

Two-Phase Nonisothermal Zero-Gap Alkaline Water Electrolyzer

This model defines a zero-gap alkaline water electrolyzer, where oxygen and hydrogen gas are evolved in porous gas diffusion nickel felt electrodes, placed adjacent to a porous separator (diaphragm).

The geometry defines a unit cell of an electrolyzer stack, in turn comprising two full electrolyzer cells, extending 10 cm along the channel direction. The two electrolyzer cells are separated by a corrugated bipolar steel plate.

The model solves for the fully intercoupled current distribution of the electrolyzer cells, two-phase flow of evolved gases and electrolyte, and heat transfer.

The model is advanced and uses several coupled physics interfaces. For new users, it is recommended to first study the Mass Transport and Electrochemical Reaction in a Fuel Cell Cathode and Fuel Cell Cathode with Liquid Water tutorial examples.

Model Definition

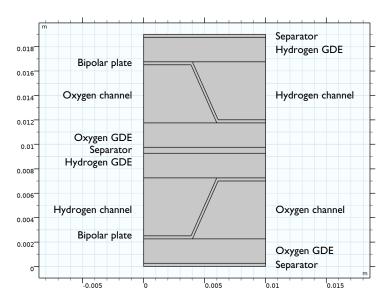


Figure 1: 2D-cross section of the two-cell unit cell.

Figure 1 shows a cross section of the model geometry, defining a two-cell unit cell within an electrolyzer stack. Each cell consists of a hydrogen electrolyte compartment, and an

oxygen electrolyte compartment, separated by a bipolar steel plate and a separator (diaphragm). The 2 mm thick gas diffusion electrodes (GDEs) consist of porous nickel felt.

The cross section is extruded to form the 3D geometry as shown in Figure 2. The cell has a length of 10 cm, with additional 6 mm extrusions of the flow channels at the oxygen and hydrogen inlets and outlets.

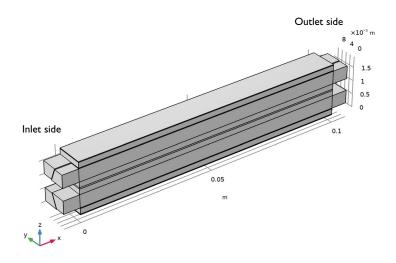


Figure 2: Extruded 3D geometry.

VOLUME FRACTIONS

The Phase Transport in Free and Porous Media interface solves for the relative gas volume fraction s_g in the gas–electrolyte mixture. The relative liquid volume fraction is defined as

$$s_1 = 1 - s_g$$

As gas is evolved in the electrodes and transported out to the gas-electrolyte channels, the volume fraction of electrolyte decreases, making room for the evolved gas.

In the GDEs, the electrolyte volume fraction ε_l is defined as

$$\varepsilon_{\rm l} = s_{\rm l} \varepsilon_{\rm por}$$

where $\epsilon_{\rm por}$ is the pore volume fraction relative to the total volume.

In the gas-electrolyte channels, the electrolyte volume fraction is defined as

$$\varepsilon_{\rm l} = \varepsilon_{\rm por}$$

MATERIAL PROPERTIES

The material properties for the steel bipolar plate and the 6 M KOH electrolyte are retrieved from the **Built-in** and **Fuel Cell & Electrolyzer** material libraries, respectively. User-defined values for the nickel felt GDEs are specified in a **Parameters** node. The Water and Electrolyzer interface is used to calculate the properties of the fully humidified H_2 and O_2 gas mixtures.

Volume-averaged properties, based on $s_{\rm g}$ and $s_{\rm l}$, are used for the thermal conductivity, density and heat capacity of the gas-electrolyte mixture. These properties are defined on the GDE and channel domains by the use of **Variables** nodes.

WATER ELECTROLYZER INTERFACE

The current distribution and electrochemical reactions are defined using the **Water Electrolyzer** interface. The porous gas diffusion electrodes are modeled using Butler–Volmer kinetics. Ohmic losses in the electrode and electrolyte phases are included. Gas transport of the gas phase as a whole is included in the model, but any effects due to partial pressure gradients of the different species in the gas phase are neglected.

The effective electrolyte conductivity in the electrolyte compartment, GDEs and the separator is set to depend on the electrolyte volume fraction according to

$$\sigma_{l, \text{ eff}} = \varepsilon_l^{3/2} \sigma_{l, \text{ bulk}}$$
 (1)

where $\sigma_{l,bulk}$ is the bulk conductivity of 6 M KOH.

The cell voltage of the two-cell unit cell is set by the offset in the periodic condition (see the section below). Also, an electrolyte phase point condition is added in order to ground the model and ensure a unique solution for the potential variables.

MULTIPHASE FLOW IN FREE AND POROUS MEDIA MULTIPHYSICS INTERFACE

The two-phase flow model is defined by adding a **Multiphase Flow in Free and Porous Media** multiphysics interface to the model. This in turn adds the following physics interfaces to the model tree:

• Darcy's Law, solving for the liquid pressure in the GDEs

- Laminar Flow, solving for the liquid pressure and velocity field in the channels
- Phase Transport, solving for the gas phase volume fraction in the gas-liquid two-phase mixture

In addition, the following multiphysics nodes are also added by Multiphase Flow in Free and Porous Media:

- Multiphase Flow in Porous Media, coupling Darcy's law and Phase Transport in the GDEs
- Free and Porous Media Flow Coupling, defining the boundary between the Laminar Flow and Darcy's Law domains
- Mixture Model, coupling Laminar Flow and Phase Transport in the channels

The gas and liquid mass sources, stemming from the electrode reactions defined by the Water Electrolyzer interface, are added as a Mass Source node in the Phase Transport interface. **Turbulent Mixing** is added in the channels to the Phase Transport interface in order to facilitate convergence.

Fully-developed flow conditions are defined on a common **Inlet** node in the Laminar Flow interface, with an average velocity of 1 cm/s set for all channels. A uniform outlet pressure of 25 atm is defined on the **Outlet** node in the same interface.

HEAT TRANSFER IN SOLIDS AND FLUIDS INTERFACE

Solid (bipolar plate), **Fluid** (channels) and **Porous Medium** (GDE and separator) nodes are used to define the heat transfer in the cell.

The heat sources related to the electrochemical reactions are added to the Heat Transfer interface by the use of an **Electrochemical Heating** multiphysics nodes.

The inlet temperature of the cell is set to 80°C.

PERIODIC CONDITIONS

Periodicity between the top- and bottom-most separator boundaries in Figure 1 is defined by the use of a **Periodic Condition** node in Heat Transfer, which sets both the ingoing and outgoing heat fluxes, as well as the temperature, equal at the matching positions at the two boundaries. In the Water Electrolyzer interface, a periodic condition for the electrolyte phase potential is set up manually by the use of a Linear Extrusion operator, which also includes a potential offset of two times the cell voltage for the two-cell unit cell.

STUDY

Three consecutive study steps are used to solve the problem. For each step, the solution of the dependent variables solved for in the previous step are passed on as the corresponding initial values to the subsequent step.

A first Current Distribution Initialization step computes suitable initial values for the electrode and electrolyte phase potentials of the Water Electrolyzer interface. A second Stationary step then solves for the pressures and velocity fields of the Darcy's Law and Laminar Flow interfaces only. The third, final, step solves for the fully coupled problem, ramping up the cell voltage from 1.5 to 2.1 V using an Auxiliary Sweep.

Results and Discussion

Figure 3 shows the polarization plot generated by the auxiliary sweep.

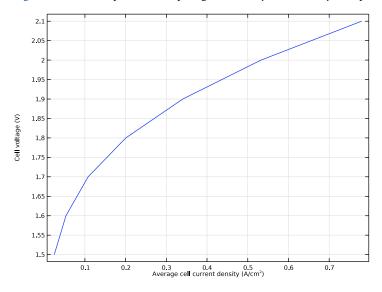


Figure 3: Polarization.

Figure 4 shows the electrolyte phase potential in the channels and GDEs for a cell voltage of 2.1 V, whereas Figure 5 shows the electrode phase potential in the GDEs and bipolar plates for the same cell potential.

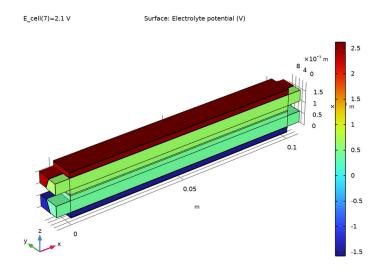


Figure 4: Electrolyte phase potential.

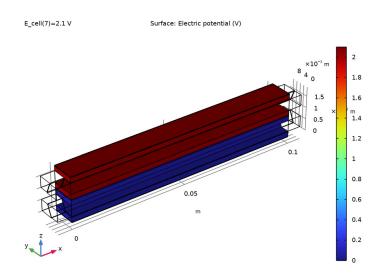


Figure 5: Electrode phase potential.

Figure 6 and Figure 7 show the gas volume fraction of the gas-electrolyte mixture in the GDEs and the channels, respectively, whereas Figure 8 show the corresponding streamlines in the channels.

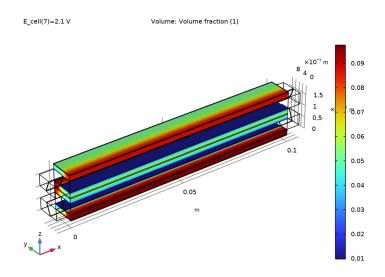


Figure 6: Gas volume fraction in the fluid mixture in the GDEs.

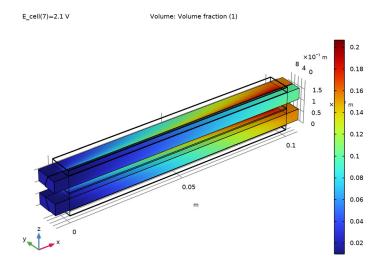


Figure 7: Gas volume fraction in the channels.

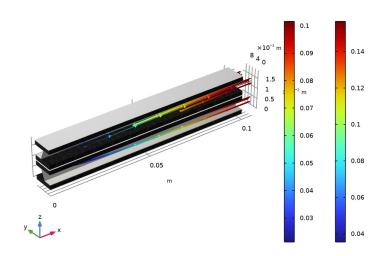


Figure 8: Gas streamlines and gas volume fraction.

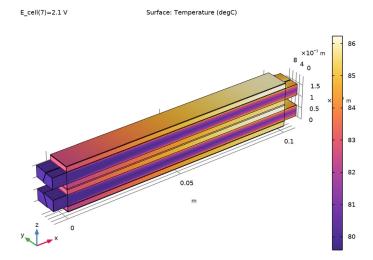


Figure 9: Temperature.

Figure 9 shows a plot of the temperature. The temperature increases towards the outlets.

Application Library path: Fuel_Cell_and_Electrolyzer_Module/ Thermal_Management/zero_gap_aec

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

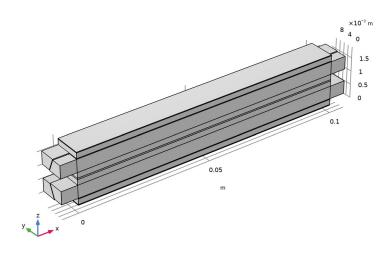
- I In the Model Wizard window, click 1 3D.
- 2 In the Select Physics tree, select Electrochemistry>Water Electrolyzers> Hydroxide Exchange (we).
- 3 Click Add.

- 4 In the Select Physics tree, select Fluid Flow>Porous Media and Subsurface Flow> Multiphase Free and Porous Media Flow.
- 5 Click Add.
- 6 In the Select Physics tree, select Heat Transfer>Heat Transfer in Solids and Fluids (ht).
- 7 Click Add.
- 8 Click Study.
- 9 In the Select Study tree, select Preset Studies for Selected Physics Interfaces> Water Electrolyzer>Stationary with Initialization.
- 10 Click Done.

GEOMETRY I

Insert the geometry sequence from a file as follows:

- 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 zero gap aec geom sequence.mph.
- 3 In the Geometry toolbar, click **Build All**.
- 4 In the Model Builder window, under Component I (compl) click Geometry I.



5 In the **Model Builder** window, collapse the **Geometry I** node.

GLOBAL DEFINITIONS

Geometry Parameters

The geometry sequence you imported uses a number of parameters, which now appear in a **Parameters** node.

- 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

Add a second **Parameters** node for the physics parameters.

- I In the Home toolbar, click Pi Parameters and choose Add>Parameters.
- 2 In the Settings window for Parameters, type Physics Parameters in the Label text field.

Import the physics parameters from a text file.

- 3 Locate the Parameters section. Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file zero_gap_aec_physics_parameters.txt.

MATERIALS

Add some material data from the material libraries as follows:

ADD MATERIAL FROM LIBRARY

In the Home toolbar, click Windows and choose Add Material from Library.

ADD MATERIAL

- I Go to the Add Material window.
- 2 In the tree, select Built-in>Steel AISI 4340.
- 3 Right-click and choose Add to Component I (compl).

MATERIALS

Steel AISI 4340 (mat1)

- I In the Model Builder window, under Component I (compl)>Materials click Steel AISI 4340 (matl).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Bipolar Plates.

ADD MATERIAL

- I Go to the Add Material window.
- 2 In the tree, select Fuel Cell and Electrolyzer>Aqueous Alkali>Potassium Hydroxide, KOH.
- 3 Right-click and choose Add to Component I (compl).
- 4 In the Home toolbar, click **# Add Material** to close the **Add Material** window.

MATERIALS

Potassium Hydroxide, KOH (mat2)

- I In the Settings window for Material, locate the Geometric Entity Selection section.
- 2 From the Selection list, choose Electrolyte Domains.

DEFINITIONS

Now add a number of **Variables** nodes. Note that the different nodes have different domain selections. In this way variables with the same name can be defined differently in different domains.

Variables - GDEs

- I In the Model Builder window, under Component I (compl) right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, type Variables GDEs in the Label text field.
- 3 Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose GDEs.
- 5 Locate the Variables section. Click **Load from File.**
- **6** Browse to the model's Application Libraries folder and double-click the file zero gap aec gde variables.txt.

Variables - Channels

- I In the Model Builder window, right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, type Variables Channels in the Label text field.
- 3 Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Channels.
- 5 Locate the Variables section. Click **Load from File.**

6 Browse to the model's Application Libraries folder and double-click the file zero gap aec channel variables.txt.

Some variable expressions you imported are indicating missing variable definitions. Change the name of the dependent variables in the phase transport interface in order to fix some of these issues.

PHASE TRANSPORT IN FREE AND POROUS MEDIA FLOW (PHTR)

- I In the Model Builder window, under Component I (compl) click Phase Transport in Free and Porous Media Flow (phtr).
- 2 In the Settings window for Phase Transport in Free and Porous Media Flow, click to expand the **Dependent Variables** section.
- **3** In the **Volume fractions (1)** table, enter the following settings:

 s_1 s_g

> In this model s 1 denotes the volume fraction of the liquid phase, and s g denotes the volume fraction of the gas phase.

WATER ELECTROLYZER (WE)

Now start setting up the Water Electrolyzer physics interface. This interface will solve for the electrolyte and electrode phase potentials, and will define the properties of the gas phase.

- I In the Model Builder window, under Component I (compl) click Water Electrolyzer (we).
- 2 In the Settings window for Water Electrolyzer, locate the H2 Gas Mixture section.
- 3 Find the Transport mechanisms subsection. Clear the Include gas phase diffusion check box.
- 4 Find the Reactions subsection. Select the Include H20(I) in reaction stoichiometry check box.
- 5 Locate the **02** Gas Mixture section. Find the Transport mechanisms subsection. Clear the **Include gas phase diffusion** check box.
- 6 Find the Reactions subsection. Select the Include H20(1) in reaction stoichiometry check box.

Current Collector I

- I In the Physics toolbar, click **Domains** and choose Current Collector.
- 2 In the Settings window for Current Collector, locate the Domain Selection section.

- 3 From the Selection list, choose Bipolar Plates.
- 4 Locate the Electrode Charge Transport section. From the σ_s list, choose From material.

H2 Gas-Electrolyte Compartment I

- In the Physics toolbar, click Domains and choose H2 Gas-Electrolyte Compartment.
- 2 In the Settings window for H2 Gas-Electrolyte Compartment, locate the Domain Selection section.
- 3 From the Selection list, choose Hydrogen Channels.
- 4 Locate the Effective Electrolyte Charge Transport section. In the ε_l text field, type eps1.

H2 Gas Diffusion Electrode I

- 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 **Hydrogen GDEs**.
- 4 Locate the Electrode Charge Transport section. In the σ_s text field, type sigma_Ni_eff.
- **5** Locate the **Effective Electrolyte Charge Transport** section. In the ε_l text field, type eps1.

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 Stoichiometric Coefficients section.
- 3 In the v_{H2O} text field, type 0.
- 4 In the $v_{\text{H2O(l)}}$ text field, type -1.
- **5** Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type i0_ref_her.
- **6** Locate the **Active Specific Surface Area** section. In the a_v text field, type Av.

Separator I

- I In the Physics toolbar, click **Domains** and choose Separator.
- 2 In the Settings window for Separator, locate the Domain Selection section.
- 3 From the Selection list, choose Separators.
- **4** Locate the **Effective Electrolyte Charge Transport** section. In the ε_l text field, type epsl sep.

O2 Gas Diffusion Electrode 1

I In the Physics toolbar, click **Domains** and choose **O2 Gas Diffusion Electrode**.

- 2 In the Settings window for O2 Gas Diffusion Electrode, locate the Domain Selection section.
- 3 From the Selection list, choose Oxygen GDEs.
- 4 Locate the **Electrode Charge Transport** section. In the σ_s text field, type sigma_Ni_eff.
- **5** Locate the **Effective Electrolyte Charge Transport** section. In the ε_l text field, type eps1.
- O2 Gas Diffusion Electrode Reaction I
- I In the Model Builder window, click **02** Gas Diffusion Electrode Reaction I.
- 2 In the Settings window for O2 Gas Diffusion Electrode Reaction, locate the Stoichiometric Coefficients section.
- 3 In the $v_{\rm H2O}$ text field, type 0.
- 4 In the $v_{H2O(1)}$ text field, type -1.
- **5** Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type i0_ref_oer.
- **6** From the **Edit** menu, choose
 - 02 Gas Diffusion Electrode Reaction 1: Reference Exchange Current Density.
- 7 Locate the Active Specific Surface Area section. In the a_v text field, type Av.
- 02 Gas-Electrolyte Compartment I
- I In the Physics toolbar, click **Domains** and choose **O2 Gas-Electrolyte Compartment**.
- 2 In the Settings window for O2 Gas-Electrolyte Compartment, locate the Domain Selection section.
- 3 From the Selection list, choose Oxygen Channels.
- 4 Locate the Effective Electrolyte Charge Transport section. In the ϵ_l text field, type eps1.

DEFINITIONS

The model defines a two-cell unit-cell, assuming symmetry and periodic conditions on all external boundaries parallel to the xy and xz-planes. Add an extrusion operator to define the periodic condition for the electrolyte phase potential.

Linear Extrusion I (linext I)

- I In the Definitions toolbar, click Monlocal Couplings and choose Linear Extrusion.
- 2 In the Settings window for Linear Extrusion, locate the Source Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 23 only.
- 5 Locate the Source Vertices section. Click to select the Activate Selection toggle button.

- **6** Select Point 37 only.
- 7 Click to select the **Activate Selection** toggle button.
- **8** Select Point 17 only.
- **9** Click to select the **Activate Selection** toggle button.
- **10** Select Point 49 only.
- II Locate the Destination Vertices section. Click to select the 💷 Activate Selection toggle button.
- **12** Select Point 48 only.
- **13** Click to select the **Activate Selection** toggle button.
- **14** Select Point 28 only.
- **15** Click to select the **Activate Selection** toggle button.
- **16** Select Point 60 only.

WATER ELECTROLYZER (WE)

Electrolyte Phase I

In the Model Builder window, under Component I (compl)>Water Electrolyzer (we) click Electrolyte Phase 1.

Electrolyte Potential I

- I In the Physics toolbar, click 🖳 Attributes and choose Electrolyte Potential.
- 2 Select Boundary 54 only.
- 3 In the Settings window for Electrolyte Potential, locate the Electrolyte Potential section.
- 4 In the $\phi_{l,bnd}$ text field, type linext1(we.phil+2*E_cell).

H2 Gas Phase I

- I In the Model Builder window, under Component I (compl)>Water Electrolyzer (we) click H2 Gas Phase I.
- 2 In the Settings window for H2 Gas Phase, locate the Model Input section.
- **3** From the p_A list, choose **User defined**. In the associated text field, type pA_gas.
- 4 Locate the Composition section. From the Mixture specification list, choose Humidified mixture.
- **5** In the T_{hum} text field, type T.
- **6** In the $p_{A,\text{hum}}$ text field, type pA_gas.

O2 Gas Phase I

- I In the Model Builder window, click 02 Gas Phase I.
- 2 In the Settings window for O2 Gas Phase, locate the Model Input section.
- **3** From the p_A list, choose **User defined**. In the associated text field, type pA_gas .
- 4 Locate the Composition section. From the Mixture specification list, choose Humidified mixture.
- **5** In the T_{hum} text field, type T.
- **6** In the $p_{A,\text{hum}}$ text field, type pA_gas.

The potentials need to be grounded somewhere in the model (otherwise no unique solution for the potentials exists). Use a pointwise constraint in a point to ground the electrode phase potential.

- 7 Click the Show More Options button in the Model Builder toolbar.
- 8 In the Show More Options dialog box, select Physics>Equation-Based Contributions in the tree.
- 9 In the tree, select the check box for the node Physics>Equation-Based Contributions.
- IO Click OK.

Pointwise Constraint - Electrode Potential Ground

- I In the Physics toolbar, click Points and choose Pointwise Constraint.
- 2 In the Settings window for Pointwise Constraint, type Pointwise Constraint -Electrode Potential Ground in the Label text field.
- **3** Select Point 19 only.
- 4 Locate the Pointwise Constraint section. In the Constraint expression text field, type we.phis.
- 5 In the Model Builder window, collapse the Water Electrolyzer (we) node.

LAMINAR FLOW (SPF)

The electrolyzer settings are now complete. Now set up the flow interfaces, starting with the laminar flow in the electrolyte-gas channels.

- I In the Model Builder window, under Component I (compl) click Laminar Flow (spf).
- 2 In the Settings window for Laminar Flow, locate the Domain Selection section.
- 3 From the Selection list, choose Channels.
- **4** Locate the **Physical Model** section. In the $p_{\rm ref}$ text field, type p_out.

Fluid Properties 1

- I In the Model Builder window, under Component I (compl)>Laminar Flow (spf) click Fluid Properties 1.
- 2 In the Settings window for Fluid Properties, locate the Model Input section.
- **3** From the *c* list, choose **Common model input**.

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 Inlets.
- 4 Locate the Boundary Condition section. From the list, choose Fully developed flow.
- **5** Locate the **Fully Developed Flow** section. In the $U_{\rm av}$ text field, type v_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 **Outlets**.

Symmetry I

- I In the Physics toolbar, click **Boundaries** and choose Symmetry.
- **2** Select Boundaries 2, 6, 19, 20, 31, 43, 69, 75, 82, 89, 105, and 106 only.
- 3 In the Model Builder window, collapse the Laminar Flow (spf) node.

DARCY'S LAW (DL)

Now set up the Darcy's Law interface, which defines the flow in the porous gas diffusion electrodes.

- I In the Model Builder window, under Component I (compl) click Darcy's Law (dl).
- 2 In the Settings window for Darcy's Law, locate the Domain Selection section.
- 3 From the Selection list, choose GDEs.
- **4** Locate the **Physical Model** section. In the p_{ref} text field, type p_out.
- 5 Click to expand the Discretization section. From the Pressure list, choose Linear.

Porous Matrix I

- I In the Model Builder window, under Component I (compl)>Darcy's Law (dl)> Porous Medium I click Porous Matrix I.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.

- **3** From the $\varepsilon_{\rm p}$ list, choose **User defined**. In the associated text field, type eps_pores.
- **4** From the κ list, choose **User defined**. In the associated text field, type perm_GDE.
- 5 In the Model Builder window, collapse the Darcy's Law (dl) node.

PHASE TRANSPORT IN FREE AND POROUS MEDIA FLOW (PHTR)

Now set up the **Phase Transport** interface, which solves for the volume fraction of the gases in the gas diffusion electrodes and the gas-electrolyte channels.

- I In the Model Builder window, under Component I (compl) click Phase Transport in Free and Porous Media Flow (phtr).
- 2 In the Settings window for Phase Transport in Free and Porous Media Flow, locate the **Domain Selection** section.
- 3 From the Selection list, choose Channels and GDEs.

Phase and Transport Properties I

- I In the Model Builder window, under Component I (compl)> Phase Transport in Free and Porous Media Flow (phtr) click Phase and Transport Properties I.
- 2 In the Settings window for Phase and Transport Properties, locate the Model Input section.
- **3** From the c list, choose **Common model input**.

Turbulent Mixing 1

- I In the Physics toolbar, click 🦳 Attributes and choose Turbulent Mixing. The turbulent mixing is needed make the evolved gas move away from the gde-channel interface and to achieve convergence. The parameter values used for turbulent mixing should be regarded as empirical tuning parameters for this very model.
- 2 In the Settings window for Turbulent Mixing, locate the Turbulent Mixing Parameters section.
- 3 In the v_T text field, type 1e-5.
- **4** In the $Sc_{\rm T}$ text field, type 1.

Phase and Porous Media Transport Properties 1

- I In the Model Builder window, under Component I (compl)> Phase Transport in Free and Porous Media Flow (phtr) click Phase and Porous Media Transport Properties I.
- 2 In the Settings window for Phase and Porous Media Transport Properties, locate the **Domain Selection** section.

- 3 From the Selection list, choose GDEs.
- 4 Locate the Model Input section. From the c list, choose Common model input.
- **5** Locate the **Capillary Pressure** section. In the p_{csg} text field, type dpc_dsg*s_g.
- 6 Locate the Phase I Properties section. From the Fluid s_I list, choose Potassium Hydroxide, KOH (mat2).
- **7** In the κ_{rsl} text field, type s_1^2.
- **8** Locate the **Phase 2 Properties** section. From the ρ_{sg} list, choose Density of gas phase (we).
- 9 From the μ_{sg} list, choose Dynamic viscosity of gas phase (we).
- **IO** In the κ_{rsg} text field, type s_g^2.

Initial Values 1

- I In the Model Builder window, click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the $s_{0,sg}$ text field, type s_g_i n.

Free-Porous Interface 1

- I In the Model Builder window, click Free-Porous Interface I.
- 2 In the Settings window for Free-Porous Interface, locate the Phase 2 section.
- 3 From the Boundary condition list, choose Outflow, no flux below threshold saturation.
- **4** In the $s_{0.sg}$ text field, type s_g_i n.

Volume Fraction 1

- I In the Physics toolbar, click **Boundaries** and choose **Volume Fraction**.
- 2 In the Settings window for Volume Fraction, locate the Boundary Selection section.
- **3** From the **Selection** list, choose **Inlets**.
- 4 Locate the Volume Fraction section. Select the Phase s_g check box.
- **5** In the $s_{0,sg}$ text field, type s_g_in.

Outflow I

- I 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 **Outlets**.

DEFINITIONS

To define the mass sources of evolved gas, we will add additional variables nodes. The reaction rates are based on the volumetric current density computed by the water electrolyzer interface, and Faraday's second law of electrolysis.

Variables - Oxygen GDEs

- I In the Model Builder window, under Component I (compl) right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, type Variables Oxygen GDEs in the Label text
- 3 Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Oxygen GDEs.
- **5** Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
R_02_oer	we.iv_o2gder1/(4* F_const)	mol/(m³·s)	Molar reaction rate, oxygen evolution reaction
Rm_gas	R_02_oer*we.M02	kg/(m³·s)	Mass gas evolution rate

Variables - Hydrogen GDEs

- I In the Model Builder window, right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, type Variables Hydrogen GDEs in the Label text field.
- 3 Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Hydrogen GDEs.
- **5** Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
R_H2_her	-we.iv_h2gder1/(2* F_const)	mol/(m³·s)	Molar reaction rate, hydrogen evolution reaction
Rm_gas	R_H2_her*we.MH2	kg/(m³·s)	Mass gas evolution rate

PHASE TRANSPORT IN FREE AND POROUS MEDIA FLOW (PHTR)

Mass Source 1

- I In the Physics toolbar, click **Domains** and choose Mass Source.
- 2 In the Settings window for Mass Source, locate the Domain Selection section.
- 3 From the Selection list, choose GDEs.
- 4 Locate the Mass Source section. Select the Mass transfer to other phases check box.
- **5** In the $Q_{\rm sl}$ text field, type -Rm_gas.
- **6** In the $Q_{\rm sg}$ text field, type Rm_gas.
- 7 In the Model Builder window, collapse the Phase Transport in Free and Porous Media Flow (phtr) node.

HEAT TRANSFER IN SOLIDS AND FLUIDS (HT)

Now set up the **Heat Transfer** interface.

Fluid 1

- I In the Model Builder window, under Component I (compl)> Heat Transfer in Solids and Fluids (ht) click Fluid 1.
- 2 In the Settings window for Fluid, locate the Domain Selection section.
- 3 From the Selection list, choose Channels.
- **4** Locate the **Model Input** section. From the p_A list, choose **User defined**. In the associated text field, type pA_liquid.
- **5** From the c list, choose **Common model input**.
- **6** Locate the **Heat Convection** section. From the **u** list, choose **Velocity field (spf)**.
- 7 Locate the **Heat Conduction, Fluid** section. From the k list, choose **User defined**. In the associated text field, type kappa_two_phase_mix.
- 8 Locate the Thermodynamics, Fluid section. From the Fluid type list, choose Gas/Liquid.
- **9** From the p list, choose **User defined**. In the associated text field, type rho mix.
- **10** From the C_p list, choose **User defined**. In the associated text field, type Cp two phase mix.
- II From the γ list, choose User defined.

Initial Values 1

- I In the Model Builder window, click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the *T* text field, type T0.

Porous Medium - Separators

- I In the Physics toolbar, click **Domains** and choose Porous Medium.
- 2 In the Settings window for Porous Medium, type Porous Medium Separators in the Label text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **Separators**.

Fluid 1

- I In the Model Builder window, click Fluid I.
- 2 In the Settings window for Fluid, locate the Model Input section.
- **3** From the p_A list, choose **User defined**. From the c list, choose **Common model input**.
- **4** Locate the **Heat Conduction, Fluid** section. From the $k_{
 m f}$ list, choose **User defined**. In the associated text field, type kappa KOH.
- **5** Locate the **Thermodynamics**, Fluid section. From the $C_{p,f}$ list, choose **User defined**. In the associated text field, type Cp_KOH.
- **6** From the γ list, choose **User defined**.

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 epsl_sep.
- 4 Locate the Heat Conduction, Porous Matrix section. From the $k_{\rm b}$ list, choose User defined. In the associated text field, type kappa_sep.
- 5 Locate the Thermodynamics, Porous Matrix section. From the ρ_b list, choose User defined. In the associated text field, type rho sep.
- **6** From the $C_{\rm p,h}$ list, choose **User defined**. In the associated text field, type Cp_sep.

Porous Medium - GDEs

- I In the Physics toolbar, click **Domains** and choose Porous Medium.
- 2 In the Settings window for Porous Medium, type Porous Medium GDEs in the Label text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **GDEs**.

Fluid 1

- I In the Model Builder window, click Fluid I.
- 2 In the Settings window for Fluid, locate the Model Input section.
- **3** From the p_A list, choose **User defined**. In the associated text field, type pA_liquid .

- **4** From the c list, choose **Common model input**.
- 5 Locate the Heat Convection section. From the u list, choose Total Darry velocity field (dl/
- **6** Locate the **Heat Conduction, Fluid** section. From the k_f list, choose **User defined**. In the associated text field, type kappa_two_phase_mix.
- 7 Locate the Thermodynamics, Fluid section. From the ρ_f list, choose User defined. In the associated text field, type rho_mix.
- **8** From the $C_{p,f}$ list, choose **User defined**. In the associated text field, type Cp_two_phase_mix.
- **9** From the γ list, choose **User defined**.

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 eps_pores.
- 4 Locate the Heat Conduction, Porous Matrix section. From the $k_{\rm b}$ list, choose User defined. In the associated text field, type kappa_Ni.
- 5 Locate the Thermodynamics, Porous Matrix section. From the ρ_b list, choose User defined. In the associated text field, type rho_Ni.
- **6** From the $C_{p,b}$ list, choose **User defined**. In the associated text field, type Cp_Ni .

Periodic Condition I

- I In the Physics toolbar, click **Boundaries** and choose Periodic Condition.
- 2 Select Boundaries 23 and 54 only.

Inflow I

- I 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 Inlets.
- **4** Locate the **Upstream Properties** section. In the $T_{\rm ustr}$ text field, type T0.

Outflow I

- I 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 **Outlets**.
- 4 In the Model Builder window, collapse the Heat Transfer in Solids and Fluids (ht) node.

MULTIPHYSICS

All physics-interface settings are now complete. To finalize the physics setup, also the some settings on the multiphysics nodes are required. These nodes define couplings between the individual physics interfaces.

Mixture Model I (mfmm I)

- I In the Model Builder window, under Component I (compl)>Multiphysics click Mixture Model I (mfmm I).
- 2 In the Settings window for Mixture Model, locate the Model Input section.
- **3** From the T list, choose Common model input.
- 4 Locate the Physical Model section. From the Dispersed phase list, choose Liquid droplets/ bubbles.
- 5 Locate the Dispersed Phase 2 Properties section. From the ρ_{sg} list, choose Density of gas phase (we).
- 6 From the μ_{sg} list, choose User defined. In the associated text field, type we.mu.

Electrochemical Heating I (ech I)

In the Physics toolbar, click Authority Multiphysics Couplings and choose Domain> **Electrochemical Heating.**

GLOBAL DEFINITIONS

As a last step to finalize the physics settings, we will define the KOH concentration in the **Default Model Inputs** node. This concentration will be used for computing the KOH density in all nodes.

Default Model Inputs

- 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>Concentration (mol/m^3) minput.c.
- **4** Find the Expression for remaining selection subsection. In the Concentration text field, type c KOH.

MULTIPHYSICS

In the Model Builder window, collapse the Component I (compl)>Multiphysics node.

MESH I

A user-defined mesh will be used in this model. The extruded channel geometry is suitable for using a swept mesh. First we define the surface meshes on the faces that are to be used for sweeping.

Mapped I

- I In the Mesh toolbar, click \triangle More Generators and choose Mapped.
- 2 In the Settings window for Mapped, locate the Boundary Selection section.
- 3 From the Selection list, choose Mapped Mesh Boundaries.

Distribution 1

- I Right-click Mapped I and choose Distribution.
- **2** Select Edges 36, 45, 51, 60, 88, 94, 98, 104, and 201 only.

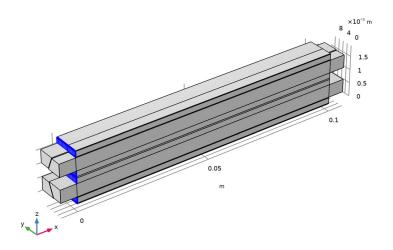
Distribution 2

- I In the Model Builder window, right-click Mapped I and choose Distribution.
- **2** Select Edges 33, 48, 63, 86, 96, 106, and 202 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 In the Number of elements text field, type 2.

Size 1

- I Right-click Mapped I and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** 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 W rib/10.

6 Click Build Selected.



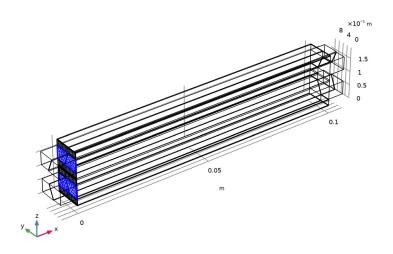
Free Triangular I

- I In the Mesh toolbar, click \times 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 Triangular Mesh Boundaries.

Size 1

- I Right-click Free Triangular I and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** 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/4.
- 6 Click Pauld Selected.

7 Click the Wireframe Rendering button in the Graphics toolbar.



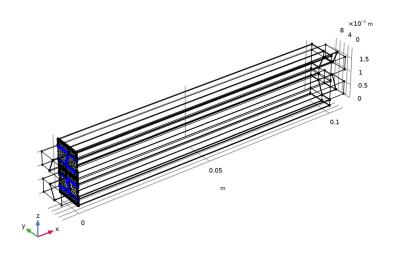
Boundary Layers 1

- 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 Boundary.
- 4 From the Selection list, choose Triangular Mesh Boundaries.

Boundary Layer Properties

- I In the Model Builder window, click Boundary Layer Properties.
- 2 In the Settings window for Boundary Layer Properties, locate the Edge Selection section.
- 3 From the Selection list, choose All edges.
- **4** Select Edges 43, 46, 55, 58, 68, 70, 72, 73, 75, 76, 82, and 84 only.
- 5 Locate the Layers section. In the Number of layers text field, type 2.
- 6 In the Stretching factor text field, type 1.5.
- 7 From the Thickness specification list, choose First layer.
- 8 In the Thickness text field, type H ch/50.

9 Click Build Selected.



Swept I

In the Mesh toolbar, click A Swept.

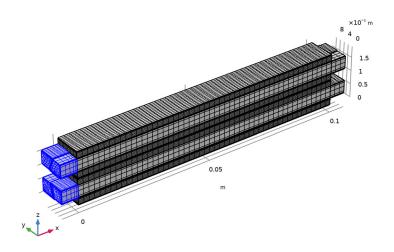
Size 1

- I Right-click Swept I and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** 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 W_ribch/ 10.

Distribution I

- I In the Model Builder window, right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 Click Clear Selection.
- **4** Select Domains 1–4 only.
- **5** Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.
- 6 In the Element ratio text field, type 4.
- 7 Click Build All.

8 Click the Wireframe Rendering button in the Graphics toolbar.



MESH I

In the Model Builder window, collapse the Component I (compl)>Mesh I node.

STUDY I

The problem is solved in three steps. The first step initializes the current distribution of the electrolyzer interface. The second step computes the flow profiles, excluding phase transport. The final step computes the solution for all physics, ramping up the cell voltage.

Step 3: Stationary 2

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

Stationary - Flow Initialization

- I In the Model Builder window, click Step 2: Stationary.
- 2 In the Settings window for Stationary, type Stationary Flow Initialization in the Label text field.
- 3 Locate the Physics and Variables Selection section. In the table, clear the Solve for check boxes for Water Electrolyzer (we), Phase Transport in Free and Porous Media Flow (phtr), and Heat Transfer in Solids and Fluids (ht).

Stationary 2- All Physics

I In the Model Builder window, click Step 3: Stationary 2.

- 2 In the Settings window for Stationary, type Stationary 2- All Physics in the Label text field.
- 3 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.
- 4 Click + Add.
- 5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E_cell (Cell voltage)	range(E_cell_lower,0.1, E_cell_upper)	V

Solution I (soll)

A fully coupled solver is suitable for this fairly small problem, and makes the simulation run faster.

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

DEFINITIONS

As a final step before solving, also add an average operator. It will be used later on when post-processing the solution.

Average I (aveop I)

- I In the Definitions toolbar, click Monlocal Couplings and choose Average.
- 2 In the Settings window for Average, locate the Source Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 54 only.

STUDY I

- I In the Model Builder window, click Study I.
- 2 In the Settings window for Study, locate the Study Settings section.
- 3 Clear the Generate default plots check box.
- 4 In the Home toolbar, click **Compute**.

Proceed as follows to reproduce all remaining figures from the model documentation:

RESULTS

Polarization Plot

- I In the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Polarization Plot in the Label text field.

Global I

- I Right-click Polarization Plot and choose Global.
- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

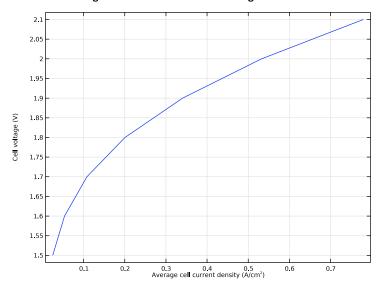
Expression	Unit	Description
E_cell	V	Cell voltage

- 4 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 5 In the Expression text field, type aveop1 (-we.nIl).
- 6 In the Unit field, type A/cm^2.

Polarization Plot

- I In the Model Builder window, click Polarization Plot.
- 2 In the Settings window for ID Plot Group, click to expand the Title section.
- **3** From the **Title type** list, choose **None**.
- 4 Locate the Plot Settings section.
- 5 Select the x-axis label check box. In the associated text field, type Average cell current density (A/cm²).

6 Locate the Legend section. Clear the Show legends check box.



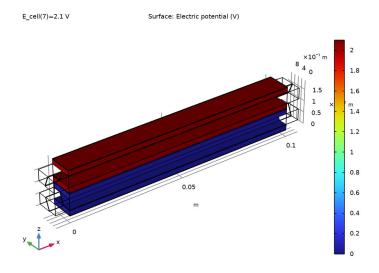
Electrode Phase Potential

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Electrode Phase Potential in the Label text field.

Surface I

- I Right-click Electrode Phase Potential 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 I (compl)> Water Electrolyzer>we.phis - Electric potential - V.

3 In the Electrode Phase Potential toolbar, click Plot.



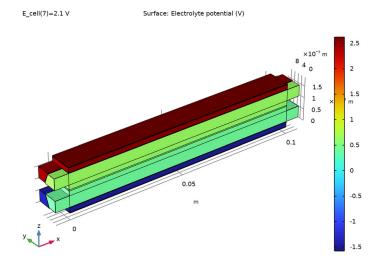
Electrolyte Phase Potential

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Electrolyte Phase Potential in the Label text field.

Surface I

- I Right-click Electrolyte Phase Potential and choose Surface.
- 2 In the Electrolyte Phase Potential toolbar, click Plot.

3 In the Model Builder window, click Surface 1.



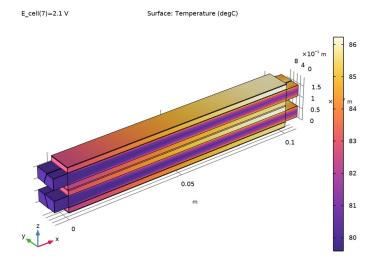
Temperature

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Temperature in the Label text field.

Surface I

- I Right-click Temperature 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 I (compl)> Heat Transfer in Solids and Fluids>Temperature>T - Temperature - K.
- 3 Locate the Expression section. From the Unit list, choose degC.
- 4 Locate the Coloring and Style section. Click Change Color Table.
- 5 In the Color Table dialog box, select Thermal>HeatCameraLight in the tree.
- 6 Click OK.

7 In the Temperature toolbar, click Plot.



Gas Volume Fraction in Channels

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Gas Volume Fraction in Channels in the Label text field.

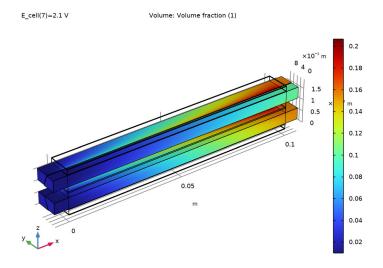
Volume 1

- I Right-click Gas Volume Fraction in Channels 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 I (compl)> Phase Transport in Free and Porous Media Flow>s_g - Volume fraction - 1.
- 3 Locate the Coloring and Style section. Click | Change Color Table.
- 4 In the Color Table dialog box, select Rainbow>Prism in the tree.
- 5 Click OK.

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 Channels.

4 In the Gas Volume Fraction in Channels toolbar, click Plot.



Gas Volume Fraction in Channels

In the Model Builder window, under Results right-click Gas Volume Fraction in Channels and choose **Duplicate**.

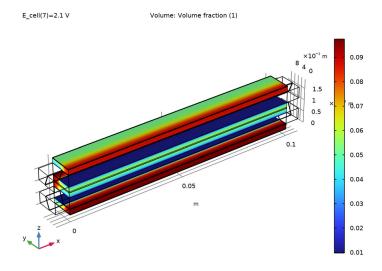
Gas Volume Fraction in GDEs

- I In the Model Builder window, under Results click Gas Volume Fraction in Channels I.
- 2 In the Settings window for 3D Plot Group, type Gas Volume Fraction in GDEs in the Label text field.
- 3 In the Model Builder window, expand the Gas Volume Fraction in GDEs node.

Selection I

- I In the Model Builder window, expand the Results>Gas Volume Fraction in GDEs>Volume I node, then click Selection 1.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose GDEs.

4 In the Gas Volume Fraction in GDEs toolbar, click Plot.



Gas Volume Fractions and Streamlines

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Gas Volume Fractions and Streamlines in the Label text field.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the Plot Settings section. Clear the Plot dataset edges check box.

Streamline I

- I Right-click Gas Volume Fractions and Streamlines and choose Streamline.
- 2 In the Settings window for Streamline, locate the Expression section.
- 3 In the x-component text field, type Ngasx.
- 4 In the **y-component** text field, type Ngasy.
- 5 In the **z-component** text field, type Ngasz.
- 6 Locate the Streamline Positioning section. From the Positioning list, choose Magnitude controlled.
- 7 In the Minimum distance text field, type 0.02.
- 8 Locate the Coloring and Style section. Find the Line style subsection. From the Type list, choose Ribbon.
- **9** Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

Color Expression 1

- I Right-click Streamline I and choose Color Expression.
- 2 In the Settings window for Color Expression, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Phase Transport in Free and Porous Media Flow>s_g - Volume fraction - 1.

Selection 1

- I In the Model Builder window, right-click Streamline I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Oxygen Channels.
- 4 In the Gas Volume Fractions and Streamlines toolbar, click **1** Plot.

Streamline 1

Right-click Streamline I and choose Duplicate.

Color Expression 1

- I In the Model Builder window, expand the Streamline 2 node, then click Color Expression I.
- 2 In the Settings window for Color Expression, locate the Coloring and Style section.
- 3 Click Change Color Table.
- **4** In the **Color Table** dialog box, select **Wave>Disco** in the tree.
- 5 Click OK.

Selection I

- I In the Model Builder window, click Selection I.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Hydrogen Channels.

Surface 1

- I In the Model Builder window, right-click Gas Volume Fractions and Streamlines and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- **3** In the **Expression** text field, type 1.

Selection 1

- I Right-click Surface I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.

- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Separators.

Material Appearance 1

- I In the Model Builder window, right-click Surface I and choose Material Appearance.
- 2 In the Settings window for Material Appearance, locate the Appearance section.
- 3 From the Appearance list, choose Custom.

Surface 1

Right-click **Surface I** and choose **Duplicate**.

Selection 1

- I In the Model Builder window, expand the Surface 2 node, then click Selection I.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose GDEs.

Material Appearance 1

- I In the Model Builder window, click Material Appearance I.
- 2 In the Settings window for Material Appearance, locate the Appearance section.
- 3 From the Material type list, choose Carbon (forged).

Surface 2

In the Model Builder window, right-click Surface 2 and choose Duplicate.

Selection 1

- I In the Model Builder window, expand the Surface 3 node, then click Selection I.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Bipolar Plates.

Material Appearance 1

- I In the Model Builder window, click Material Appearance I.
- 2 In the Settings window for Material Appearance, locate the Appearance section.
- 3 From the Material type list, choose Steel.

