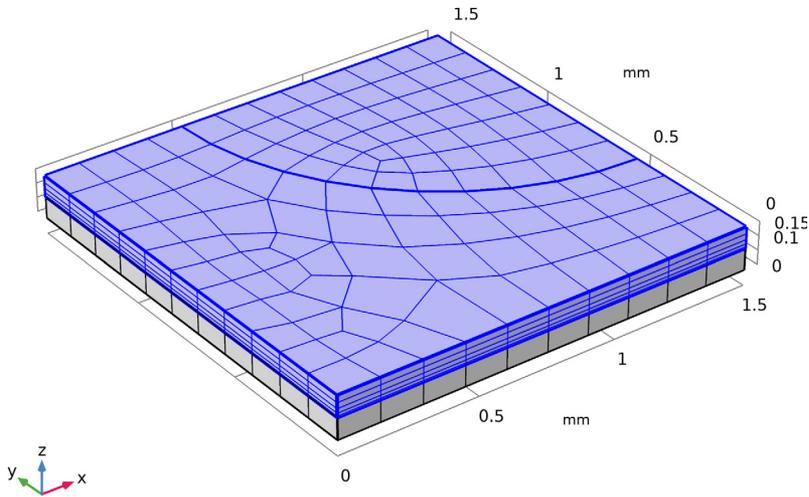
- 1 Right-click Component 1 (comp1)>Mesh 1>Swept 1 and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 From the Selection list, choose Porous Electrode.

- 4 Locate the Distribution section. From the Distribution type list, choose Predefined.

We will use the Arithmetic sequence to create a mesh with thinner elements in the porous electrode domain towards the boundary facing the electrolyte domain.

- 5 In the Element ratio text field, type 5.
- 6 Select the Reverse direction check box.
- 7 Click Build All.

The mesh should now look as follows:



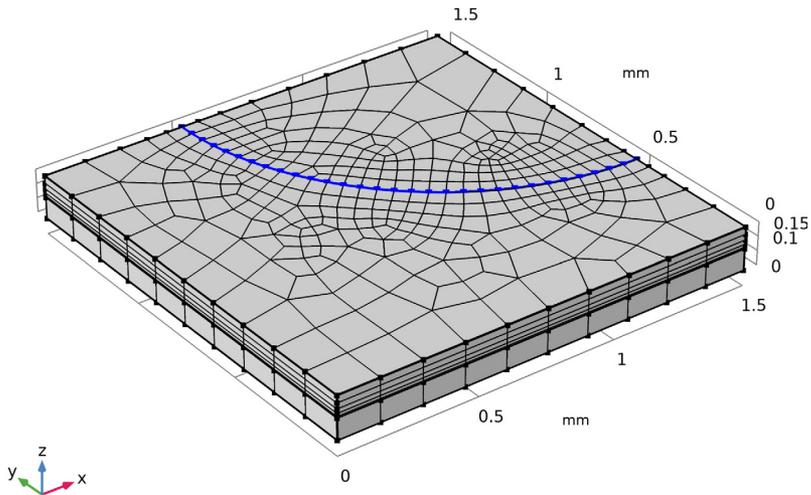
Swept 1

To improve the resolution along the current collector-inlet hole edge, also add a size node.

Size 1

- 1 Right-click Swept 1 and choose Size.
- 2 In the Settings window for Size, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Edge.
- 4 Select Edge 14 only.
- 5 Locate the Element Size section. From the Predefined list, choose Extra fine.

6 Click Build All.



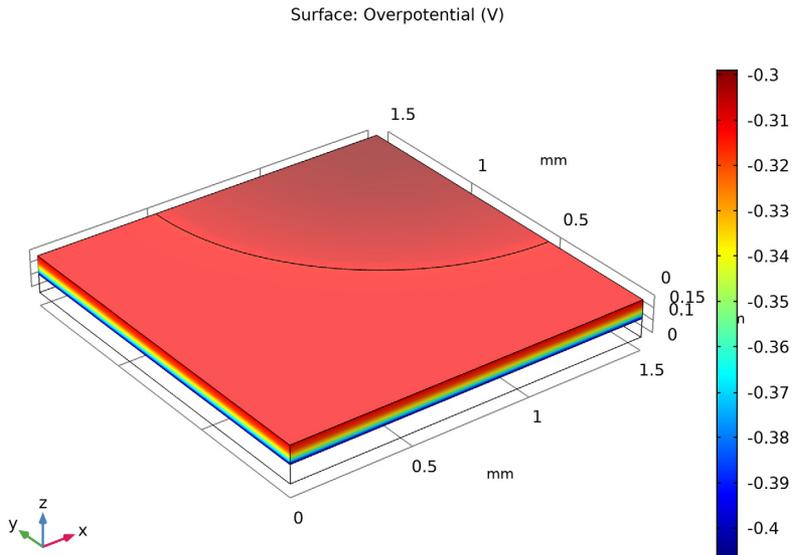
Recompute With the Improved Mesh

Now that we have improved the mesh, recompute the solution.

| In the Home toolbar, click Compute.

Overpotential Plot (Improved)

The overpotential plot now looks better.

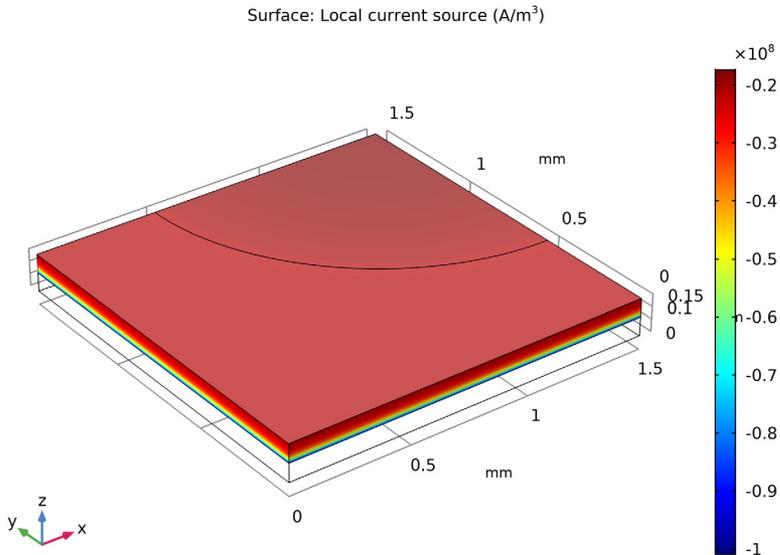


Volumetric Current Density Plot

Now plot the local volumetric current density as follows:

- 1 In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Local Volumetric Current Density in the Label text field.
- 3 Right-click Local Volumetric Current Density and choose Surface.
- 4 In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component 1>Secondary Current Distribution>Electrode kinetics>cd.iv_per1 - Local current source - A/m³.
- 5 In the Local Volumetric Current Density toolbar, click Plot.

The volumetric current density plot should now look as follows:



As for the overpotentials, the highest current density magnitudes are found close to the electrolyte domain.

Local Current Density at the Anode Boundary

Finally for this post processing analysis of the secondary current distribution, also plot the local current density at the anode boundary as follows:

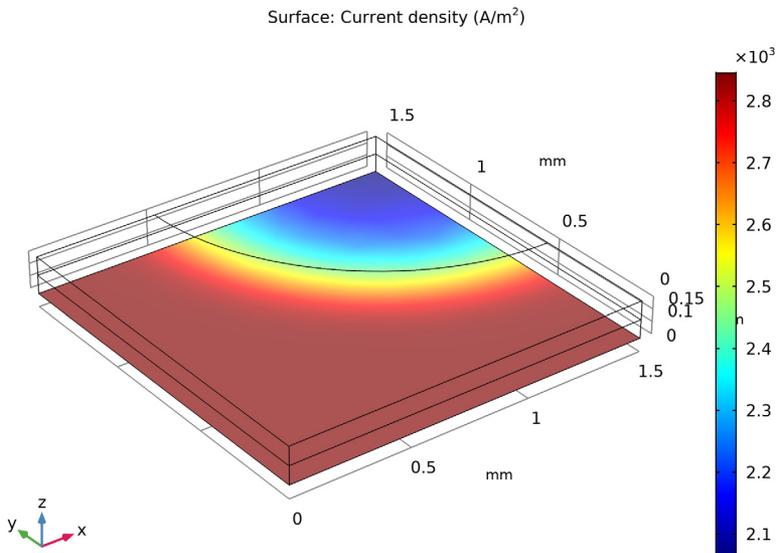
- 1 In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Current Density at Anode Boundary in the Label text field.
- 3 Right-click Current Density at Anode Boundary and choose Surface.
- 4 In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component 1>Secondary Current Distribution>cd.nI1 - Normal electrolyte current density - A/m².
- 5 Locate the Expression section. In the Expression text field, type $\text{abs}(\text{cd.nI1})$. The $\text{abs}()$ is an operator which will return the absolute (positive) value of the argument.
- 6 Select the Description check box, and in the associated text field, type Current density.

Use a Selection node to plot the current density at the anode boundary only.

Selection 1

- 1 Right-click Results>Current Density at Anode Boundary>Surface 1 and choose Selection.
- 2 Select Boundary 3 only.
- 3 In the Settings window for Selection, locate the Selection section.
- 4 From the Selection list, choose Anode Boundary.
- 5 In the Current Density at Anode Boundary toolbar, click Plot.

The current density at the anode boundary plot should now look as follows:

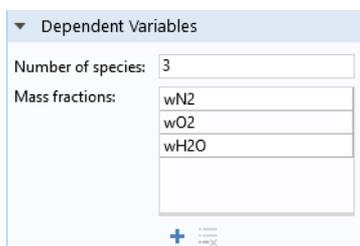


The lowest current densities at the anode boundary are found for the area facing the inlet hole at the cathode side. This is due to the ohmic drop in the electrode phase. For the area under the current collector, the current density is fairly uniform.

Add Mass Transport and Fluid Flow Physics Features to the Model

Now we start the second part of the tutorial, including mass transfer effects. The coupled gas phase diffusion-convection model will be defined using the Transport of Concentrated Species and Darcy's law interfaces.

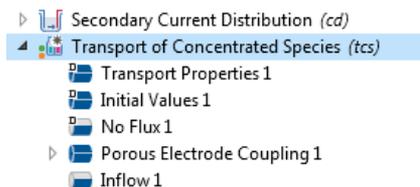
- 1 On the Home toolbar click Add Physics .
- 2 Go to the Add Physics window. In the tree under Chemical Species Transport, click Transport of Concentrated Species .
- 3 Click to expand the Dependent variables section. In the Number of species text field, type 3. In the Mass fractions table, enter wN2, wO2, and wH2O.



- 4 In the Add Physics window click  Add to Component 1.
- 5 Go to the Add Physics window again. In the tree under Fluid Flow>Porous Media and Subsurface Flow, click Darcy's Law .
- 6 In the Add physics window click  Add to Component 1.

Transport of Concentrated Species

- 1 In the Model Builder click Transport of Concentrated Species .



The gas phase is only present in the porous electrode domain.

- 2 Locate the Domain Selection section. From the Selection list choose Porous Electrode.

Transport Properties 1

- 1 In the Model Builder expand the Transport of Concentrated Species  node then click Transport Properties 1 .
- 2 Both the velocity and pressure are coupled to Darcy's law. In the Model Input section, the Absolute pressure is automatically set to the Common model input value. You can use the Go to source button to check that this corresponds to the pressure computed by the Darcy's law, $d1$. pA.
- 3 In the Settings window for Transport Properties, locate the Density section
 - In the M_{wN2} text field, type M_N2.
 - In the M_{wO2} text field, type M_O2.
 - In the M_{wH2O} text field, type M_H2O.
- 4 Locate the Convection section. From the \mathbf{u} list, choose Darcy's velocity field (dl).
- 5 Locate the Diffusion section. In the table enter the following settings:

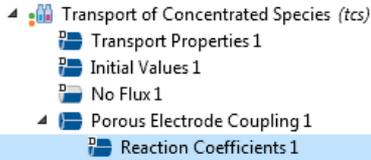
SPECIES 1	SPECIES 2	DIFFUSION COEFFICIENT (M ² /S)
wN2	wO2	D_02N2_eff
wN2	wH2O	D_N2H2O_eff
wO2	wH2O	D_02H2O_eff

Couple the Reaction Rate of Oxygen to the Electrochemical Currents

Use a porous electrode coupling to create a mass sink in the domain corresponding to the oxygen leaving the gas phase due to the electrochemical reactions.

- 1 In the Settings window for Transport of Concentrated Species, locate the Transport Mechanisms section. Select the Mass transfer in porous media check box.
- 2 On the Physics toolbar click Domains  and choose Porous Electrode Coupling .
- 3 Click Porous Electrode Coupling 1 .
- 4 In the Settings window for Porous Electrode Coupling locate the Domain Selection section. From the Selection list choose Porous Electrode.

5 Expand the Porous Electrode Coupling node and click Reaction Coefficients 1 .



6 In the Settings window for Reaction Coefficients, locate the Model Inputs section. From the i_p list, choose Local current source, Porous Electrode Reaction 1 (cd/pce1/per1).

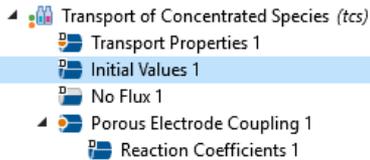
7 Locate the Stoichiometric Coefficients section.

- In the n text field, type 4.
- In the v_{wO_2} text field, type -1.
- In the v_{wH_2O} text field, type 2.

Define the Initial Values Node

Specify the initial and inflow values using molar fractions.

1 Click the Initial Values 1 node .



2 From the Mixture specification list, choose Mole fractions.

3 In the Settings window under Initial Values, enter Mass fraction values $x_{O_2_in}$ in the x_{0,wO_2} field and $x_{H_2O_in}$ in the x_{0,wH_2O} field.

Define the Inflow Node

1 On the Physics toolbar click Boundaries  and choose Inflow .

2 In the Model Builder click Inflow 1 .

3 In the Settings window for Inflow locate the Boundary Selection section. From the Selection list choose Inlet.

4 From the Mixture specification list, choose Mole fractions.

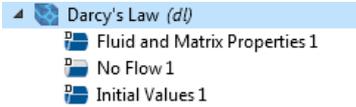
5 Locate the Inflow section.

- In the x_{0,wO_2} text field, type $x_{O_2_in}$.
- In the x_{0,wH_2O} text field, type $x_{H_2O_in}$.

Darcy's Law

Now do the settings for Darcy's law. Also here the electrochemical currents result in a mass sink due to the oxygen molecules leaving the domain.

1 In the Model Builder click Darcy's Law .



2 In the Settings window for Darcy's Law locate the Domain Selection section. From the Selection list, choose Porous Electrode.

3 Locate the Physical Model section. In the p_{ref} text field, type `p_atm`.

Define the Fluid and Matrix Properties

1 Expand the Darcy's Law (dl) node  then click Fluid and Matrix Properties 1.

2 Locate the Fluid Properties section

- From the ρ list, choose Density (tcs/cdm1). (The density is now taken from the Transport of Concentrated Species interface.)
- From the μ list, choose User defined. In the associated text field, type `mu`.

3 Locate the Matrix Properties section.

- From the ϵ_p list, choose User defined. In the associated text field, type `eps_gas`.
- From the κ list, choose User defined. In the associated text field, type `perm`.

Porous Electrode Coupling 1

Since there will be a net flow of mass from the electrolyte phase into the gas phase, a mass source node, coupled to the electrochemical reactions, needs to be defined also here using a Porous Electrode Coupling node.

1 On the Physics toolbar click Domains  and choose Porous Electrode Coupling .

2 Under Darcy's Law click Porous Electrode Coupling 1 .

3 Locate the Domain Selection section and from the Selection list, choose Porous Electrode.

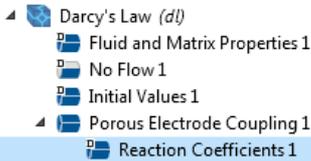
4 Locate the Species section. Click Add  twice.

5 In the Species table, enter the following settings:

SPECIES	MOLAR MASS (KG/MOL)
1	M_N2
2	M_O2
3	M_H2O

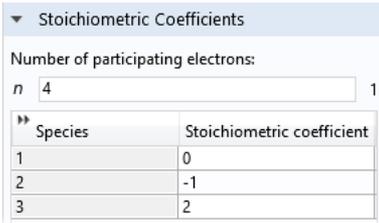
Reaction Coefficients 1

1 In the Model Builder expand the Porous Electrode Coupling 1 node then click Reaction Coefficients 1 .



2 Under Model Inputs, from the Coupled reaction i_v list, choose Local current source, Porous Electrode Reaction 1(cd/pce1/per1).

3 Under Stoichiometric Coefficients enter 4 in the n field, -1 in the 2 field and 2 in 3 field.



Specify the Pressure at the Inlet Hole 1

1 On the Physics toolbar click Boundaries  and choose Pressure .

2 In the Settings window for Pressure locate the Boundary Selection section. From the Selection list, choose Inlet.

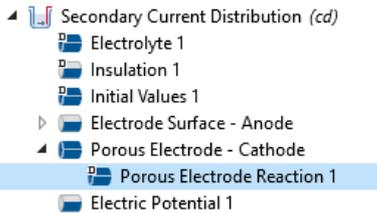
3 (Keep the default pressure setting of 0 Pa).

Secondary Current Distribution

To finalize the mass transport dependent model, make the electrode kinetics dependent on the partial pressure of the reacting gases as follows.

Make the Electrode Reaction Dependent on Partial Pressures

- 1 In the Model Builder under Secondary Current Distribution>Porous Electrode - Cathode, click Porous Electrode Reaction 1 .



- 2 In the Settings window for Porous Electrode Reaction, locate the Equilibrium Potential section.
- 3 In the C_R text field, type $(tcs.p_{wH2O}/p_{ref})^2$ and in the C_O text field, type $tcs.p_{wO2}/p_{ref}$. ($tcs.p_{XXX}$ is the partial pressure variables, defined by the Transport of Concentrated Species interface.)

Add a New Study and Recompute

Add a second study, and recompute.

- 1 From the Windows menu, choose Add Study to open the Add Study window.
- 2 In the Add Study windows, find the Studies subsection. In the Select Study tree, select Preset Studies for Selected Physics Interfaces>Secondary Current Distribution>Stationary with Initialization.
- 3 Click Add Study, and then close the Add Study window.
- 4 In the Model Builder window, right-click Study 2 and choose Compute.

Evaluate the Mass Transport-Dependent Results

Group Some old Default Plots Together

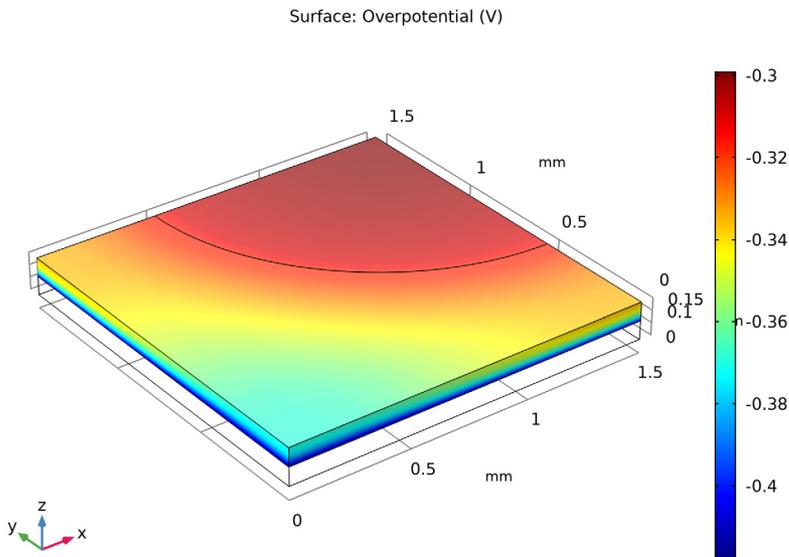
A set of new default plots were created by the second study. Place the default plots pertaining to Study 1 into a Group as follows: (Do not include the plots you created manually in this group)

- 1 Shift-click to select the five plots Electrolyte Potential (cd) to Electrode Potential vs. Adjacent Reference (cd).

- 2 Right-click and choose Group.
- 3 In the Settings window for Group, type **Plots** from **Study 1** in the Label text field.

Change Dataset for the Plots You Created Manually

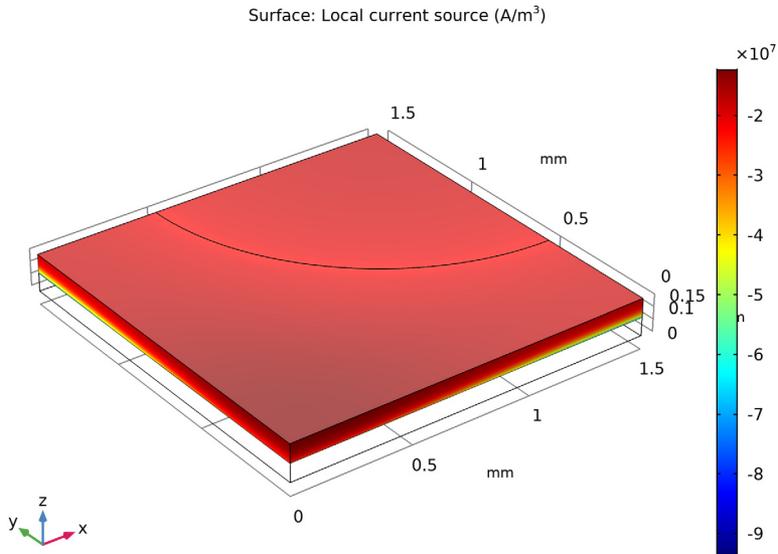
- 1 By changing the Dataset you can make the plots you created before point to the results from Study 2.
- 2 In the Model Builder window, under Results click **Overpotential**.
- 3 In the Settings window for 3D Plot Group, locate the Data section.
- 4 From the Dataset list, choose **Study 2/Solution 3 (sol3)**.
- 5 In the Overpotential toolbar, click **Plot**.



Note how the overpotential, volumetric current density and the current density at the anode boundary plots all change as a result of the mass transfer effects.

- 6 In the Model Builder window, under Results click **Local Volumetric Current Density**.
- 7 In the Settings window for 3D Plot Group, locate the Data section.
- 8 From the Dataset list, choose **Study 2/Solution 3 (sol3)**.

9 In the Local Volumetric Current Density toolbar, click Plot.

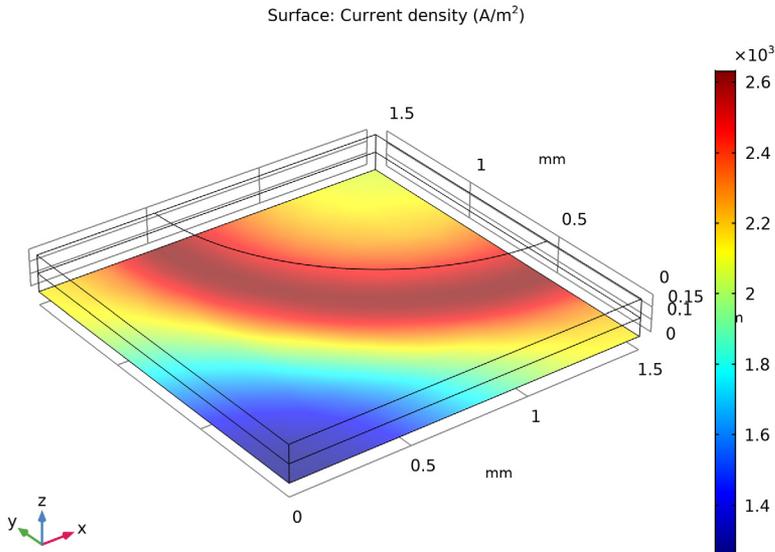


10 In the Model Builder window, under Results click Current Density at Anode Boundary.

11 In the Settings window for 3D Plot Group, locate the Data section.

12 From the Dataset list, choose Study 2/Solution 3 (sol3).

13 In the Current Density at Anode Boundary toolbar, click Plot.



Create a Group for all Study 2 Plots

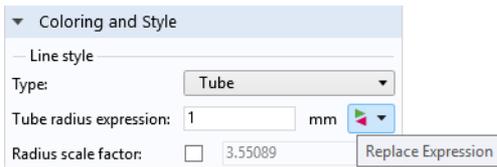
- 1** In the Model Builder window, under Results, collapse the Overpotential, the Local Volumetric Current and Current Density at Anode Boundary nodes.
- 2** In the Model Builder window, under Results, Shift-click to select all non-grouped plot groups (the Overpotential to Pressure (dl) nodes) and right-click to choose Group.
- 3** In the Model Builder window, under Results click Group 2.
- 4** In the Settings window for Group, type **Plots from Study 2** in the Label text field.

Concentration, O₂, Streamline

Also the Transport of Concentrated Species and the Darcy's law interfaces create a number of default plots. Polish the default plot for the oxygen concentration streamlines as follows:

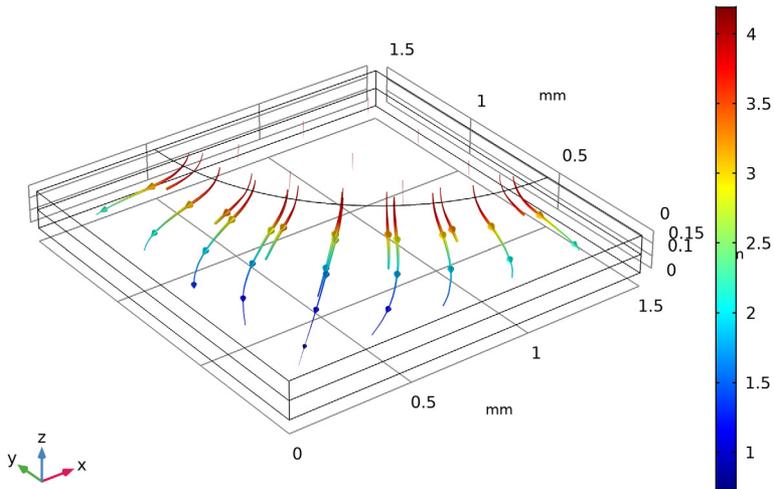
- 1** In the Model Builder window, expand the Concentration, O₂, Streamline (tcs) node, then click Streamline 1.
- 2** In the Settings window for Streamline, locate the Streamline Positioning section.
- 3** From the Positioning list, choose On selected boundaries.

- 4 Locate the Selection section. Select the Active toggle button.
- 5 Select Boundary 6 only.
- 6 Locate the Streamline Positioning section. In the Number text field, type 30.
- 7 Locate the Coloring and Style section. Find the Line style subsection. From the Type list, choose Tube.
- 8 Click Replace Expression in the upper-right corner of the Coloring and Style section and choose Component 1>Transport of Concentrated Species>Species wO2>Fluxes>tcs.tfluxMag_wO2 - Total flux magnitude - $\text{kg}/(\text{m}^2\cdot\text{s})$ from the menu.



- 9 In the Concentration, O2, Streamline (tcs) toolbar, click Plot.

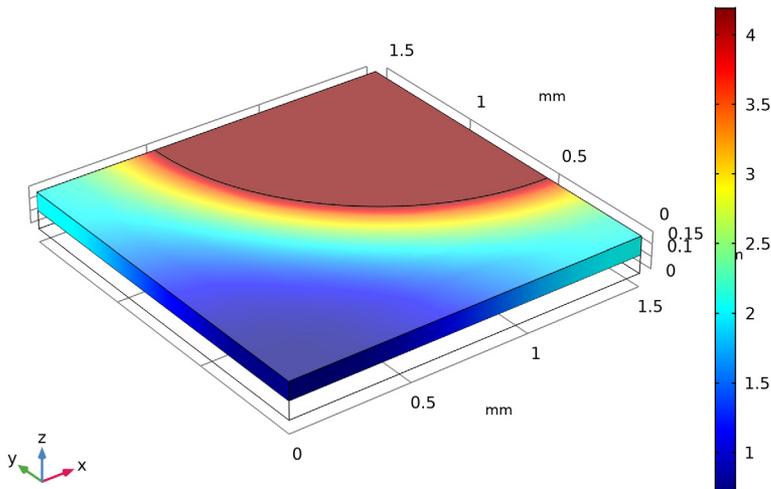
Species O2: Streamline: Total flux Streamline Color: Molar concentration (mol/m^3)



Note the direction of the arrows. Oxygen flows from the inlet hole into the porous cathode to react to form water.

Concentration, O₂, Surface (tcs)

Species O₂: Molar concentration (mol/m³)



The oxygen concentration gets low far away from the inlet hole. Since the electrode kinetics now is concentration dependent, this explains the lower current densities seen in the current density plots.

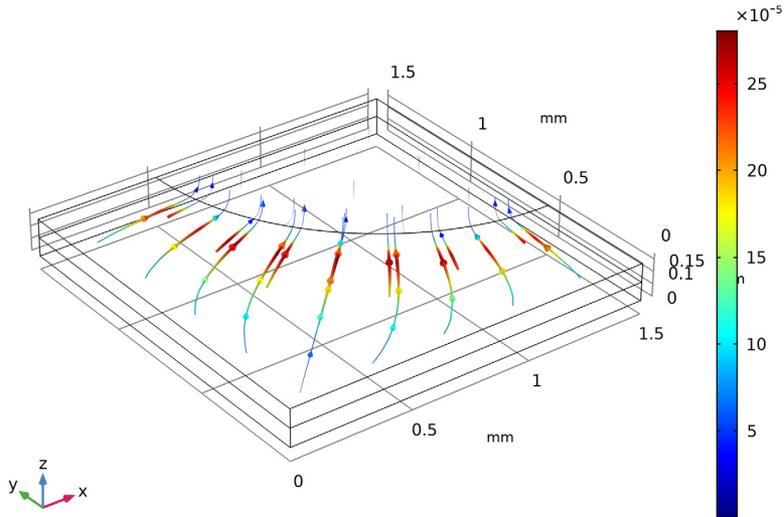
Velocity (dl)

Polish the velocity plot as follows:

- 1 In the Model Builder window, expand the Velocity (dl) node, then click Streamline 1.
- 2 In the Settings window for Streamline, locate the Streamline Positioning section.
- 3 From the Positioning list, choose On selected boundaries.
- 4 Locate the Selection section. Click Clear Selection.
- 5 Select Boundary 6 only.
- 6 Locate the Streamline Positioning section. In the Number text field, type 30.
- 7 Locate the Coloring and Style section. Find the Line style subsection. From the Type list, choose Tube.
- 8 Click Replace Expression in the upper-right corner of the Coloring and Style section and choose Component 1>Darcy's Law>Velocity and pressure>dl.U - Darcy's velocity magnitude - m/s from the menu.

9 In the Velocity (dl) toolbar, click Plot.

Streamline: Darcy's velocity field



The direction of the net velocity is toward the inlet hole, that is, opposite to the oxygen flux. This is a result of the net flux of mass (protons) from the anode to the cathode.