

Solid Oxide Electrolyzer

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:

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

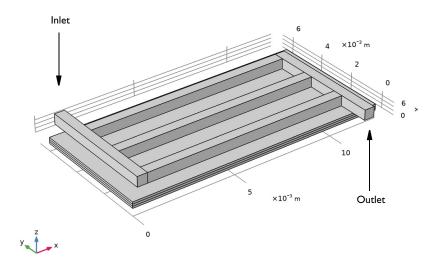


Figure 1: Model geometry. From top: Cathode gas channels, cathode gas diffusion electrode, solid oxide electrolyte layer, and anode gas diffusion layer. The positions of the inlet and outlet are indicated in the figure.

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.

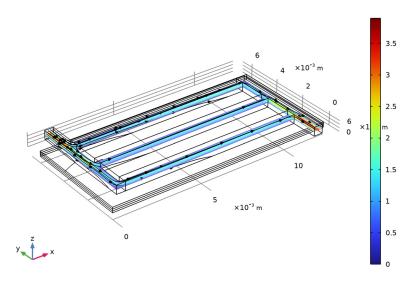
The current distribution is defined assuming a constant conductivity of the solid electrolyte. The Water Electrolyzer interface is used to define the electrode reactions and the electrolyte charge transport in the porous gas diffusion electrodes and the electrolyte layer, as well as the mass transport of hydrogen and water. The momentum flow is defined in the model using the Free and Porous Media Flow interface. Brinkman equations are used for the porous gas diffusion electrodes and Navier-Stokes equations are used for the nonporous gas channels.

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 properties of the cathode gas mixture, as well as the equilibrium potentials of the electrode reactions are automatically defined by the default built-in options of the Water Electrolyzer interface.

Results and Discussion

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



Slice: Velocity magnitude (m/s) Streamline: Velocity field

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.

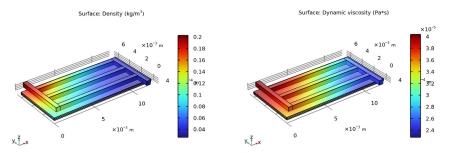


Figure 3: Density (left) and dynamic viscosity (right).

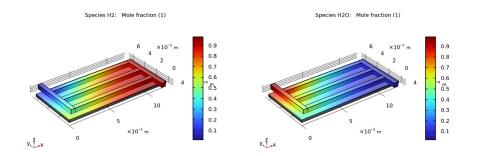
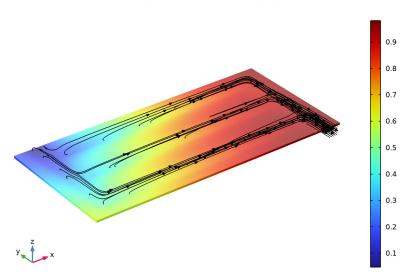


Figure 4: Hydrogen (left) and water vapor (right) molar fractions.

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.



Streamline: Total flux Volume: Mole fraction (1)

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.

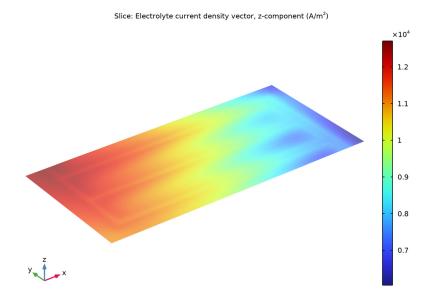


Figure 6: Electrolyte current density through electrolyte layer.

Application Library path: Fuel_Cell_and_Electrolyzer_Module/Electrolyzers/ soec

Modeling Instructions

This tutorial models the current distribution in a solid oxide electrolyzer. The tutorial comprises two major parts. First, 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.

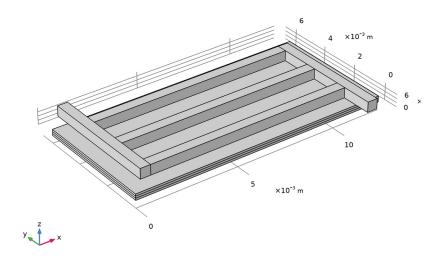
MODEL WIZARD

- I In the Model Wizard window, click 间 3D.
- 2 In the Select Physics tree, select Electrochemistry>Water Electrolyzers>Solid Oxide (we).
- 3 Click Add.
- 4 Click 🔿 Study.
- 5 In the Select Study tree, select Preset Studies for Selected Physics Interfaces> Stationary with Initialization.
- 6 Click **M** Done.

GEOMETRY I

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

- I In the Geometry toolbar, click Insert Sequence and choose Insert Sequence.
- 2 Browse to the model's Application Libraries folder and double-click the file soec_geom_sequence.mph.
- 3 In the Geometry toolbar, click 🟢 Build All.



GLOBAL DEFINITIONS

Geometry Parameters

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

Physics Parameters

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

- I In the Home toolbar, click P; 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 **b** Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file soec_physics_parameters.txt.

WATER ELECTROLYZER (WE)

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

- I In the Model Builder window, under Component I (compl) click Water Electrolyzer (we).
- 2 In the Settings window for Water Electrolyzer, locate the Domain Selection section.
- 3 Click 📉 Clear Selection.
- **4** Select Domains 1–3 only.
- 5 Locate the H2 Gas Mixture section. Find the Transport mechanisms subsection. Clear the Include gas phase diffusion check box.

Membrane I

- I In the Physics toolbar, click 📄 Domains and choose Membrane.
- **2** Select Domain 2 only.

ADD MATERIAL

- I In the Home toolbar, click 🙀 Add Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select Fuel Cell and Electrolyzer>Solid Oxides>Yttria-Stabilized Zirconia, 8YSZ, (ZrO2)0.92-(Y2O3)0.08.
- 4 Right-click and choose Add to Component I (compl).

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

WATER ELECTROLYZER (WE)

Electrolyte Phase I

In the **Electrolyte Phase** node, the electrolyte conductivity is set to be taken from the **Materials** node.

H2 Gas Diffusion Electrode I

Set up the properties of the **H2 Gas Diffusion Electrode** node. The details of electrode kinetics are set in the child node. Note that the reference equilibrium potential is calculated automatically when the default **Built in** option is used.

- I In the Physics toolbar, click 🔚 Domains and choose H2 Gas Diffusion Electrode.
- **2** In the Settings window for **H2 Gas Diffusion Electrode**, locate the Domain Selection section.
- 3 From the Selection list, choose Cathode.
- 4 Locate the Electrode Charge Transport section. In the σ_s text field, type sigmaeff_s.
- 5 Locate the Effective Electrolyte Charge Transport section. In the ε_l text field, type por_1.

H2 Gas Diffusion Electrode Reaction I

- I In the Model Builder window, click H2 Gas Diffusion Electrode Reaction I.
- 2 In the Settings window for H2 Gas Diffusion Electrode Reaction, locate the Electrode Kinetics section.
- **3** In the $i_{0,ref}(T)$ text field, type i0_H2.
- **4** Locate the **Active Specific Surface Area** section. In the a_v text field, type S.

O2 Gas Diffusion Electrode 1

Similarly, set up the properties of the **O2 Gas Diffusion Electrode** node. The details of electrode kinetics are set in the child node. Note that the reference equilibrium potential is calculated automatically when the default **Built in** option is used.

- I In the Physics toolbar, click 📄 Domains and choose O2 Gas Diffusion Electrode.
- **2** In the **Settings** window for **02 Gas Diffusion Electrode**, locate the **Domain Selection** section.
- 3 From the Selection list, choose Anode.
- **4** Locate the **Electrode Charge Transport** section. In the σ_s text field, type sigmaeff_s.
- **5** Locate the **Effective Electrolyte Charge Transport** section. In the ε_1 text field, type por_1.

O2 Gas Diffusion Electrode Reaction 1

- I In the Model Builder window, click O2 Gas Diffusion Electrode Reaction I.
- 2 In the Settings window for O2 Gas Diffusion Electrode Reaction, locate the Electrode Kinetics section.
- **3** In the $i_{0,ref}(T)$ text field, type i0_02.
- **4** In the α_a text field, type **3.5**.
- **5** Locate the **Active Specific Surface Area** section. In the a_v text field, type S.

Electronic Conducting Phase I

Finally, set up the boundary conditions.

I In the Model Builder window, under Component I (compl)>Water Electrolyzer (we) click Electronic Conducting Phase I.

Electric Ground 1

- I In the Physics toolbar, click 📃 Attributes 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.

Electronic Conducting Phase I

In the Model Builder window, click Electronic Conducting Phase I.

Electrode Current I

- I In the Physics toolbar, click 📃 Attributes and choose Electrode Current.
- 2 In the Settings window for Electrode Current, locate the Electrode Current section.
- 3 From the list, choose Average current density.
- 4 Locate the Boundary Selection section. From the Selection list, choose Anode Current Collector.
- **5** Locate the **Electrode Current** section. In the $i_{s.average}$ text field, type I_avg.

GLOBAL DEFINITIONS

Default Model Inputs

Default Model Inputs node can be used to set the **Temperature** for the entire model. This node may be accessed by multiple physics nodes.

- I 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 I

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

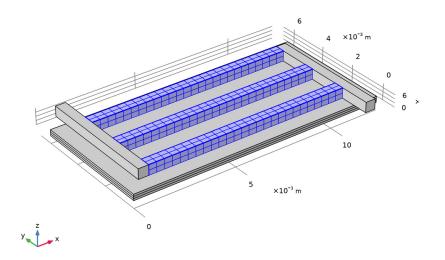
Size I

- I In the Model Builder window, under Component I (comp1) right-click Mesh I 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 I

- I 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.



Boundary Layers 1

Also add boundary layer mesh nodes 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.

- I 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** Select Domains 5–7 only.

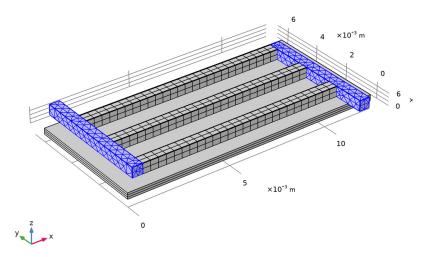
Boundary Layer Properties

- I In the Model Builder window, click Boundary Layer Properties.
- **2** In the Settings window for Boundary Layer Properties, locate the Boundary Selection section.
- **3** Click **Paste Selection**.
- 4 In the Paste Selection dialog box, type 21-23, 25, 28-30, 32, 35-37, 39 in the Selection text field.
- 5 Click OK.

- 6 In the Settings window for Boundary Layer Properties, locate the Layers section.
- 7 In the Number of layers text field, type 2.
- 8 In the Stretching factor text field, type 1.3.
- 9 From the Thickness specification list, choose First layer.
- **IO** In the **Thickness** text field, type H_Ch/10.
- II Click 🖷 Build Selected.

Free Tetrahedral I

- I In the Mesh toolbar, click \land 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 2

- I In the Model Builder window, under Component I (comp1)>Mesh I right-click Boundary Layers I and choose Duplicate.
- 2 In the Settings window for Boundary Layers, locate the Geometric Entity Selection section.
- 3 Click Clear Selection.

4 Select Domains 4 and 8 only.

Boundary Layer Properties

- I In the Model Builder window, expand the Boundary Layers 2 node, then click Boundary Layer Properties.
- **2** In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.
- 3 Click Clear Selection.
- 4 Click **Paste Selection**.
- 5 In the Paste Selection dialog box, type 14-18, 24, 31, 38, 41, 43-45, 47, 49, 51, 52 in the Selection text field.
- 6 Click OK.

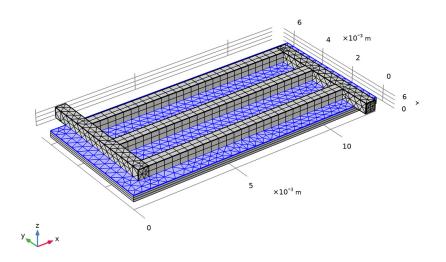
Boundary Layers 2

In the Model Builder window, right-click Boundary Layers 2 and choose Build Selected.

Free Triangular 1

- I In the Mesh toolbar, click \bigwedge Boundary 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 Assert.

Distribution I

- I Right-click Swept 2 and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 Click Telear 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.

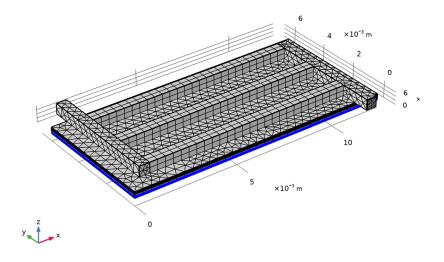
Distribution 2

- I 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 3

- I In the Model Builder window, under Component I (compl)>Mesh l>Swept 2 right-click Distribution I and choose Duplicate.
- 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 I

The problem is now ready for solving.

I In the Home toolbar, click **=** Compute.

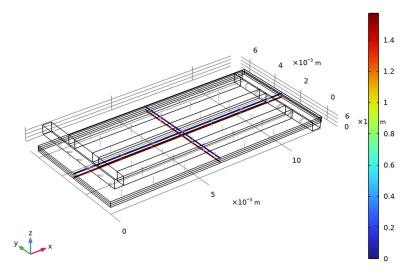
RESULTS

Electrode Potential with Respect to Ground (we)

I In the Electrode Potential with Respect to Ground (we) toolbar, click 💿 Plot.

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

Multislice: Electric potential (V) Arrow Volume: Electrode current density vector



COMPONENT I (COMPI)

Now start with the second part of the tutorial which adds a **Free and Porous Media Flow** interface to the cathode side of the model, enables hydrogen gas phase diffusion in the **Water Electrolyzer** interface, and couples the distribution of hydrogen and water vapor to the electrochemistry.

ADD PHYSICS

- I 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 Fluid Flow>Porous Media and Subsurface Flow> Free and Porous Media Flow (fp).
- 4 Click Add to Component I in the window toolbar.
- 5 In the Home toolbar, click 🙀 Add Physics to close the Add Physics window.

FREE AND POROUS MEDIA FLOW (FP)

- I Select Domains 3–8 only.
- **2** In the **Settings** window for **Free and Porous Media Flow**, locate the **Domain Selection** section.
- 3 Click here are a create Selection.
- 4 In the **Create Selection** dialog box, type **Gas** domains in the **Selection name** text field.
- 5 Click OK.
- 6 In the Settings window for Free and Porous Media Flow, locate the Physical Model section.
- 7 From the Compressibility list, choose Compressible flow (Ma<0.3).

Porous Medium I

- I Right-click Component I (compl)>Free and Porous Media Flow (fp) and choose Porous Medium.
- 2 In the Settings window for Porous Medium, locate the Domain Selection section.
- 3 From the Selection list, choose Cathode.

Porous Matrix I

- I In the Model Builder window, click Porous Matrix I.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- 3 From the ε_p list, choose User defined. In the associated text field, type por.
- **4** From the κ list, choose **User defined**. In the associated text field, type kappa.

Inlet 1

- I 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 I

- I 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.

MULTIPHYSICS

Reacting Flow, H2 Gas Phase 1 (rfh1)

In the Physics toolbar, click And Multiphysics Couplings and choose Domain>Reacting Flow, H2 Gas Phase.

WATER ELECTROLYZER (WE)

- I In the Model Builder window, under Component I (compl) click Water Electrolyzer (we).
- 2 In the Settings window for Water Electrolyzer, locate the Domain Selection section.
- 3 From the Selection list, choose All domains.
- 4 Locate the H2 Gas Mixture section. Find the Transport mechanisms subsection. Select the Include gas phase diffusion check box.

H2 Gas Flow Channel I

- I In the Physics toolbar, click 📄 Domains and choose H2 Gas Flow Channel.
- 2 In the Settings window for H2 Gas Flow Channel, locate the Domain Selection section.
- 3 From the Selection list, choose Channel Domains.

H2 Gas Diffusion Electrode I

- I In the Model Builder window, click H2 Gas Diffusion Electrode I.
- 2 In the Settings window for H2 Gas Diffusion Electrode, locate the Gas Transport section.
- **3** In the ε_g text field, type por.

H2 Gas Phase I

Note that the settings on the **H2 Gas Phase** node are either the default option or automatically set by the multiphysics coupling node. Set up the required boundary conditions and initial values.

I In the Model Builder window, click H2 Gas Phase I.

H2 Inlet I

- I In the Physics toolbar, click 📃 Attributes and choose H2 Inlet.
- 2 In the Settings window for H2 Inlet, locate the Boundary Selection section.
- 3 From the Selection list, choose Inlet.
- 4 Locate the Mixture Specification section. From the list, choose Mass flow rates.
- **5** In the $J_{0,\text{H2O}}$ text field, type Mflux_in.

H2 Gas Phase I

In the Model Builder window, click H2 Gas Phase I.

H2 Outlet I

- I In the Physics toolbar, click 📃 Attributes and choose H2 Outlet.
- 2 In the Settings window for H2 Outlet, locate the Boundary Selection section.
- 3 From the Selection list, choose Outlet.

Initial Values 1

- I In the Model Builder window, click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Composition section.
- 3 In the $x_{0,H2O}$ text field, type 0.95*(1-x/(W_cell*stoich)).

STUDY I

The concentration-dependent model is now ready for solving. Use a sequence of study steps, solving first for the current distribution initialization, 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

- I In the Model Builder window, under Study I click Step I: 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 box for Reacting Flow, H2 Gas Phase I (rfh1).

Step 2: Stationary

- I 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, clear the Solve for check box for Water Electrolyzer (we).
- 4 In the table, clear the Solve for check box for Reacting Flow, H2 Gas Phase I (rfhI).

Stationary 2

I 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 I right-click Solver Configurations and choose Delete Configurations.

Solution 1 (soll)

- I In the Study toolbar, click The Show Default Solver.
- 2 In the Model Builder window, expand the Solution I (soll) node.
- 3 In the Model Builder window, expand the Study I>Solver Configurations> Solution I (soll)>Stationary Solver 3 node.
- 4 Right-click Stationary Solver 3 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

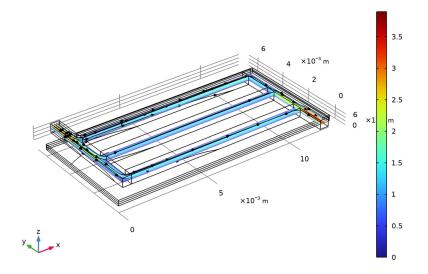
- I In the Model Builder window, expand the Results>Velocity (fp) node, then click Slice.
- 2 In the Settings window for Slice, locate the Plane Data section.
- 3 From the Plane list, choose xy-planes.
- 4 From the Entry method list, choose Coordinates.
- 5 In the z-coordinates text field, type H_cell-H_ch/2.
- 6 In the Velocity (fp) toolbar, click 🗿 Plot.

Streamline 1

- I In the Model Builder window, right-click Velocity (fp) and choose Streamline.
- In the Settings window for Streamline, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
 Free and Porous Media Flow>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 (fp) toolbar, click **I** Plot.

Slice: Velocity magnitude (m/s) Streamline: Velocity field



Density

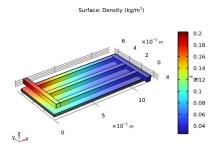
The density of the gas mixture will change as water is replaced by hydrogen in the gas stream. Plot the density as follows:

- I 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

- I Right-click **Density** and choose **Surface**.
- In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
 Free and Porous Media Flow>Material properties>fp.rho Density kg/m³.

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



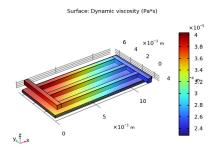
Viscosity

Also, the viscosity will change in the gas stream.

- I 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.

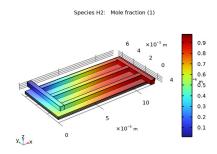
Surface 1

- I Right-click **Viscosity** and choose **Surface**.
- In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
 Free and Porous Media Flow>Material properties>fp.mu Dynamic viscosity Pa·s.
- **3** In the **Viscosity** toolbar, click **I** Plot.

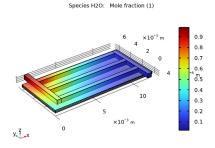


Mole Fraction, H2, Surface (we)

Default plots are created for the hydrogen and water molar fractions.



Mole Fraction, H2O, Surface (we)



Molar Fraction and Flux, H2

Create a plot for the hydrogen molar fraction and flux as follows:

- I 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

- I Right-click Molar Fraction and Flux, H2 and choose Streamline.
- In the Settings window for Streamline, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
 Water Electrolyzer>Species H2>we.tfluxH2x,...,we.tfluxH2z 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

- I Right-click Streamline I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Channel Domains.

Volume 1

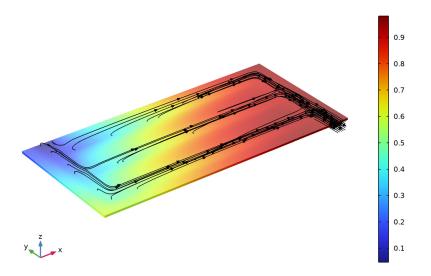
- I In the Model Builder window, right-click Molar Fraction and Flux, H2 and choose Volume.
- In the Settings window for Volume, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
 Water Electrolyzer>Species H2>we.xH2 Mole fraction.

Selection I

- I Right-click Volume I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.
- **3** From the **Selection** list, choose **Cathode**.
- **4** Click the **Show Grid** button in the **Graphics** toolbar.

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

```
Streamline: Total flux Volume: Mole fraction (1)
```



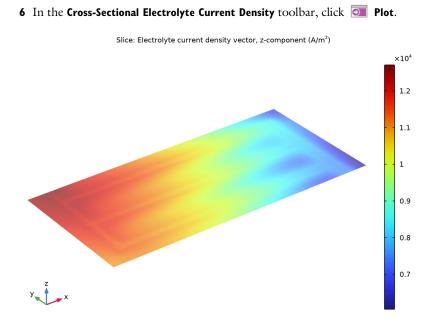
Cross-Sectional Electrolyte Current Density

Finally, plot the current distribution across the electrolyte layer as follows:

- I 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

- I 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 I (compl)>Water Electrolyzer> Electrolyte current density vector A/m²>we.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_e1/2.



Appendix - Geometry Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click 🔗 Model Wizard.

MODEL WIZARD

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

GLOBAL DEFINITIONS

Geometry Parameters

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, type Geometry Parameters in the Label text field.
- **3** Locate the **Parameters** section. Click **>** Load from File.

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

GEOMETRY I

Anode

- I 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

- I 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

- I 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_e1.

Work Plane I (wp1)

- I 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 I (wp1)>Plane Geometry

In the Model Builder window, click Plane Geometry.

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

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type W_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 I (wp1)>Rectangle 2 (r2)

- I Right-click Component I (comp1)>Geometry I>Work Plane I (wp1)>Plane Geometry> Rectangle I (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 I (wp1)>Rectangle 3 (r3)

- I In the Work Plane toolbar, click 📃 Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type 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 I (wp1)>Array I (arr1)

- I In the Work Plane toolbar, click $[\mathcal{Q}]$ 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

- I In the Model Builder window, right-click Geometry I 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

- I 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

- I 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

- I 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

- I 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.

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