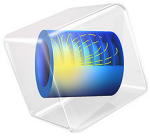


Solid Oxide Electrolyzer Using Thermodynamics

Introduction

This example models a solid oxide electrolyzer cell wherein water vapor is reduced to form hydrogen gas on the cathode, and oxygen gas is evolved on the anode. The current distribution in the cell is coupled to the cathode mass transfer of hydrogen and water and momentum transport.

Model Definition

On the anode, oxygen ions are oxidized to form oxygen gas,

$$2O^{2-} \leftrightarrow O_2(g) + 4e^- \tag{1}$$

whereas on the cathode, water vapor is reduced to form hydrogen gas and oxygen ions:

$$2H_2O(g) + 4e^- \leftrightarrow 2H_2(g) + 2O^{2-} \tag{2}$$

Figure 1 shows the model geometry. Since the oxygen is the only gas present in the anode gas chamber, and isobaric conditions are assumed, there is no need to explicitly model the anode gas transport. Four computational domains are hence used in the model: the

cathode gas channels, the cathode gas diffusion electrode, the solid oxide electrolyte layer, and the anode gas diffusion electrode.

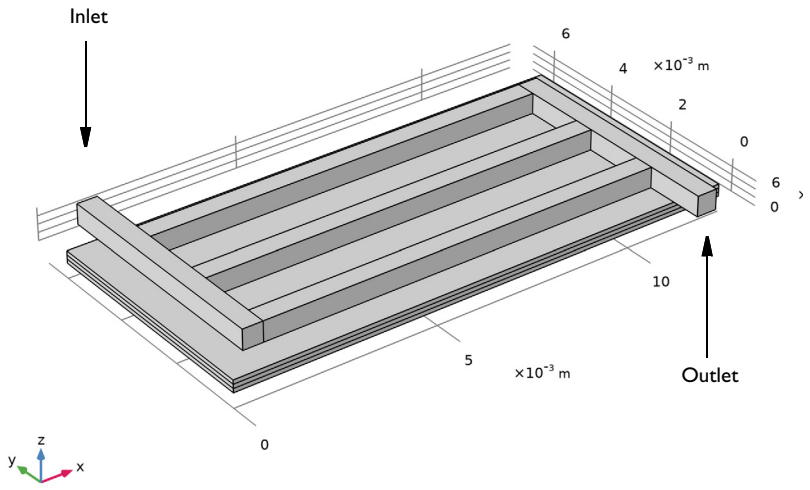


Figure 1: Model geometry. From top: Cathode gas channels, cathode gas diffusion electrode, solid oxide electrolyte layer, and anode gas diffusion layer. The positions of the inlet and outlet are indicated in the figure.

The composition of the hydrogen-water vapor mixture will change as a result of the electrochemical reactions. The mass transport of hydrogen and water vapor is modeled in the cathode gas channels and the gas diffusion electrode, coupled to the resulting (laminar) flow of the gas mixture. The mass transport of hydrogen and water is modeled using the Transport of Concentrated Species interface, using Maxwell-Stefan diffusion. The momentum flow is defined in the model using the Brinkman Equations interface for the porous gas diffusion electrodes. The Navier-Stokes equations are used for the nonporous gas channels.

The current distribution is defined assuming a constant conductivity of the solid electrolyte. The Secondary Current Distribution interface is used to define the electrode reactions and the electrolyte charge transport in the porous gas diffusion electrodes and the electrolyte layer.

On the cathode side, the electrode kinetics depends on the local concentration of water and hydrogen according to the law of mass action (and Nernst equation). On the anode

side, and a uniform partial pressure of oxygen is assumed and a concentration-independent Butler-Volmer expression is hence used to define the electrode kinetics.

The Thermodynamics and Chemistry nodes are used to automatically define the properties of the cathode gas mixture, as well as the equilibrium potentials of the electrode reactions.

Results and Discussion

Figure 2 shows the velocity magnitude distribution in the cell. The highest velocities are located close to the inlet and outlet.

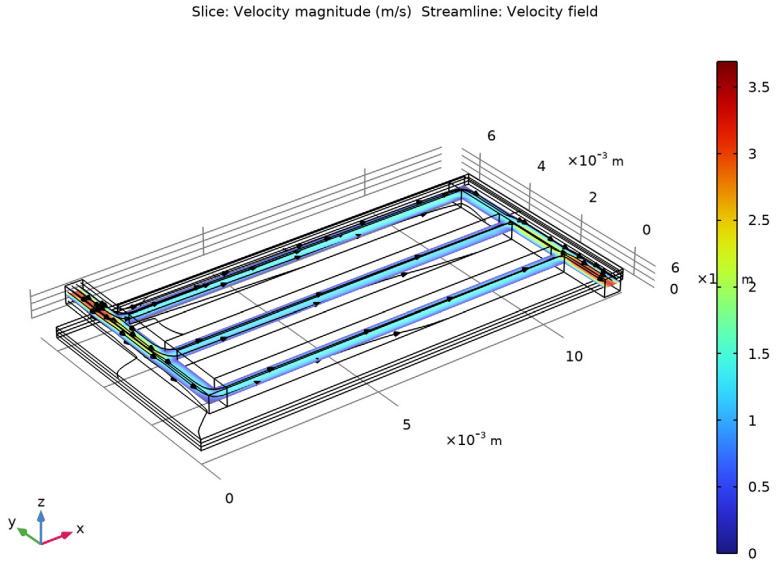


Figure 2: Velocity in the cell.

Figure 3 shows how the density and the dynamic viscosity of the gas relate to the hydrogen and water molar fractions shown in Figure 4. As the hydrogen content of the gas increases toward the outlet, the density and the viscosity both decrease.

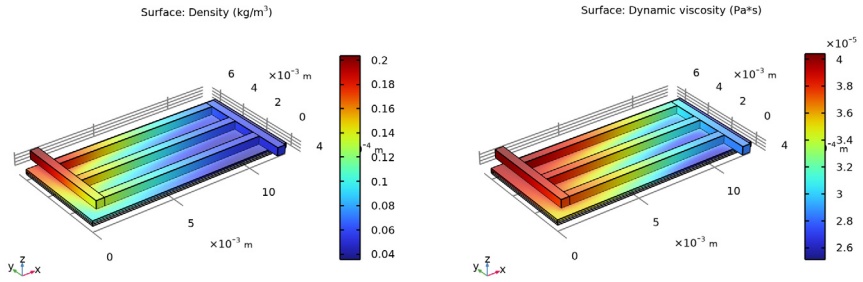


Figure 3: Density (left) and dynamic viscosity (right).

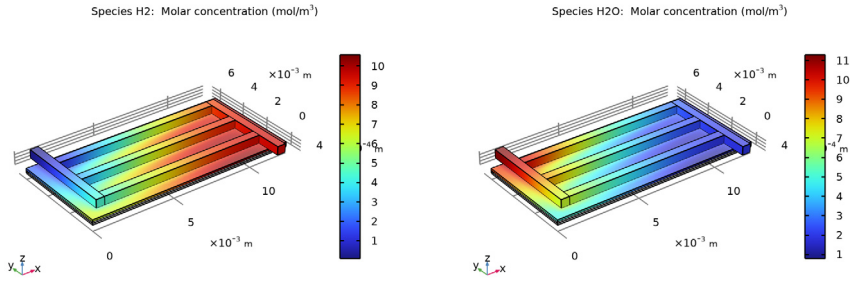


Figure 4: Hydrogen (left) and water vapor (right) concentrations.

Figure 5 shows the molar fraction of hydrogen in the gas mixture, and the corresponding hydrogen flux streamlines. The molar fraction is close to zero at the inlet and almost 100% at the outlet.

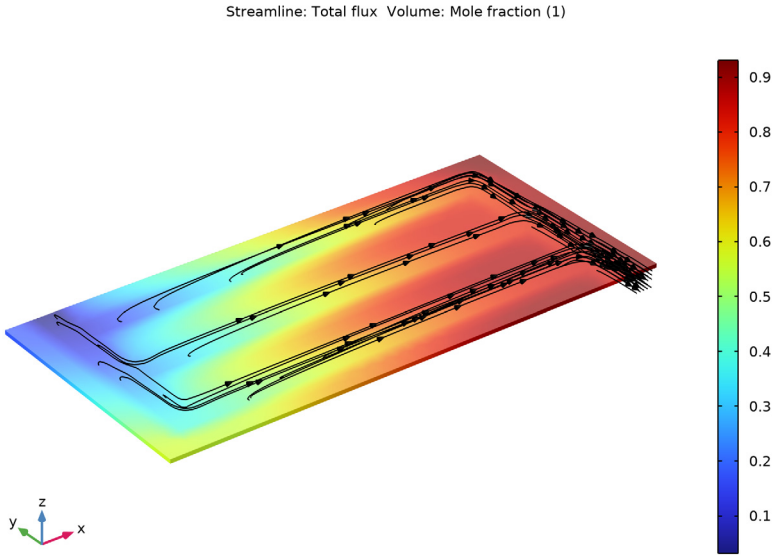


Figure 5: Hydrogen molar fraction (slice) and flux (streamlines).

Finally, Figure 6 shows the cross-sectional electrolyte current density in the middle of the electrolyte between the anode and the cathode. The current density is highest close to the inlet, where the water/hydrogen ratio is high, and decreases toward the outlet.

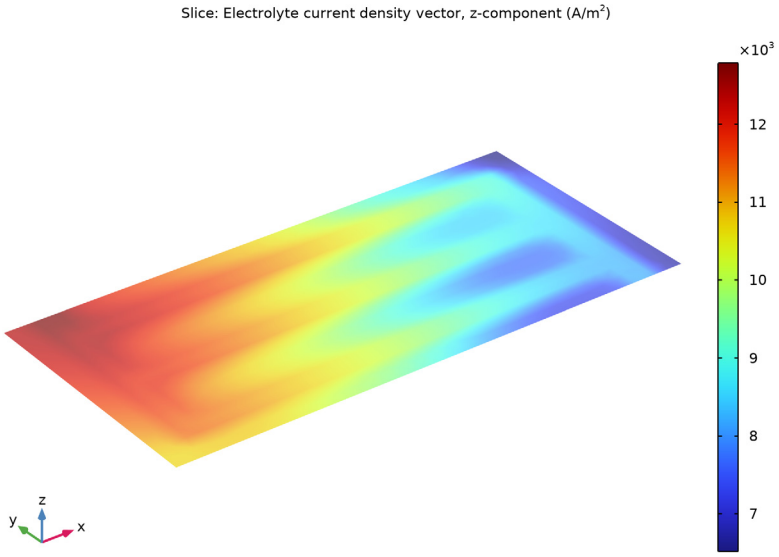


Figure 6: Electrolyte current density through electrolyte layer.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Electrolyzers/soec_thermodynamics`

Modeling Instructions

This tutorial models the current distribution in a solid oxide electrolyzer. The tutorial comprises two major parts. First, the thermodynamics and the electrode reactions are defined to provide the equilibrium potentials of the anode and the cathode, and a secondary (not concentration dependent) current distribution is modeled. In the second part, mass and momentum transport are added to model a concentration-dependent current distribution of the cell, where the mixture properties of the anode gas depends on the molar fractions of water and hydrogen.

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 In the **Select Physics** tree, select **Electrochemistry> Primary and Secondary Current Distribution>Secondary Current Distribution (cd)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Stationary with Initialization**.

6 Click **Done**.

GEOMETRY 1

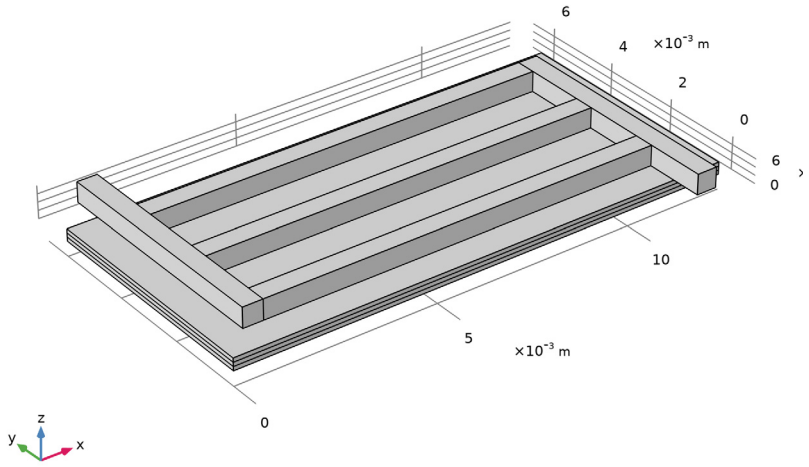
The model geometry is available as a parameterized geometry sequence in a separate MPH-file. If you want to build it from scratch, follow the instructions in the section Appendix —Geometry Modeling Instructions. Otherwise load it from file using the following steps.

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

2 Browse to the model's Application Libraries folder and double-click the file `soec_thermodynamics_geom_sequence.mph`.

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

4 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.



GLOBAL DEFINITIONS

Geometry Parameters

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, type `Geometry Parameters` in the **Label** text field.

Physics Parameters

Some parameters were imported with the geometry sequence. Import some additional physics parameters from a text file.

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

2 In the **Settings** window for **Parameters**, type `Physics Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

Add a thermodynamic system for the hydrogen/water gas mixture.

5 In the **Physics** toolbar, click **Thermodynamics** and choose **Thermodynamic System**.

SELECT SYSTEM

1 Go to the **Select System** window.

2 Click **Next** in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 In the **Species** list, select **water (7732-18-5, H2O)**.

3 Click **Add Selected**.

4 In the **Species** list, select **hydrogen (1333-74-0, H2)**.

5 Click **Add Selected**.

6 Click **Next** in the window toolbar.

SELECT THERMODYNAMIC MODEL

1 Go to the **Select Thermodynamic Model** window.

2 Click **Finish** in the window toolbar.

GLOBAL DEFINITIONS

Gas System - H2 and H2O

1 In the **Model Builder** window, under **Global Definitions>Thermodynamics** click **Gas System 1 (pp1)**.

2 In the **Settings** window for **Thermodynamic System**, type `Gas System - H2 and H2O` in the **Label** text field.

3 Right-click **Global Definitions>Thermodynamics>Gas System - H2 and H2O** and choose **Generate Chemistry**.

SELECT SPECIES

1 Go to the **Select Species** window.

2 In the list, choose **hydrogen** and **water**.

3 Click **Add Selected**.

4 Click **Next** in the window toolbar.

CHEMISTRY SETTINGS

1 Go to the **Chemistry Settings** window.

2 From the **Mass transfer** list, choose **Concentrated species**.

3 Click **Finish** in the window toolbar.

CHEMISTRY - H2 AND H2O

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Chemistry (chem)**.

2 In the **Settings** window for **Chemistry**, type `Chemistry - H2 and H2O` in the **Label** text field.

3 Locate the **Model Input** section. Select the **Enable electrode reactions** check box.

4 From the E list, choose **Electrode potential (cd)**.

5 Click to expand the **Calculate Transport Properties** section.

Electrode Reaction 1

Add the electrode reaction for the cathode. Use the `(ads)` annotation in the reaction formula to define that the oxygen ions do not belong the main (gas) phase.

1 In the **Physics** toolbar, click **Domains** and choose **Electrode Reaction**.

2 In the **Model Builder** window, expand the **Component 1 (comp1)>Chemistry - H2 and H2O (chem)** node, then click **Electrode Reaction 1**.

3 In the **Settings** window for **Electrode Reaction**, locate the **Reaction Formula** section.

4 In the **Formula (written as reduction)** text field, type `H2O+2e<=>H2+O(ads)`.

5 Click **Apply**.

6 Locate the **Equilibrium Potential** section. From the list, choose **Automatic**.

7 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_H2`.

8 In the α_a text field, type `1.5`.

For the first computation we will assume constant mass fractions (concentrations) for the species.

9 In the **Model Builder** window, under **Component 1 (comp1)** click **Chemistry - H2 and H2O (chem)**.

10 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.

11 Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Mass fraction	Value (1)	From Thermodynamics
H2	Variable	User defined	0.5	H2
H2O	Variable	User defined	0.5	H2O

12 Find the **Surface species** subsection. In the table, enter the following settings:

Species	Species concentration type	Surface concentration (mol/m^2)
O(ads)	Free species	`1e-5[mol/m^2]`

GLOBAL DEFINITIONS

Now add a second thermodynamics system for the anode oxygen gas.

In the **Physics** toolbar, click **Thermodynamics** and choose **Thermodynamic System**.

SELECT SYSTEM

1. Go to the **Select System** window.
2. Click **Next** in the window toolbar.

SELECT SPECIES

1. Go to the **Select Species** window.
2. In the **Species** list, select **oxygen (7782-44-7, O2)**.
3. Click **Add Selected**.
4. Click **Next** in the window toolbar.

SELECT THERMODYNAMIC MODEL

1. Go to the **Select Thermodynamic Model** window.
2. Click **Finish** in the window toolbar.

GLOBAL DEFINITIONS

Gas System - O2

1. In the **Model Builder** window, under **Global Definitions>Thermodynamics** click **Gas System 1 (pp2)**.
2. In the **Settings** window for **Thermodynamic System**, type `Gas System - O2` in the **Label** text field.
3. Right-click **Global Definitions>Thermodynamics>Gas System - O2** and choose **Generate Chemistry**.

SELECT SPECIES

1. Go to the **Select Species** window.
2. In the list, select **oxygen**.
3. Click **Add Selected**.

4 Click **Next** in the window toolbar.

CHEMISTRY SETTINGS

1 Go to the **Chemistry Settings** window.

2 Click **Finish** in the window toolbar.

CHEMISTRY - O2

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Chemistry 2 (chem2)**.

2 In the **Settings** window for **Chemistry**, type `Chemistry - O2` in the **Label** text field.

3 Locate the **Model Input** section. Select the **Enable electrode reactions** check box.

4 From the E list, choose **Electrode potential (cd)**.

Electrode Reaction 1

1 In the **Physics** toolbar, click **Domains** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Reaction Formula** section.

3 In the **Formula (written as reduction)** text field, type `O2+4e<=>2O(ads)`.

4 Click **Apply**.

5 Locate the **Equilibrium Potential** section. From the list, choose **Automatic**.

6 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_O2`.

7 In the **Model Builder** window, under **Component 1 (comp1)** click **Chemistry - O2 (chem2)**.

8 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.

9 Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Mass fraction	Value (1)	From Thermodynamics
O2	Variable	User defined	1	O2

10 Find the **Surface species** subsection. In the table, enter the following settings:

Species	Species concentration type	Surface concentration (mol/m^2)
O(ads)	Free species	`1e-5[mol/m^2]`

SECONDARY CURRENT DISTRIBUTION (CD)

Now define the current distribution in the gas diffusion electrodes and the electrolyte.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Secondary Current Distribution (cd)**.

2 In the **Settings** window for **Secondary Current Distribution**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domains 1–3 only.

Electrolyte 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Secondary Current Distribution (cd)** click **Electrolyte 1**.

2 In the **Settings** window for **Electrolyte**, locate the **Electrolyte** section.

3 From the σ_l list, choose **User defined**. In the associated text field, type `sigma_l`.

Porous Electrode - H2 and H2O (Cathode)

1 In the **Physics** toolbar, click **Domains** and choose **Porous Electrode**.

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode - H2 and H2O (Cathode)` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Cathode**.

4 Locate the **Electrolyte Current Conduction** section. From the σ_l list, choose **User defined**. In the associated text field, type `sigma_l`.

5 In the ε_l text field, type `por_l`.

6 Locate the **Electrode Current Conduction** section. From the σ_s list, choose **User defined**. In the associated text field, type `sigma_s`.

7 In the ε_s text field, type `1-por_l`.

Porous Electrode Reaction 1

Couple the electrode reaction current density to the chemistry interface for the cathode as follows.

1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.

3 In the E_{eq} text field, type `chem.Eeq_er1`.

4 Locate the **Electrode Kinetics** section. From the $i_{loc,expr}$ list, choose **User defined**. In the associated text field, type `chem.iloc_er1`.

5 Locate the **Active Specific Surface Area** section. In the a_v text field, type `S`.

Porous Electrode - H2 and H2O (Cathode)

In the **Model Builder** window, right-click **Porous Electrode - H2 and H2O (Cathode)** and choose **Duplicate**.

Porous Electrode - O2 (Anode)

1. In the **Model Builder** window, under **Component 1 (comp1)>** **Secondary Current Distribution (cd)** click **Porous Electrode - H2 and H2O (Cathode) 1**.
2. In the **Settings** window for **Porous Electrode**, type `Porous Electrode - O2 (Anode)` in the **Label** text field.
3. Locate the **Domain Selection** section. From the **Selection** list, choose **Anode**.

Porous Electrode Reaction 1

1. In the **Model Builder** window, expand the **Porous Electrode - O2 (Anode)** node, then click **Porous Electrode Reaction 1**.
2. In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.
3. In the E_{eq} text field, type `chem2.Eeq_er1`.
4. Locate the **Electrode Kinetics** section. In the $i_{\mathrm{loc,expr}}$ text field, type `chem2.iloc_er1`.

Electric Ground 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Electric Ground**.
2. In the **Settings** window for **Electric Ground**, locate the **Boundary Selection** section.
3. From the **Selection** list, choose **Cathode Current Collector**.
4. Locate the **Contact Resistance** section. Select the **Include contact resistance** check box.
5. In the R_{c} text field, type `Rc`.

Electrode Current 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current**.
2. In the **Settings** window for **Electrode Current**, locate the **Boundary Selection** section.
3. From the **Selection** list, choose **Anode Current Collector**.
4. Locate the **Electrode Current** section. From the list, choose **Average current density**.
5. In the $i_{\mathrm{s,average}}$ text field, type `I_avg`.
6. Locate the **Contact Resistance** section. Select the **Include contact resistance** check box.
7. In the R_{c} text field, type `Rc`.

GLOBAL DEFINITIONS

Default Model Inputs

1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General>Temperature (K) - minput.T**.

4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T`.

MESH 1

The physics settings for the first part of the tutorial are now complete. Add a user-defined mesh.

Size 1

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

2 In the **Settings** window for **Size**, click to expand the **Element Size Parameters** section.

3 Locate the **Element Size** section. Click the **Custom** button.

4 Locate the **Element Size Parameters** section.

5 Select the **Maximum element size** check box. In the associated text field, type `H_ch*0.8`.

Swept 1

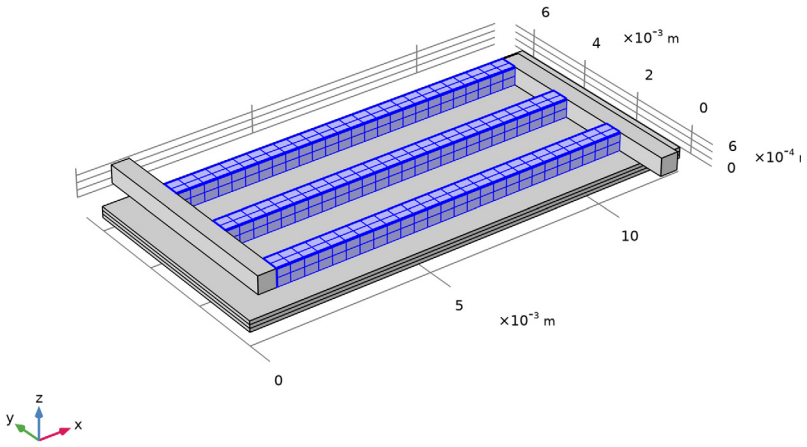
1 In the **Mesh** toolbar, click  **Swept**.

2 In the **Settings** window for **Swept**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domains 5–7 only.

5 Click **Build Selected**.



6 Click **Build Selected**.

Free Tetrahedral 1

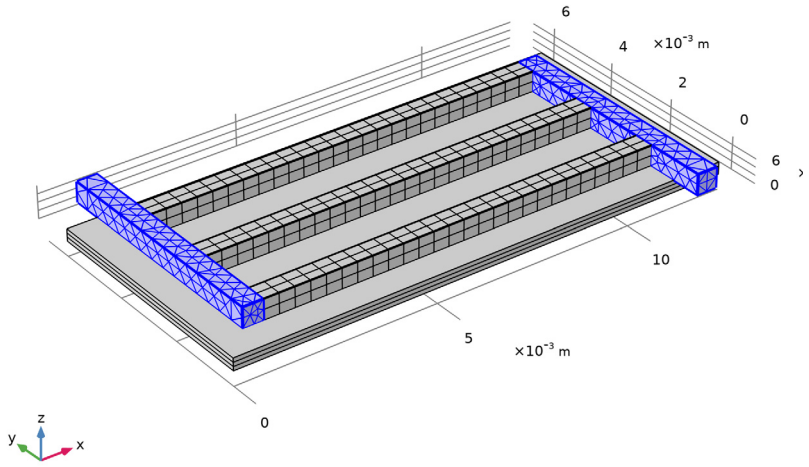
1 In the **Mesh** toolbar, click **Free Tetrahedral**.

2 In the **Settings** window for **Free Tetrahedral**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domains 4 and 8 only.

5 Click **Build Selected**.



Boundary Layers 1

Also add a boundary layer mesh at this stage. These are actually not needed for the first calculation, but will improve the accuracy and convergence of the solution for the second part of the tutorial when mass transport and convection has been added.

1 In the **Mesh** toolbar, click **Boundary Layers**.

2 In the **Settings** window for **Boundary Layers**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Channel Domains**.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Boundary Layer Boundaries**.

4 Locate the **Layers** section. In the **Number of layers** text field, type `2`.

5 In the **Stretching factor** text field, type `1.3`.

6 From the **Thickness specification** list, choose **First layer**.

7 In the **Thickness** text field, type `H_ch/10`.

8 Click **Build Selected**.

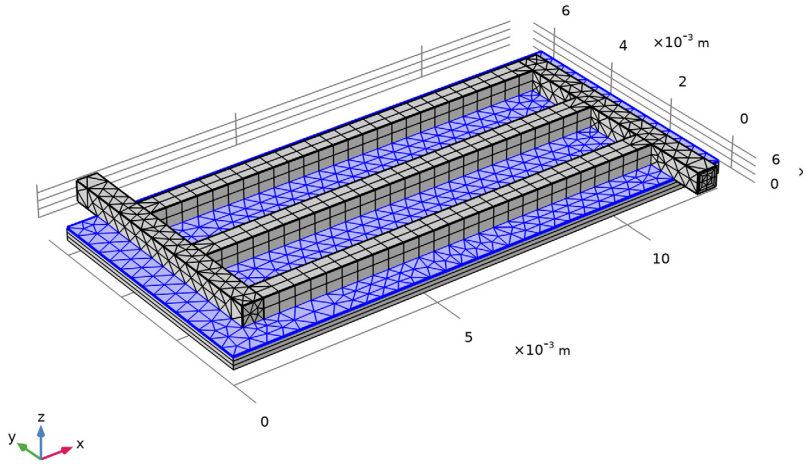
Free Triangular 1

1 In the **Mesh** toolbar, click **More Generators** and choose **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Cathode Current Collector**.

4 Click **Build Selected**.



Swept 2

In the **Mesh** toolbar, click **Swept**.

Distribution 1

1 Right-click **Swept 2** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domain 3 only.

5 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.

6 In the **Element ratio** text field, type `2`.

7 Select the **Reverse direction** check box.

Distribution 2

1 In the **Model Builder** window, right-click **Swept 2** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domain 2 only.

5 Locate the **Distribution** section. In the **Number of elements** text field, type 2.

Distribution 1

In the **Model Builder** window, right-click **Distribution 1** and choose **Duplicate**.

Distribution 3

1 In the **Model Builder** window, click **Distribution 3**.

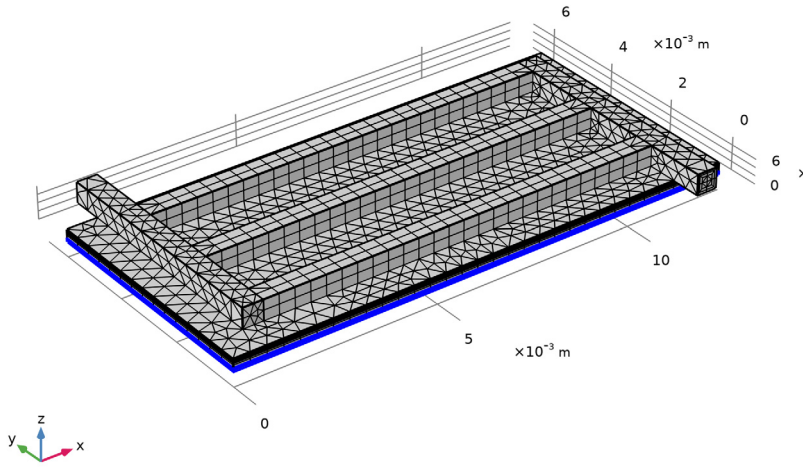
2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domain 1 only.

5 Locate the **Distribution** section. Clear the **Reverse direction** check box.

6 Click **Build All**.



STUDY 1

The problem is now ready for solving.

1 In the **Home** toolbar, click **Compute**.

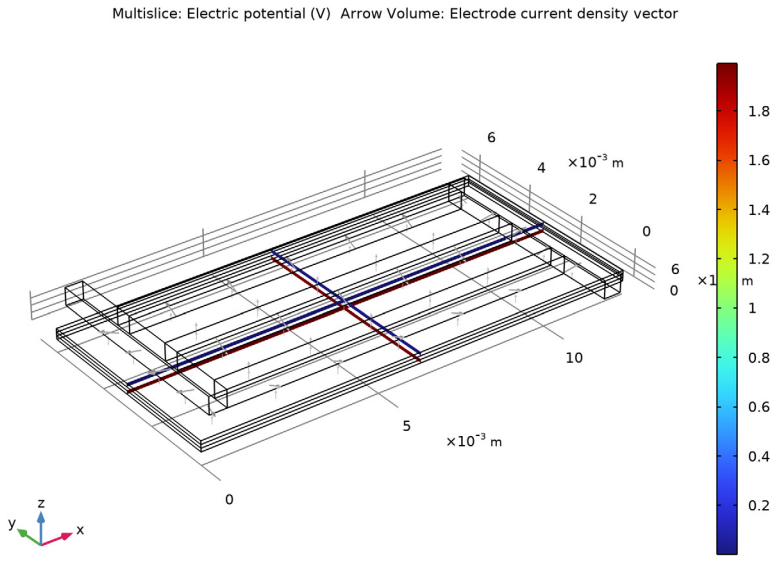
RESULTS

Electrode Potential with Respect to Ground (cd)

1 In the **Model Builder** window, under **Results** click **Electrode Potential with Respect to Ground (cd)**.

2 In the **Electrode Potential with Respect to Ground (cd)** toolbar, click **Plot**.

Inspect the potential plot. The plot should look as follows:



COMPONENT 1 (COMP1)

Now start with the second part of the tutorial which adds a reacting flow interface to the cathode side of the model, and couples the distribution of hydrogen and water vapor to the electrochemistry.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Chemical Species Transport>Reacting Flow in Porous Media> Transport of Concentrated Species**.

4 Click **Add to Component 1** in the window toolbar.

5 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

MULTIPHYSICS

Reacting Flow 1 (nirf1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Reacting Flow 1 (nirf1)**.

2 In the **Settings** window for **Reacting Flow**, locate the **Temperature** section.

3 In the T text field, type `T`.

MATERIALS

Note that a **Porous Material** node has been created automatically when adding an entry from the **Reacting Flow in Porous Media** branch of the **Add Physics** window.

Porous Material 1 (pmat1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials** node, then click **Porous Material 1 (pmat1)**.

2 In the **Settings** window for **Porous Material**, locate the **Geometric Entity Selection** section.

3 From the **Selection** list, choose **Cathode**.

4 Locate the **Porosity** section. In the ε_p text field, type `por`.

5 Locate the **Homogenized Properties** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Permeability	kappa_iso ; kappaii = kappa_iso, kappaij = 0	kappa	m²	Basic

BRINKMAN EQUATIONS (BR)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Brinkman Equations (br)**.

2 Select Domains 3–8 only.

3 In the **Settings** window for **Brinkman Equations**, locate the **Domain Selection** section.

4 Click **Create Selection**.

5 In the **Create Selection** dialog box, type `Gas domains` in the **Selection name** text field.

6 Click **OK**.

7 In the **Settings** window for **Brinkman Equations**, locate the **Physical Model** section.

8 Clear the **Neglect inertial term (Stokes flow)** check box.

Fluid Properties 1

1 In the **Physics** toolbar, click **Domains** and choose **Fluid Properties**.

2 In the **Settings** window for **Fluid Properties**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Channel Domains**.

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 In the **Settings** window for **Inlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Boundary Condition** section. From the list, choose **Mass flow**.

5 Locate the **Mass Flow** section. In the m text field, type `Mflux_in`.

Outlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outlet**.

2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** check box.

TRANSPORT OF CONCENTRATED SPECIES IN POROUS MEDIA (TCS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Concentrated Species in Porous Media (tcs)**.

2 In the **Settings** window for **Transport of Concentrated Species in Porous Media**, locate the **Domain Selection** section.

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

4 Locate the **Transport Mechanisms** section. From the **Diffusion model** list, choose **Maxwell-Stefan**.

5 Click to expand the **Dependent Variables** section. In the **Mass fractions (1)** table, enter the following settings:

wH2
wH2O

Species Molar Masses 1

1 In the **Model Builder** window, under **Component 1 (comp1)>** **Transport of Concentrated Species in Porous Media (tcs)** click **Species Molar Masses 1**.

2 In the **Settings** window for **Species Molar Masses**, locate the **Molar Mass** section.

3 From the M_{wH2} list, choose **Molar mass (chem/H2)**.

4 From the M_{wH2O} list, choose **Molar mass (chem/H2O)**.

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>** **Transport of Concentrated Species in Porous Media (tcs)>Porous Medium 1** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.

3 In the table, enter the following settings:

Species 1	Species 2	Diffusivity	Diffusion coefficient (m^2/s)
wH2	wH2O	Maxwell-Stefan diffusivity , H2-H2O (chem)	comp1.chem.D_H2_H2O

4 From the **Effective diffusivity model** list, choose **Bruggeman model**.

5 Locate the **Pore-Wall Interaction** section. Select the **Include pore-wall interaction** check box.

6 In the d_{pore} text field, type `d_pore`.

Porous Electrode Coupling 1

1 In the **Physics** toolbar, click **Domains** and choose **Porous Electrode Coupling**.

2 In the **Settings** window for **Porous Electrode Coupling**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Cathode**.

Reaction Coefficients 1

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

2 In the **Settings** window for **Reaction Coefficients**, locate the **Model Inputs** section.

3 From the i_v list, choose **Local current source, Porous Electrode Reaction 1 (cd/pce1/per1)**.

4 Locate the **Stoichiometric Coefficients** section. In the n text field, type `2`.

5 In the ν_{wH2} text field, type `1`.

6 In the ν_{wH2O} text field, type `-1`.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Inflow** section. From the **Mixture specification** list, choose **Mass flow rates**.

5 In the $J_{\text{in,wH2O}}$ text field, type `Mflux_in`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

Transport Properties 1

1 In the **Physics** toolbar, click **Domains** and choose **Transport Properties**.

2 In the **Settings** window for **Transport Properties**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Channel Domains**.

4 Locate the **Diffusion** section. In the table, enter the following settings:

Species 1	Species 2	Diffusivity	Diffusion coefficient (m^2/s)
wH2	wH2O	Maxwell-Stefan diffusivity , H2-H2O (chem)	comp1.chem.D_H2_H2O

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 From the **Mixture specification** list, choose **Mole fractions**.

4 In the $x_{0,\text{wH2O}}$ text field, type `0.95*(1-x/(W_cell*stoich))`.

CHEMISTRY - H2 AND H2O (CHEM)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Chemistry - H2 and H2O (chem)**.

2 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.

3 From the **Species solved for** list, choose **Transport of Concentrated Species in Porous Media**.

4 Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Mass fraction	Value (1)	From Thermodynamics
H2	Variable	wH2	Solved for	H2
H2O	Variable	wH2O	Solved for	H2O

STUDY 1

The concentration-dependent model is now ready for solving. Use a sequence of study steps, solving for the secondary current distribution first, then the flow, and finally the fully coupled problem. By solving for only one set of physics at a time in individual steps, suitable initial values automatically propagate to the final study step where the complete problem is solved.

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, under **Study 1** click **Step 1: Current Distribution Initialization**.

2 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Brinkman Equations (br)** and **Transport of Concentrated Species in Porous Media (tcs)**.

4 In the table, clear the **Solve for** check box for **Reacting Flow 1 (nirf1)**.

Step 2: Stationary

1 In the **Model Builder** window, click **Step 2: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics interface	Solve for	Equation form
Secondary Current Distribution (cd)	√	Automatic (Stationary)
Brinkman Equations (br)		Automatic (Stationary)
Transport of Concentrated Species in Porous Media (tcs)		Automatic (Stationary)

4 In the table, clear the **Solve for** check box for **Reacting Flow 1 (nirf1)**.

Step 3: Stationary 2

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Secondary Current Distribution (cd)** and **Transport of Concentrated Species in Porous Media (tcs)**.

4 In the table, clear the **Solve for** check box for **Reacting Flow 1 (nirf1)**.

Step 4: Stationary 3

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

Remove the old study sequence and generate a new one.

Solver Configurations

In the **Model Builder** window, under **Study 1** right-click **Solver Configurations** and choose **Delete Configurations**.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, expand the **Study 1>Solver Configurations> Solution 1 (sol1)>Stationary Solver 4** node.

4 Right-click **Stationary Solver 4** and choose **Fully Coupled**.

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

The problem should solve in about two minutes.

RESULTS

Start the postprocessing of the solution by inspecting and polishing the default plot for the velocity field.

Slice

1 In the **Model Builder** window, expand the **Results>Velocity (br)** node, then click **Slice**.

2 In the **Settings** window for **Slice**, locate the **Plane Data** section.

3 From the **Plane** list, choose **xy-planes**.

4 From the **Entry method** list, choose **Coordinates**.

5 In the **z-coordinates** text field, type `H_cell-H_ch/2`.

6 In the **Velocity (br)** toolbar, click **Plot**.

Streamline 1

1 In the **Model Builder** window, right-click **Velocity (br)** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Brinkman Equations>Velocity and pressure>u,v,w - Velocity field**.

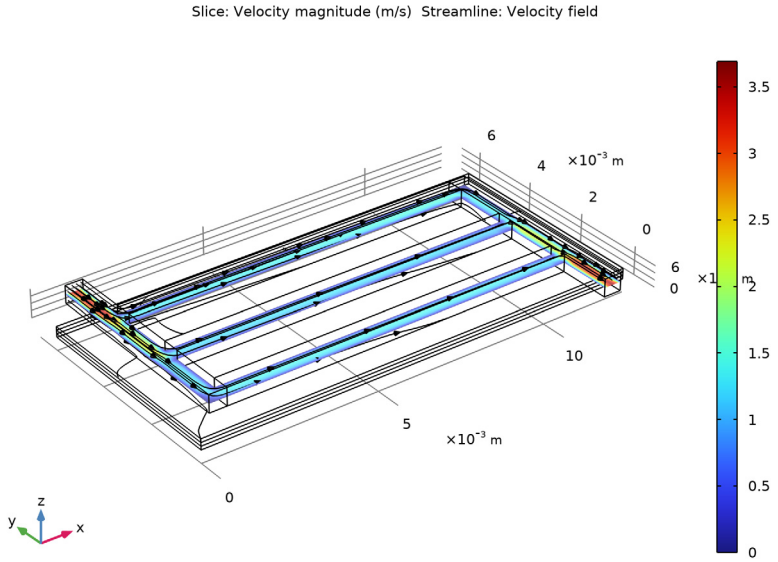
3 Locate the **Selection** section. From the **Selection** list, choose **Inlet**.

4 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

5 From the **Arrow distribution** list, choose **Equal inverse time**.

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

7 In the **Velocity (br)** toolbar, click **Plot**.



Density

The density of the gas mixture will change as water is replaced by hydrogen in the gas stream. Plot the density as follows:

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

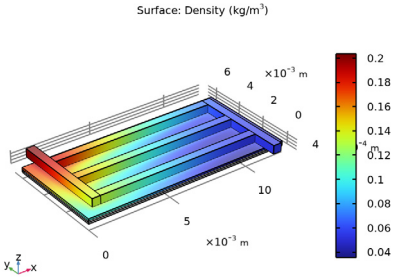
2 In the **Settings** window for **3D Plot Group**, type `Density` in the **Label** text field.

Surface 1

1 Right-click **Density** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Brinkman Equations>Material properties>br.rho - Density - kg/m³**.

3 In the **Density** toolbar, click **Plot**.



Viscosity

Also, the viscosity will change in the gas stream.

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

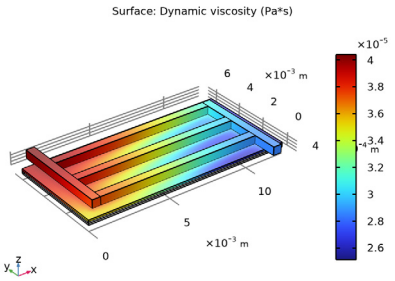
2 In the **Settings** window for **3D Plot Group**, type `Viscosity` in the **Label** text field.

Surface 1

1 Right-click **Viscosity** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Brinkman Equations>Material properties>br.mu - Dynamic viscosity - Pa·s**.

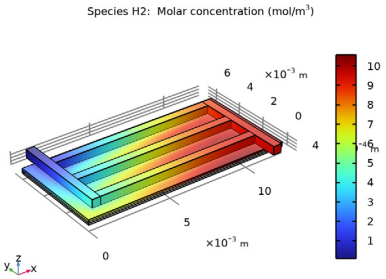
3 In the **Viscosity** toolbar, click **Plot**.



Concentration, H2, Surface (tcs)

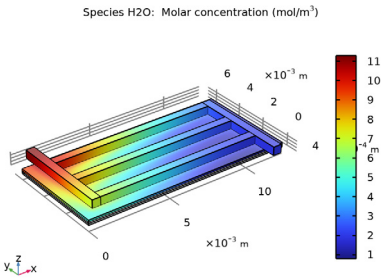
Default plots where created for the hydrogen and water concentrations.

1 In the **Model Builder** window, under **Results** click **Concentration, H2, Surface (tcs)**.



Concentration, H2O, Surface (tcs)

In the **Model Builder** window, click **Concentration, H2O, Surface (tcs)**.



Molar Fraction and Flux, H2

Create a plot for the hydrogen molar fraction and flux 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 `Molar Fraction and Flux, H2` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Streamline 1

1 Right-click **Molar Fraction and Flux, H2** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Concentrated Species in Porous Media>Species wH2>Fluxes>tcs.tflux_wH2x, ...,tcs.tflux_wH2z - Total flux**.

3 Locate the **Streamline Positioning** section. In the **Number** text field, type `30`.

4 Locate the **Selection** section. From the **Selection** list, choose **Outlet**.

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

6 From the **Arrow distribution** list, choose **Equal inverse time**.

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

Selection 1

1 Right-click **Streamline 1** and choose **Selection**.

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

3 From the **Selection** list, choose **Channel Domains**.

Volume 1

1 In the **Model Builder** window, right-click **Molar Fraction and Flux, H2** and choose **Volume**.

2 In the **Settings** window for **Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Concentrated Species in Porous Media>Species wH2>tcs.x_wH2 - Mole fraction - 1**.

Selection 1

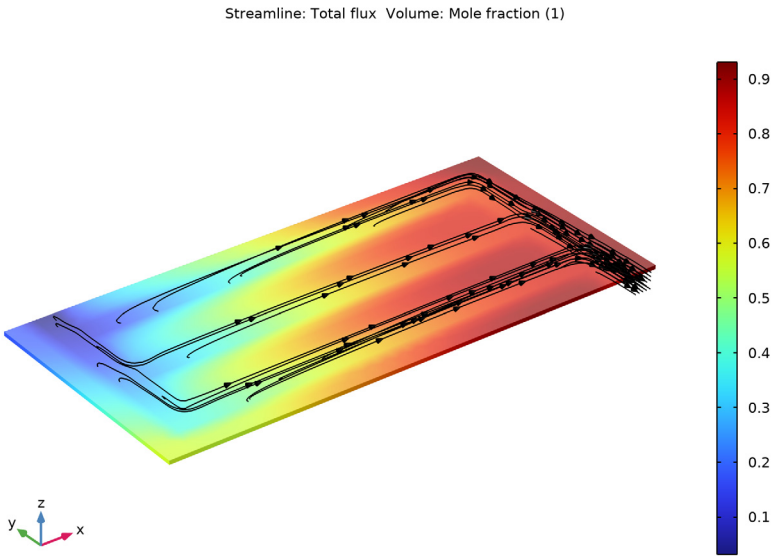
1 Right-click **Volume 1** and choose **Selection**.

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

3 From the **Selection** list, choose **Cathode**.

4 Click the **Show Grid** button in the **Graphics** toolbar.

5 In the **Molar Fraction and Flux, H2** toolbar, click **Plot**.



Cross-Sectional Electrolyte Current Density

Finally, plot the current distribution across the electrolyte layer 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 `Cross-Sectional Electrolyte Current Density` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Slice 1

1 Right-click **Cross-Sectional Electrolyte Current Density** and choose **Slice**.

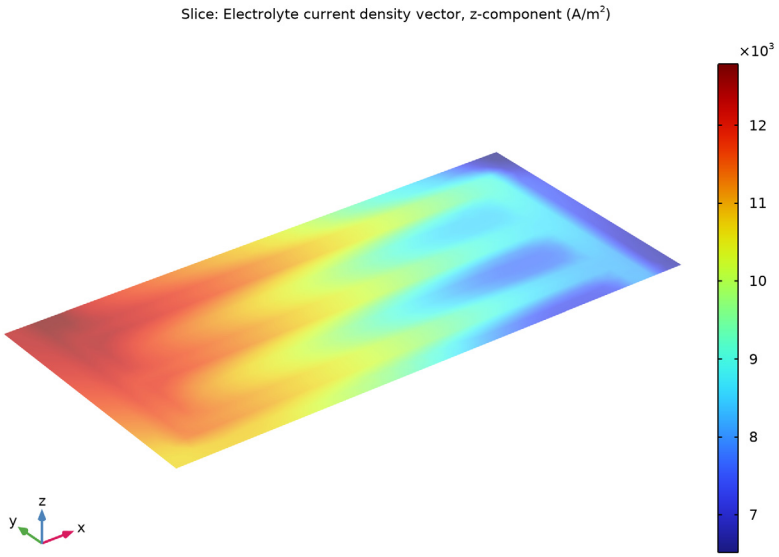
2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Secondary Current Distribution>Electrolyte current density vector - A/m²>cd.llz - Electrolyte current density vector, z-component**.

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

4 From the **Entry method** list, choose **Coordinates**.

5 In the **z-coordinates** text field, type `H_gde+H_el/2`.

6 In the **Cross-Sectional Electrolyte Current Density** toolbar, click **Plot**.



Appendix —Geometry Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 Click **Done**.

GLOBAL DEFINITIONS

Geometry Parameters

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, type `Geometry Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

GEOMETRY 1

Anode

1 In the **Geometry** toolbar, click **Block**.

2 In the **Settings** window for **Block**, type `Anode` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_cell`.

4 In the **Depth** text field, type `D_cell`.

5 In the **Height** text field, type `H_gde`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Electrolyte

1 Right-click **Anode** and choose **Duplicate**.

2 In the **Settings** window for **Block**, type `Electrolyte` in the **Label** text field.

3 Locate the **Position** section. In the **z** text field, type `H_gde`.

Cathode

1 Right-click **Electrolyte** and choose **Duplicate**.

2 In the **Settings** window for **Block**, type `Cathode` in the **Label** text field.

3 Locate the **Position** section. In the **z** text field, type `H_gde+H_el`.

Work Plane 1 (wp1)

1 In the **Geometry** toolbar, click **Work Plane**.

2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 In the **z-coordinate** text field, type `H_cell-H_ch`.

Work Plane 1 (wp1)>Plane Geometry

In the **Model Builder** window, click **Plane Geometry**.

Work Plane 1 (wp1)>Rectangle 1 (r1)

1 In the **Work Plane** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `W_ch`.

4 In the **Height** text field, type `N_ch*(W_ch+W_rib)`.

5 Locate the **Position** section. In the **xw** text field, type `W_rib/2`.

6 In the **yw** text field, type `W_rib/2`.

Work Plane 1 (wp1)>Rectangle 2 (r2)

1 Right-click **Component 1 (comp1)>Geometry 1>Work Plane 1 (wp1)>Plane Geometry>Rectangle 1 (r1)** and choose **Duplicate**.

2 In the **Settings** window for **Rectangle**, locate the **Position** section.

3 In the **xw** text field, type `W_rib/2+L_ch+W_ch`.

4 In the **yw** text field, type `-W_rib/2`.

Work Plane 1 (wp1)>Rectangle 3 (r3)

1 In the **Work Plane** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `L_ch`.

4 In the **Height** text field, type `W_ch`.

5 Locate the **Position** section. In the **xw** text field, type `W_rib/2+W_ch`.

6 In the **yw** text field, type `W_rib/2`.

Work Plane 1 (wp1)>Array 1 (arr1)

1 In the **Work Plane** toolbar, click **Transforms** and choose **Array**.

2 Select the object **r3** only.

3 In the **Settings** window for **Array**, locate the **Size** section.

4 In the **yw size** text field, type `N_ch`.

5 Locate the **Displacement** section. In the **yw** text field, type `W_ch+W_rib`.

6 In the **Work Plane** toolbar, click **Build All**.

Channel Domains

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Extrude**.

2 In the **Settings** window for **Extrude**, type `Channel Domains` in the **Label** text field.

3 Locate the **Distances** section. In the table, enter the following settings:

Distances (m)
H_ch

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Form Union (fin)

In the **Model Builder** window, right-click **Form Union (fin)** and choose **Build Selected**.

Inlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Inlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 19 only.

Outlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Outlet` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 42 only.

Cathode Current Collector

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Cathode Current Collector` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundaries 10, 26, 33, and 40 only.

Anode Current Collector

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Anode Current Collector` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 3 only.

Channel Domain Boundaries

1 In the **Geometry** toolbar, click **Selections** and choose **Adjacent Selection**.

2 In the **Settings** window for **Adjacent Selection**, locate the **Input Entities** section.

3 Click **Add**.

4 In the **Add** dialog box, select **Channel Domains** in the **Input selections** list.

5 Click **OK**.

6 In the **Settings** window for **Adjacent Selection**, type `Channel Domain Boundaries` in the **Label** text field.

Boundary Layer Boundaries

1 In the **Geometry** toolbar, click **Selections** and choose **Difference Selection**.

2 In the **Settings** window for **Difference Selection**, type `Boundary Layer Boundaries` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click the **Add** button for **Selections to add**.

5 In the **Add** dialog box, select **Channel Domain Boundaries** in the **Selections to add** list.

6 Click **OK**.

7 In the **Settings** window for **Difference Selection**, locate the **Input Entities** section.

8 Click the **Add** button for **Selections to subtract**.

9 In the **Add** dialog box, in the **Selections to subtract** list, choose **Inlet** and **Outlet**.

10 Click **OK**.