



Two-Phase Flow in a Polymer Electrolyte Membrane Fuel Cell

Introduction

In a polymer electrolyte membrane fuel cell (PEMFC), water is produced at the cathode, and the cell is usually also fed with water vapor via the inlet gas streams.

This tutorial investigates the effects of water condensation in a polymer electrolyte membrane fuel cell with parallel flow channels.

In the model, condensation may result due to production of water at the cathode, but also due to the removal of other reactant species (H_2 or O_2) from the gas mixtures.

The resulting two-phase flow, fully coupled to the cell current distribution and mass transfer, is included in both the channels and the gas diffusion layers.

Model Definition

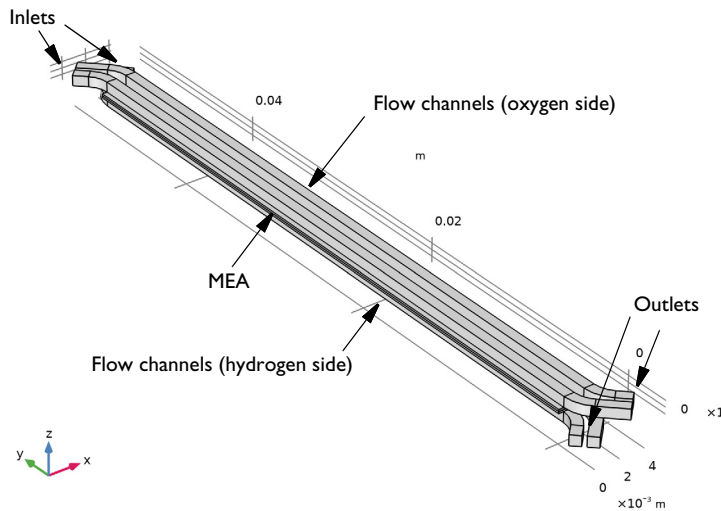


Figure 1: Model geometry.

Figure 1 shows the full model geometry. The cell geometry consists of two parallel flow channels on each side of the membrane-electrode-assembly (MEA). The MEA is defined as three rectangular block domains defining the hydrogen-side gas diffusion layer (GDL), the membrane and the oxygen-side GDL.

The model is setup using the **Hydrogen Fuel Cell** interface together with the **Free and Porous Multiphase Flow** multiphysics interface.

VOLUME FRACTIONS

The **Phase Transport in Free and Porous Media Flow** interface solves for the relative liquid water volume fraction s_w in the gas pores in the GDLs and the channels. The relative gas volume fraction is then defined as

$$s_g = 1 - s_w$$

As liquid water condenses in the GDLs and is transported out to the channels, the volume fraction of gas decreases, making room for the produced liquid.

In the GDLs, the gas volume fraction ε_g is defined as

$$\varepsilon_g = s_g \varepsilon_{\text{por}}$$

where ε_{por} is the pore volume fraction relative to the total volume.

HYDROGEN FUEL CELL INTERFACE

The current distribution, electrochemical and water condensation-evaporation reactions are defined using the **Hydrogen Fuel Cell** interface. The gas diffusion electrode reactions are modeled using Butler–Volmer kinetics. Ohmic losses in the electrode and electrolyte phases are included. Electroosmotic water drag is enabled in the model, allowing for membrane transport of water between the oxygen and hydrogen compartment.

The fuel cell part of the model is very similar to the [Low-Temperature PEM Fuel Cell with Serpentine Flow Field](#) tutorial and more details about the setup of the Hydrogen Fuel Cell interface can be found in this example.

Gas diffusion in relation to the mass-averaged gas-phase velocity is defined by the fuel cell interface, solving for the mass fractions of the gas species in the gas mixtures, whereas the mass-averaged velocity and pressure are defined by the **Darcy's Law** and **Laminar Flow** interfaces (see below).

The effective gas diffusivities in the GDLs on each side of the membrane is set to depend on the electrolyte volume fraction according to

$$D_{ij, \text{eff}} = \varepsilon_g^{3/2} D_{ij} \quad (1)$$

where D_{ij} are the binary (bulk) diffusivities of the gas species.

In the channels, the water volume fraction is assumed to be so low that the impact on the gas diffusivity may be neglected.

An average cell current density of 1 A/cm^2 is applied on the cathode current conductor.

The cell fed with humidified air and hydrogen mixtures, humidified to 100% relative humidity (RH).

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 pressure in the GDLs
- **Laminar Flow**, solving for the gas pressure and velocity field in the channels
- **Phase Transport in Free and Porous Media Flow**, solving for the liquid water 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 GDLs
- **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 **Hydrogen Fuel Cell** interface, are added as a **Mass Source** node in the **Phase Transport in Free and Porous Media Flow** interface. **Turbulent Mixing** is added in the channels in the **Phase Transport in Free and Porous Media Flow** interface in order to facilitate convergence.

Fully-developed flow conditions are defined on the **Inlet** nodes in the **Laminar Flow** interface, specifying mass flow rates corresponding to a hydrogen and oxygen stoichiometry of 2 and 2.5, respectively. A uniform absolute outlet pressure of 1 atm is defined on the **Outlet** node in the same interface.

CAPILLARY PRESSURE AND RESIDUAL SATURATION

In the GDLs, the liquid water transport will be governed by the capillary pressure and the relative permeabilities of the two phases, both being functions of the water saturation level as defined on the **Porous Medium>Fluid** node of the **Phase Transport in Free and Porous Media**

Flow interface. In this tutorial, the **Brooks and Corey** model is used, using parameters found in [Ref. 1](#).

The residual saturation, s_{rs} (dimensionless), defines the amount of liquid water remaining in the porous structure at zero capillary pressure. One reason for the remaining water is the formation of a thin water film on the pore wall surfaces within the matrix, also at relative humidities below 100%. Assuming the film thickness to scale linearly with the relative humidity, we use the following relation between the relative humidity and the residual saturation

$$s_{rs} = RH s_{rs, 100\% RH} \quad (2)$$

where $s_{rs, 100\%RH}$ is the residual saturation at 100% relative humidity, and RH is the relative humidity, regularized between 0 and 100%.

The variable s_{rs} is used both in the Brooks and Corey model for the capillary pressure and permeabilities, and as a boundary condition for setting the liquid saturation level at the GDL-channel boundaries.

WATER CONDENSATION AND EVAPORATION

Due to the significantly larger internal surface area of the GDLs in comparison to the channels, water is assumed to condensate or evaporate in the GDL domains only.

The rate expression for water condensation is defined as

$$r_{cc} = k_w (a_{H_2O(g)} - a_{H_2O(l)}) \quad (3)$$

where k_w is a rate constant and $a_{H_2O(g)}$ and $a_{H_2O(l)}$ are the thermodynamic activities of water in the gas and liquid phases, respectively.

The gas phase thermodynamic activity is related to the partial pressure of gaseous water as

$$a_{H_2O(g)} = \frac{p_{H_2O(g)}}{1 \text{ atm}} \quad (4)$$

whereas the thermodynamic liquid water activity is related to the water vapor pressure as

$$a_{H_2O(l)} = \frac{p_{vap}}{1 \text{ atm}} \quad (5)$$

for the case when the liquid saturation level is higher than the residual saturation at 100% RH ($s_w > s_{rs, 100\%RH}$). When the liquid saturation is lower than the residual saturation ($s_w < s_{rs, 100\%RH}$) at 100% RH, the liquid water activity is defined as

$$a_{\text{H}_2\text{O}(l)} = \frac{s_w}{s_{rs, 100\% \text{ RH}}} \frac{P_{\text{vap}}}{1 \text{ atm}} \quad (6)$$

STUDY

Four consecutive study steps are used to solve the model. 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, neglecting nonlinear activation overpotentials.
- The second **Current Distribution Initialization** step includes nonlinear activation overpotentials.
- A third **Stationary** step then solves for the pressures and velocity fields of the **Darcy's Law** and **Laminar Flow** interfaces only, with all resulting mass sources from the fuel cell model disabled.
- The fourth and final **Time Dependent** step solves for the fully coupled problem using a time-dependent solver, representing the transient behavior of the cell during 60 s after a current step going from a 0 to 1 A/cm² average cell current density at $t = 0$ s.

Results and Discussion

Figure 2 shows the cell voltage versus time. The lowered cell voltage over time is due to a lowered oxygen partial pressure at the cathode. It takes about 10 s before a steady-state voltage establishes.

Figure 3 shows the cross-membrane current density at the end of the simulation. The current density decreases toward the outlet. As we will see, this is also related to the oxygen partial pressure.

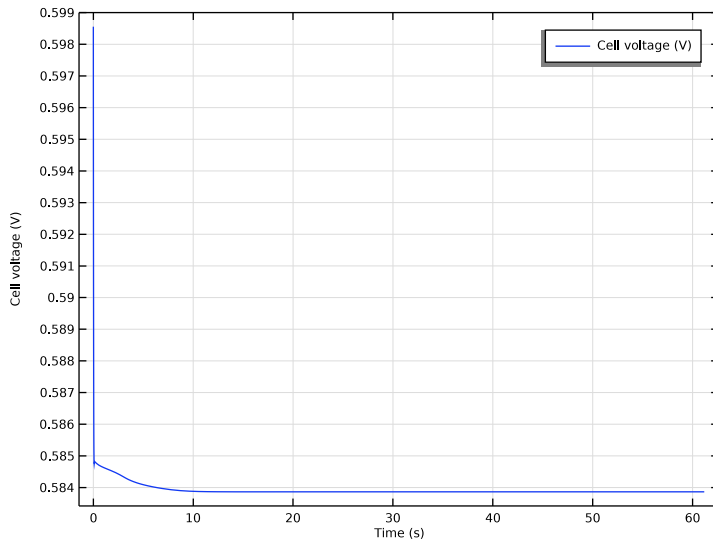


Figure 2: Cell voltage versus time.

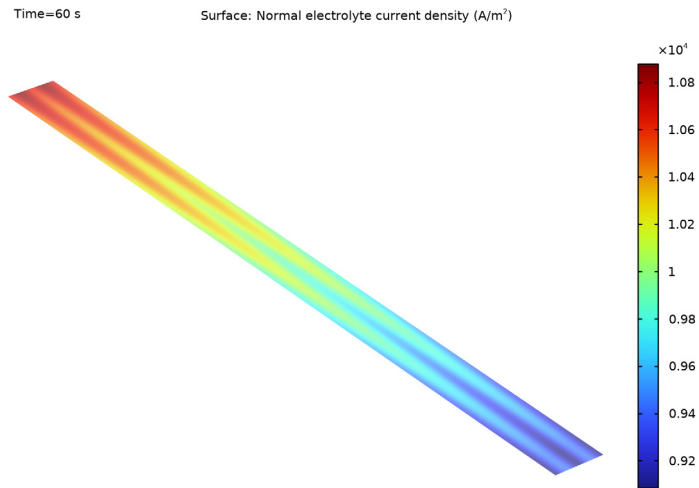


Figure 3: Cross-membrane current density.

Figure 4 and Figure 5 show the hydrogen and oxygen molar fractions in the cell at the end of the simulation, respectively.

The hydrogen molar fraction is more or less uniform in Figure 4. This is a result of continuous condensation of water as hydrogen is oxidized and removed from the fuel stream, maintaining a relative humidity close to 100%.

The oxygen molar fraction in Figure 5 on the other hand decreases gradually toward the outlet. Also here the relative humidity remains close to 100%, but as oxygen is reduced and removed from the oxidant stream, the molar fraction of nitrogen increases.

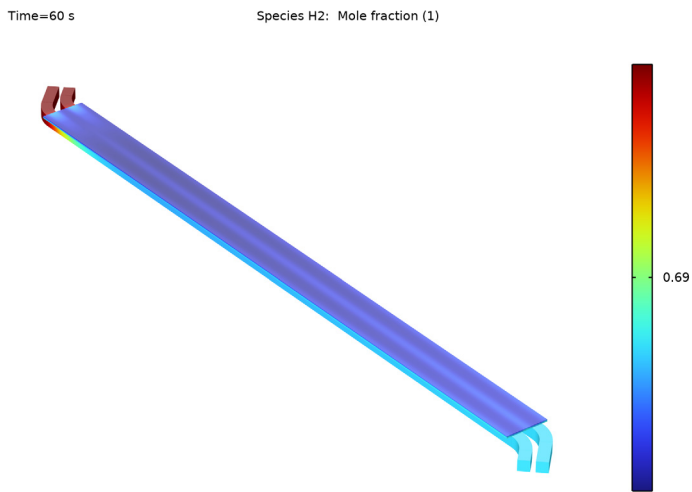


Figure 4: Hydrogen molar fraction.

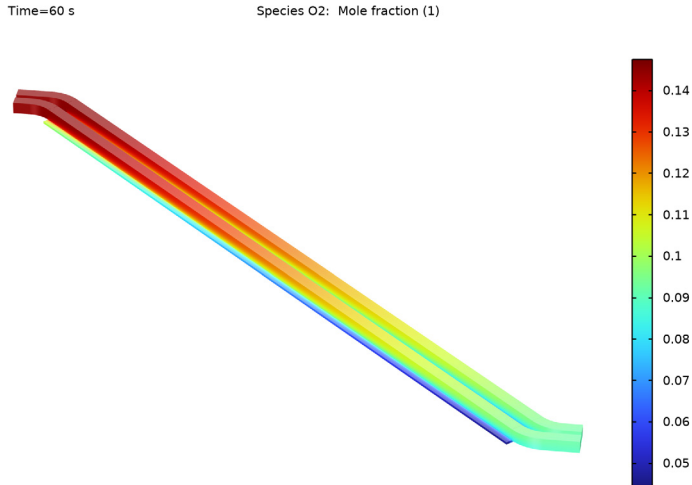


Figure 5: Oxygen molar fraction.

[Figure 6](#) shows the velocity magnitude in the channels. On the oxygen side, the velocity magnitude decreases slightly toward the outlet. This results from oxygen being removed from the gaseous oxidant stream. However, since the relative molar fraction of oxygen is relatively low, the relative velocity decrease is limited. On the hydrogen side, the velocity decrease is more significant.

Finally, the liquid water volume fraction in the GDLs and channels are shown in [Figure 7](#). The liquid water volume fraction is generally low in the channels, this is directly related to the orders of magnitudes larger density of the liquid phase.

The volume fraction increases slightly toward the outlet side, and interestingly it is slightly higher in the hydrogen channels, compared to the oxygen side. This is a result of the relatively larger volumetric utilization of hydrogen gas stream.

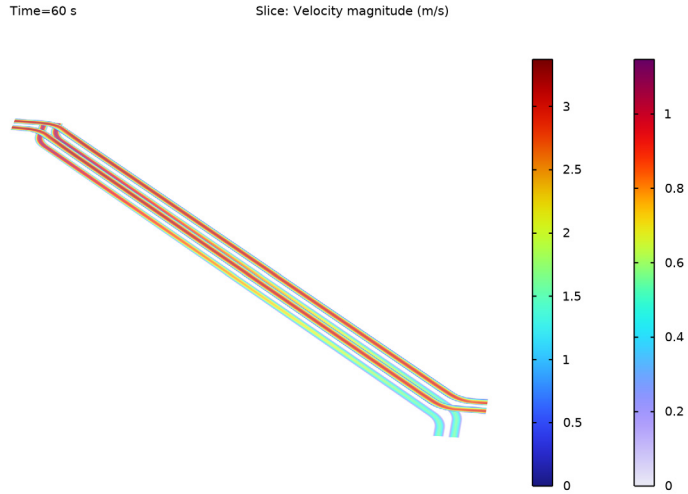


Figure 6: Velocity magnitude in channels.

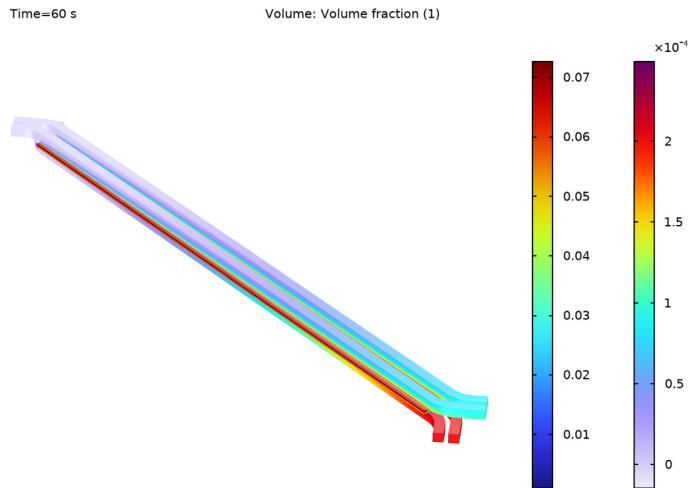


Figure 7: Liquid volume fraction.

Reference


1. N. Zamel, X. Li, J. Becker, and A. Wiegmann, “Effect of liquid water on transport properties of the gas diffusion layer of polymer electrolyte membrane fuel cells,” *Int. J. Hydrogen Energy*, vol. 36, no. 9, pp. 5466–5478, 2011.

Application Library path: Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/
two_phase_pemfc


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 In the **Select Physics** tree, select **Electrochemistry** > **Hydrogen Fuel Cells** > **Proton Exchange Membrane (fc)**.

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 **Added physics interfaces** tree, select **Phase Transport in Free and Porous Media Flow (phtr)**.

7 In the **Volume fractions (1)** table, enter the following settings:

s_g

s_w

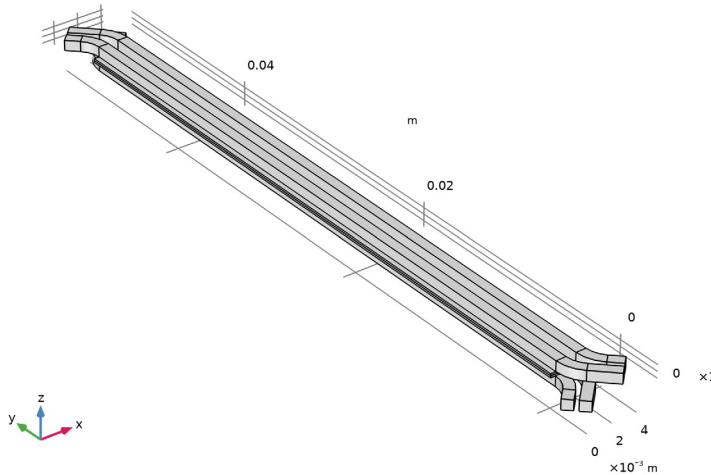
8 Click  **Study**.

9 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Hydrogen Fuel Cell** > **Time Dependent with Initialization**.

10 Click  **Done**.

GEOMETRY I

- 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 `two_phase_pemfc_geom_sequence.mph`.
- 3 In the **Model Builder** window, under **Component I (comp1)** click **Geometry I**.



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

GLOBAL DEFINITIONS

Geometry Parameters


- 1 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


- 1 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.
- 3 Locate the **Parameters** section. Click **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `two_phase_pemfc_physics_parameters.txt`.

DEFINITIONS

GDL Variables



- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type `GDL Variables` 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 **GDLs**.
- 5 Locate the **Variables** section. Click  **Load from File**.
- 6 Browse to the model's Application Libraries folder and double-click the file `two_phase_pemfc_gdl_variables.txt`.

Channel Variables

- 1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type `Channel Variables` 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 `two_phase_pemfc_channel_variables.txt`.

The two variable nodes you just added define the absolute pressure (pA) and velocity (U/V/W) differently in the channels and gdl, respectively. These variables will be used to define the gas phase properties in the **Hydrogen Fuel Cell** interface.

ADD MATERIAL

- 1 In the **Materials** 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 > Polymer Electrolytes > Nafion®**, EW 1100, Vapor Equilibrated, Protonated.
- 4 Right-click and choose **Add to Component 1 (comp1)**.
- 5 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.

MATERIALS

Nafion®, EW 1100, Vapor Equilibrated, Protonated (mat1)

- 1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 2 From the **Selection** list, choose **Membrane**.

Nafion®, EW 1100, Vapor Equilibrated, Protonated 1 (mat2)

- 1 Right-click **Component 1 (comp1)** > **Materials** > **Nafion®**, EW 1100, Vapor Equilibrated, Protonated (mat1) and choose **Duplicate**.

Two instances of the Nafion material is required for this model. The domain node defines the transport properties (such as conductivity) of the membrane, and the boundary node defines the water adsorption-desorption properties between the membrane and the gas phase.

- 2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 From the **Selection** list, choose **GDEs**.


HYDROGEN FUEL CELL (FC)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Hydrogen Fuel Cell (fc)**.
- 2 In the **Settings** window for **Hydrogen Fuel Cell**, locate the **H2 Gas Mixture** section.
- 3 Find the **Reactions** subsection. Select the **Include H2O(l) in reaction stoichiometry** checkbox.
- 4 Locate the **O2 Gas Mixture** section. Select the **Include H2O(l) in reaction stoichiometry** checkbox.

Enabling the above checkboxes allows for defining rate expressions for liquid water due to evaporation-condensation.

- 5 Click to expand the **Membrane Transport** section. Select the **Electroosmotic water drag** checkbox.

Membrane 1

- 1 In the **Physics** toolbar, click  **Domains** and choose **Membrane**.
- 2 In the **Settings** window for **Membrane**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Membrane**.

Initial Values 1

- 1 In the **Model Builder** window, expand the **Membrane 1** node, then click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.


- 3 In the $a_{w,0}$ text field, type RH.
- 4 In the T_0 text field, type T.

HYDROGEN FUEL CELL (FC)

Membrane 1

In the **Model Builder** window, collapse the **Component 1 (comp1) > Hydrogen Fuel Cell (fc) > Membrane 1** node.


H2 Gas Diffusion Layer 1

- 1 In the **Physics** toolbar, click  **Domains** and choose **H2 Gas Diffusion Layer**.
- 2 In the **Settings** window for **H2 Gas Diffusion Layer**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Hydrogen GDL**.
- 4 Locate the **Electrode Charge Transport** section. From the list, choose **Diagonal**.
- 5 Specify the σ_s matrix as

sigmas_gdl_IP	0	0
0	sigmas_gdl_IP	0
0	0	sigmas_gdl_TP

- 6 Locate the **Gas Transport** section. In the ϵ_g text field, type epsg_gdl.


O2 Gas Diffusion Layer 1

- 1 In the **Physics** toolbar, click  **Domains** and choose **O2 Gas Diffusion Layer**.
- 2 In the **Settings** window for **O2 Gas Diffusion Layer**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Oxygen GDL**.
- 4 Locate the **Electrode Charge Transport** section. From the list, choose **Diagonal**.
- 5 Specify the σ_s matrix as

sigmas_gdl_IP	0	0
0	sigmas_gdl_IP	0
0	0	sigmas_gdl_TP

- 6 Locate the **Gas Transport** section. In the ϵ_g text field, type epsg_gdl.

Thin H2 Gas Diffusion Electrode 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Thin H2 Gas Diffusion Electrode**.
- 2 In the **Settings** window for **Thin H2 Gas Diffusion Electrode**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Hydrogen GDE**.

4 Locate the **Electrode Thickness** section. In the d_{gde} text field, type H_c1.

Thin H2 Gas Diffusion Electrode Reaction I

1 In the **Model Builder** window, click **Thin H2 Gas Diffusion Electrode Reaction I**.

2 In the **Settings** window for **Thin H2 Gas Diffusion Electrode Reaction**, locate the **Electrode Kinetics** section.

3 In the $i_{0,ref}(T)$ text field, type i0_ref_HOR.

4 Locate the **Active Specific Surface Area** section. In the a_v text field, type Av_HOR.

Thin O2 Gas Diffusion Electrode I

1 In the **Physics** toolbar, click  **Boundaries** and choose **Thin O2 Gas Diffusion Electrode**.

2 In the **Settings** window for **Thin O2 Gas Diffusion Electrode**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Oxygen GDE**.

4 Locate the **Electrode Thickness** section. In the d_{gde} text field, type H_c1.

Thin O2 Gas Diffusion Electrode Reaction I

1 In the **Model Builder** window, click **Thin O2 Gas Diffusion Electrode Reaction I**.

2 In the **Settings** window for **Thin O2 Gas Diffusion Electrode Reaction**, locate the **Electrode Kinetics** section.

3 In the $i_{0,ref}(T)$ text field, type i0_ref_ORR.

4 In the α_a text field, type alphaa_ORR.

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

H2 Gas Flow Channel I

1 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 **Hydrogen Channels**.

O2 Gas Flow Channel I

1 In the **Physics** toolbar, click  **Domains** and choose **O2 Gas Flow Channel**.


2 In the **Settings** window for **O2 Gas Flow Channel**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Oxygen Channels**.

Electronic Conducting Phase I

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


Electric Ground 1

- 1 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 **Anode Current Collector**.

Electronic Conducting Phase 1

In the **Model Builder** window, click **Electronic Conducting Phase 1**.

Electrode Current 1


- 1 In the **Physics** toolbar, click  **Attributes** and choose **Electrode Current**.
- 2 In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.
- 3 In the $I_{s,total}$ text field, type $-I_{cell}$.
- 4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Cathode Current Collector**.

H2 Gas Phase 1

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Hydrogen Fuel Cell (fc)** click **H2 Gas Phase 1**.
- 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 .
- 4 Locate the **Convection** section. Specify the **u** vector as

U	x
V	y
W	z


H2 Inlet 1

- 1 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 **Hydrogen Inlets**.

H2 Gas Phase 1

In the **Model Builder** window, click **H2 Gas Phase 1**.


H2 Outlet 1

- 1 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 **Hydrogen Outlets**.

H2 Gas Phase I

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

Water Condensation-Evaporation I

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Water Condensation-Evaporation**.
- 2 In the **Settings** window for **Water Condensation-Evaporation**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Hydrogen GDL**.
- 4 Locate the **Condensation-Evaporation Rate** section. From the r_{ce} list, choose **User defined**. In the text field, type r_c .

Initial Values I


- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Composition** section.
- 3 From the **Mixture specification** list, choose **Humidified mixture**.
- 4 In the RH_{hum} text field, type RH .
- 5 In the T_{hum} text field, type T .

O2 Gas Phase I

- 1 In the **Model Builder** window, under **Component 1 (comp 1) > Hydrogen Fuel Cell (fc)** click **O2 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 p_A .
- 4 Locate the **Convection** section. Specify the **u** vector as

U	x
V	y
W	z


O2 Inlet I

- 1 In the **Physics** toolbar, click  **Attributes** and choose **O2 Inlet**.
- 2 In the **Settings** window for **O2 Inlet**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Oxygen Inlets**.

O2 Gas Phase I

In the **Model Builder** window, click **O2 Gas Phase I**.


O2 Outlet 1

- 1 In the **Physics** toolbar, click  **Attributes** and choose **O2 Outlet**.
- 2 In the **Settings** window for **O2 Outlet**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Oxygen Outlets**.

O2 Gas Phase 1

In the **Model Builder** window, click **O2 Gas Phase 1**.

Water Condensation-Evaporation 1

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Water Condensation-Evaporation**.
- 2 In the **Settings** window for **Water Condensation-Evaporation**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Oxygen GDL**.
- 4 Locate the **Condensation-Evaporation Rate** section. From the r_{ce} list, choose **User defined**.
In the text field, type r_c .

Initial Values 1

- 1 In the **Model Builder** window, click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Composition** section.
- 3 From the **Mixture specification** list, choose **Humidified air**.
- 4 In the RH_{hum} text field, type RH.
- 5 In the T_{hum} text field, type T.

HYDROGEN FUEL CELL (FC)


In the **Model Builder** window, collapse the **Component 1 (comp1) > Hydrogen Fuel Cell (fc)** node.

LAMINAR FLOW (SPF)

The settings of the fuel cell interface are now complete. Proceed to set up the conditions for the flow in the channels.


- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.
- 2 In the **Settings** window for **Laminar Flow**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Channels**.

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 **Oxygen Inlets**.
- 4 Locate the **Boundary Condition** section. From the list, choose **Mass flow**.
- 5 Clear the **Apply condition on each disjoint selection separately** checkbox.
Disabling the above checkbox means that a common pressure will be applied on all inlet boundaries. The pressure will be set so that it fulfills the total mass flow M_{cath} specified.
- 6 Locate the **Mass Flow** section. In the m text field, type M_{cath} .

Inlet 2

- 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 **Hydrogen Inlets**.
- 4 Locate the **Boundary Condition** section. From the list, choose **Mass flow**.
- 5 Clear the **Apply condition on each disjoint selection separately** checkbox.
- 6 Locate the **Mass Flow** section. In the m text field, type M_{an} .

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 **Outlets**.

LAMINAR FLOW (SPF)

In the **Model Builder** window, collapse the **Component 1 (comp1) > Laminar Flow (spf)** node.

DARCY'S LAW (DL)

Darcy's law is used in this model to define the pressure and velocity field in the gdl.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** 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 **GDLs**.

Porous Matrix 1

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Darcy's Law (dl) > Porous Medium 1** click **Porous Matrix 1**.
- 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_gdl .
- 4 From the κ list, choose **User defined**. In the associated text field, type $perm_gdl$.

5 In the **Model Builder** window, collapse the **Darcy's Law (dl)** node.

PHASE TRANSPORT IN FREE AND POROUS MEDIA FLOW (PHTR)


The phase transport model solves for the volume fraction of liquid water in the channels and the gdl's.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** 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 **Flow Domains**.

Fluid 1

In the **Model Builder** window, under **Component 1 (comp1)** > **Phase Transport in Free and Porous Media Flow (phtr)** click **Fluid 1**.

Turbulent Mixing 1

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Turbulent Mixing**.
- 2 In the **Settings** window for **Turbulent Mixing**, locate the **Turbulent Mixing Parameters** section.
- 3 In the v_T text field, type D_{eddy} .
- 4 In the Sc_T text field, type 1.

Porous Medium 1


- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Phase Transport in Free and Porous Media Flow (phtr)** click **Porous Medium 1**.
- 2 In the **Settings** window for **Porous Medium**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **GDLs**.

Fluid 1


- 1 In the **Model Builder** window, click **Fluid 1**.
- 2 In the **Settings** window for **Fluid**, locate the **Capillary Pressure** section.
- 3 From the **Capillary pressure model** list, choose **Brooks and Corey**.
- 4 In the p_{ec} text field, type p_{BC} .
- 5 In the λ_p text field, type λ_{BC} .
- 6 Locate the **Phase 1 Properties** section. From the ρ_{sg} list, choose **Density of gas phase (fc)**.
- 7 From the μ_{sg} list, choose **Dynamic viscosity of gas phase (fc)**.

- 8 Locate the **Phase 2 Properties** section. From the ρ_{sw} list, choose **Density of liquid water (fc)**.
- 9 From the μ_{sw} list, choose **Dynamic viscosity of liquid water (fc)**.
- 10 In the s_{rsw} text field, type `sw_res`.


Initial Values - GDLs

- 1 In the **Physics** toolbar, click  **Domains** and choose **Initial Values**.
- 2 In the **Settings** window for **Initial Values**, type Initial Values - GDLs in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **GDLs**.
- 4 Locate the **Initial Values** section. In the $s_{0,sw}$ text field, type `sw_res_100_aw*RH`.

Volume Fraction I

- 1 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_w** checkbox.


Outflow I

- 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 **Outlets**.

Mass Source I


Use a **Mass Source** node to add the gas and liquid phase mass sources defined by the **Hydrogen Fuel Cell** interface.

By enabling the **Mass transfer to other phases** checkbox, the net mass source (or sink) will also be added to the **Darcy's law** interface via the **Multiphase Flow in Porous Media** multiphysics node.

- 1 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 **GDLs**.
- 4 Locate the **Mass Source** section. Select the **Mass transfer to other phases** checkbox.
- 5 From the Q_{sg} list, choose **Mass source, gas phase (fc)**.
- 6 From the Q_{sw} list, choose **Mass source, liquid phase (fc)**.

Boundary Mass Source 1

Use a **Boundary Mass Source** node to add the gas and liquid phase mass sources defined by the **Hydrogen Fuel Cell** interface.

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Boundary Mass Source**.
- 2 In the **Settings** window for **Boundary Mass Source**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **GDEs**.
- 4 Locate the **Boundary Mass Source** section. From the $q_{b,sg}$ list, choose **Boundary mass source, gas phase (fc)**.
- 5 From the $q_{b,sw}$ list, choose **Boundary mass source, liquid phase (fc)**.

PHASE TRANSPORT IN FREE AND POROUS MEDIA FLOW (PHTR)

In the **Model Builder** window, collapse the **Component 1 (comp1)** > **Phase Transport in Free and Porous Media Flow (phtr)** node.

MULTIPHYSICS

Mixture Model 1 (mfmm1)

The mixture model defines the two-phase properties in the channels.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Multiphysics** click **Mixture Model 1 (mfmm1)**.
- 2 In the **Settings** window for **Mixture Model**, locate the **Physical Model** section.
- 3 From the **Dispersed phase** list, choose **Liquid droplets/bubbles**.
- 4 Locate the **Continuous Phase Properties** section. From the ρ_c list, choose **Density of gas phase (fc)**.
- 5 From the μ_c list, choose **Dynamic viscosity of gas phase (fc)**.
- 6 Locate the **Dispersed Phase 2 Properties** section. From the ρ_{sw} list, choose **Density of liquid water (fc)**.
- 7 From the μ_{sw} list, choose **Dynamic viscosity of liquid water (fc)**.

GLOBAL DEFINITIONS

Default Model Inputs

Define the temperature on the **Default Model Inputs** node in order to use the same temperature setting on all nodes in the model.

- 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.

MULTIPHYSICS


In the **Model Builder** window, collapse the **Component 1 (comp1) > Multiphysics** node.

MESH 1

The physics settings are now complete. Now create a mesh by sweeping the oxygen channels first, then through the GDLs and membrane, and finally the hydrogen channels.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
- 2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.
- 3 From the list, choose **User-controlled mesh**.
- 4 In the **Mesh** toolbar, click  **Clear Sequence**.


Mapped 1

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Mapped**.
- 2 In the **Settings** window for **Mapped**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlets**.

Distribution 1

- 1 Right-click **Mapped 1** and choose **Distribution**.
- 2 In the **Settings** window for **Distribution**, locate the **Edge Selection** section.
- 3 From the **Selection** list, choose **All edges**.
- 4 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 8.
- 6 In the **Element ratio** text field, type 2.
- 7 Select the **Symmetric distribution** checkbox.

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 From the **Selection** list, choose **Oxygen Channels**.




Size 1

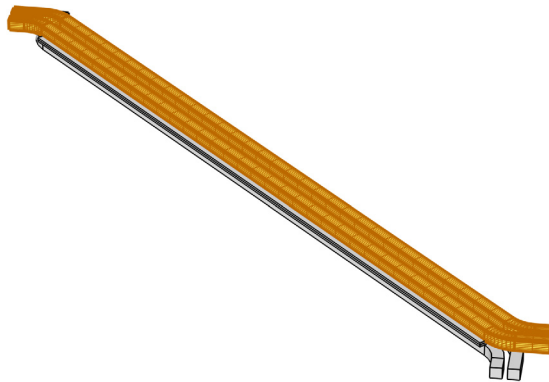
- 1 Right-click **Swept 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 Click the **Custom** button.
- 4 Locate the **Element Size Parameters** section.
- 5 Select the **Maximum element size** checkbox. In the associated text field, type W_{ribch} .

Size 2


- 1 In the **Model Builder** window, right-click **Swept 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Selection** list, choose **Bends**.
- 4 Locate the **Element Size** section. Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section.
- 6 Select the **Maximum element size** checkbox. In the associated text field, type $H_{ch}/3$.

Swept 1

- 1 Right-click **Swept 1** and choose **Build Selected**.
- 2 Click the  **Show Axis Orientation** button in the **Graphics** toolbar.
- 3 Click the  **Show Grid** button in the **Graphics** toolbar.
- 4 Click the  **Zoom Extents** button in the **Graphics** toolbar.



Mapped 2

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Mapped**.
- 2 In the **Settings** window for **Mapped**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Cathode Current Collector**.



Size 1

- 1 Right-click **Mapped 2** 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** checkbox. In the associated text field, type $W_{rib}/10$.


Mapped 2

In the **Model Builder** window, right-click **Mapped 2** and choose **Build Selected**.

Copy Face 1

- 1 In the **Mesh** toolbar, click  **Copy** and choose **Copy Face**.
- 2 In the **Settings** window for **Copy Face**, locate the **Source Boundaries** section.
- 3 From the **Selection** list, choose **Oxygen GDL Top Boundaries**.
- 4 Locate the **Destination Boundaries** section. From the **Selection** list, choose **Hydrogen GDL Bottom Boundaries**.
- 5 Click  **Build Selected**.

Swept 2

- 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 7–9 only.

Distribution 1

- 1 Right-click **Swept 2** and choose **Distribution**.
- 2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **GDLs**.
- 4 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 10.
- 6 In the **Element ratio** text field, type 3.

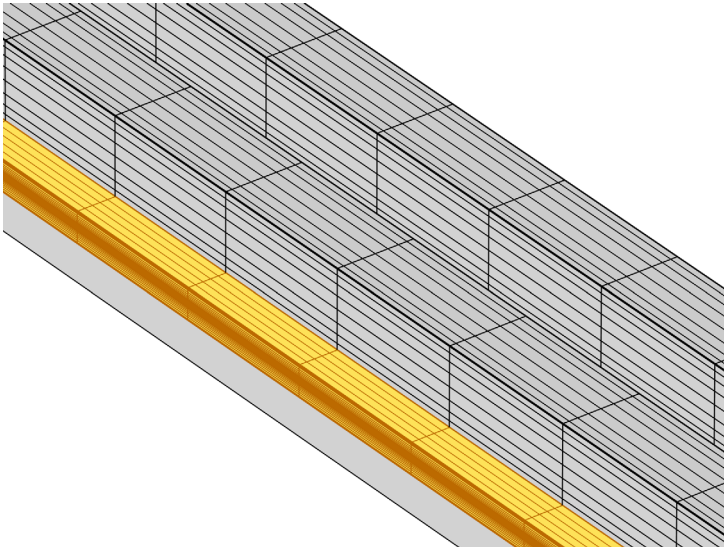
7 Select the **Reverse direction** checkbox.

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 From the **Selection** list, choose **Membrane**.
- 4 Locate the **Distribution** section. In the **Number of elements** text field, type 4.

Swept 2

Right-click **Swept 2** and choose **Build Selected**.



Swept 3

- 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 From the **Selection** list, choose **Hydrogen Channels**.
- 5 Click to expand the **Source Faces** section. From the **Selection** list, choose **Hydrogen Inlets**.
- 6 Click to expand the **Destination Faces** section. From the **Selection** list, choose **Hydrogen Outlets**.

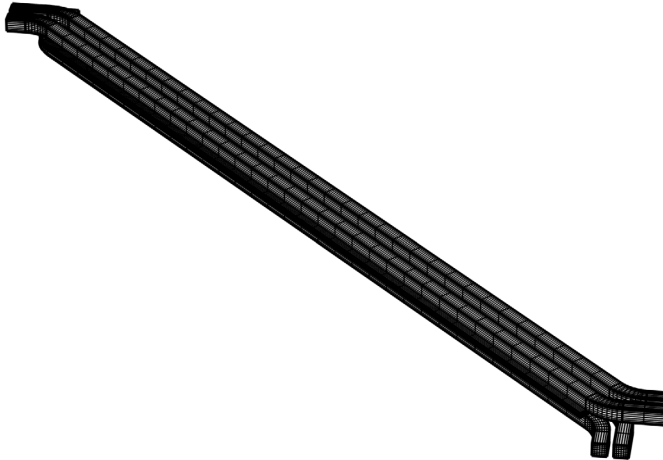
Size 1

- 1 Right-click **Swept 3** 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** checkbox. In the associated text field, type W_{ribch} .

Size 2

- 1 In the **Model Builder** window, right-click **Swept 3** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Selection** list, choose **Bends**.
- 4 Locate the **Element Size** section. Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section.
- 6 Select the **Maximum element size** checkbox. In the associated text field, type $H_{ch}/3$.
- 7 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.



STUDY 1

The physics and mesh are now complete. Modify the predefined study sequence by adding a second **Current Distribution** step and a **Stationary** step.


Each study step uses the results of the previous step as initial values. The **Current Distribution** step solves for a stationary current distribution for the initial gas distribution.

By setting the distribution type to **Secondary** in the second step, nonlinear kinetics are included.


The additional **Stationary** step will be defined to solve for the single-phase (gas-only) initial flow distribution, setting all mass sources in the fuel cell to zero.

The final time-dependent step solves for the resulting transient flow changes when the average cell current density is changed from 0 to 1 A/cm² at $t = 0$.

Step 3: Current Distribution Initialization 2

- 1 In the **Study** toolbar, click  **Study Steps** and choose **Other** > **Current Distribution Initialization**.
- 2 Right-click **Step 3: Current Distribution Initialization 2** and choose **Move Up**.
- 3 In the **Settings** window for **Current Distribution Initialization**, locate the **Study Settings** section.
- 4 From the **Current distribution type** list, choose **Secondary**.

Stationary - Single Phase Flow Initialization

- 1 In the **Study** toolbar, click  **Study Steps** and choose **Stationary** > **Stationary**.
- 2 Right-click **Step 4: Stationary** and choose **Move Up**.
- 3 In the **Settings** window for **Stationary**, type Stationary - Single Phase Flow Initialization in the **Label** text field.
- 4 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Hydrogen Fuel Cell (fc)** and **Phase Transport in Free and Porous Media Flow (phtr)**.
- 5 Select the **Modify model configuration for study step** checkbox.
- 6 In the tree, select **Component 1 (comp1)** > **Phase Transport in Free and Porous Media Flow (phtr)** > **Mass Source 1**.
- 7 Right-click and choose **Disable**.
- 8 In the tree, select **Component 1 (comp1)** > **Phase Transport in Free and Porous Media Flow (phtr)** > **Boundary Mass Source 1**.
- 9 Right-click and choose **Disable**.

Step 4: Time Dependent


- 1 In the **Model Builder** window, click **Step 4: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type 0 1 10 60.

Before solving, add a probe to monitor the cell voltage versus time for all time-steps taken by the solver.

DEFINITIONS


Global Variable Probe 1 (var1)

- 1 In the **Definitions** toolbar, click  **Probes** and choose **Global Variable Probe**.
- 2 In the **Settings** window for **Global Variable Probe**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Hydrogen Fuel Cell > fc.phis0_ec1 - Electric potential on boundary - V**.
- 3 Locate the **Expression** section.
- 4 Select the **Description** checkbox. In the associated text field, type Cell voltage.

STUDY I

Step 3: Stationary - Single Phase Flow Initialization

Probes are automatically disabled in the **Current Distribution Initialization** steps. Disable the probe in step 3 as follows:

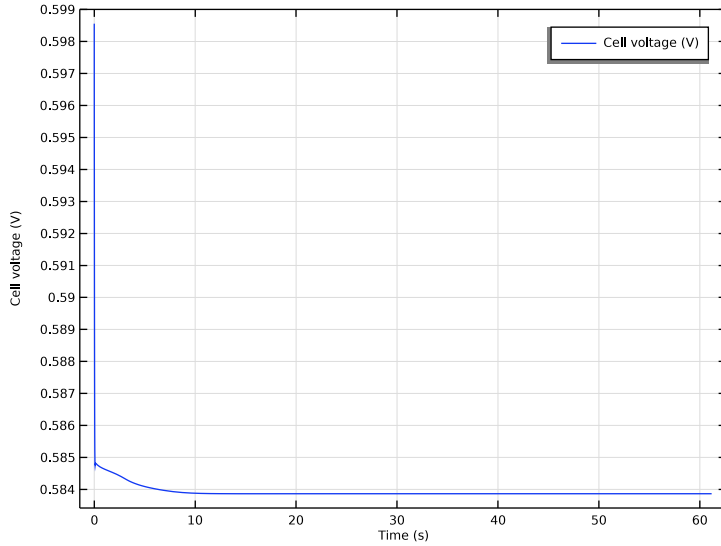
- 1 In the **Model Builder** window, under **Study I** click **Step 3: Stationary - Single Phase Flow Initialization**.
- 2 In the **Settings** window for **Stationary**, click to expand the **Results While Solving** section.
- 3 From the **Probes** list, choose **None**.
The model is now ready for solving.
- 4 In the **Study** toolbar, click  **Compute**.

RESULTS

Cell Voltage vs. Time

- 1 In the **Model Builder** window, under **Results** click **Probe Plot Group 1**.

-
- 2** In the **Settings** window for **ID Plot Group**, type **Cell Voltage vs. Time** in the **Label** text field.



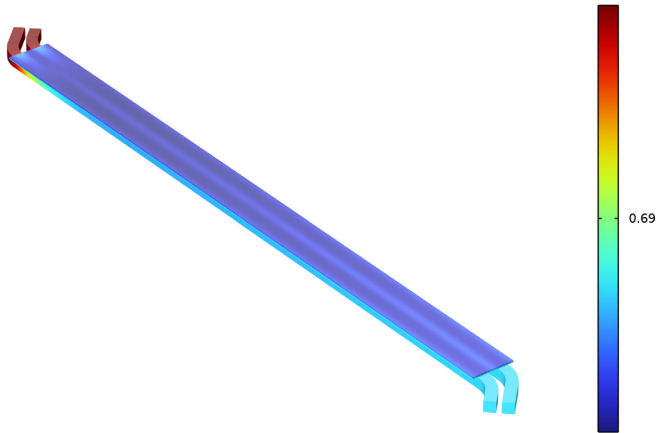
Mole Fraction, H₂, Surface (fc)

- 1** In the **Model Builder** window, click **Mole Fraction, H₂, Surface (fc)**.
- 2** In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
- 3** Clear the **Plot dataset edges** checkbox.

4 In the **Mole Fraction, H2, Surface (fc)** toolbar, click  **Plot**.

Time=60 s

Species H2: Mole fraction (1)



Mole Fraction, O2, Surface (fc)

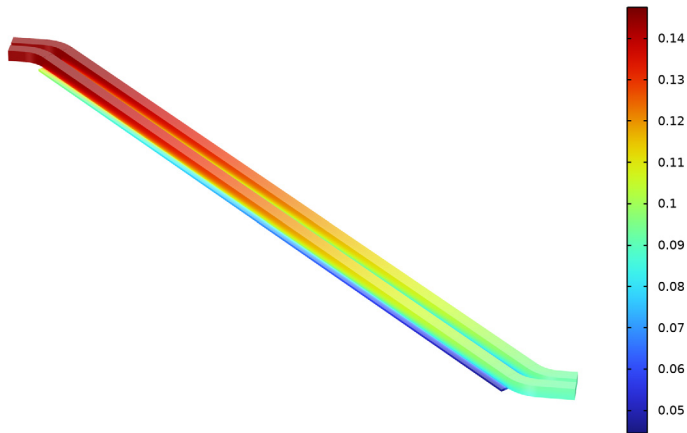
1 In the **Model Builder** window, click **Mole Fraction, O2, Surface (fc)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 Clear the **Plot dataset edges** checkbox.

Time=60 s

Species O2: Mole fraction (1)




Slice

- 1 In the **Model Builder** window, expand the **Velocity (spf)** 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 $H_{ch}/2+H_{mem}/2+H_{gd1}$.

Slice 2

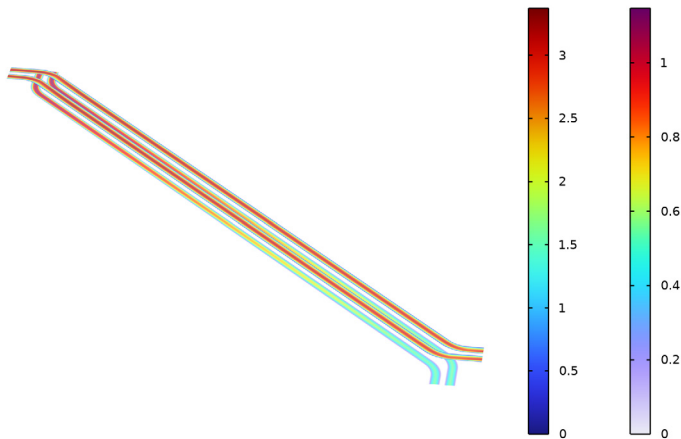
- 1 Right-click **Slice** and choose **Duplicate**.
- 2 In the **Settings** window for **Slice**, click to expand the **Title** section.
- 3 From the **Title type** list, choose **None**.
- 4 Locate the **Plane Data** section. In the **z-coordinates** text field, type $-(H_{ch}/2+H_{mem}/2+H_{gd1})$.
- 5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

Velocity (spf)

- 1 In the **Model Builder** window, click **Velocity (spf)**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
- 3 Clear the **Plot dataset edges** checkbox.
- 4 In the **Velocity (spf)** toolbar, click  **Plot**.

Time=60 s


Slice: Velocity magnitude (m/s)



Volume Fraction (phtr), Volume Fraction (phtr) 1

- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Volume Fraction (phtr)** and **Volume Fraction (phtr) 1**.
- 2 Right-click and choose **Delete**.

Liquid Volume Fraction

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type **Liquid Volume Fraction** in the **Label** text field.

Volume 1

- 1 Right-click **Liquid Volume Fraction** 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) > Phase Transport in Free and Porous Media Flow > s_w - Volume 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 **GDLs**.

Volume 2

- 1 In the **Model Builder** window, under **Results > Liquid Volume Fraction** right-click **Volume 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Volume**, click to expand the **Title** section.
- 3 From the **Title type** list, choose **None**.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

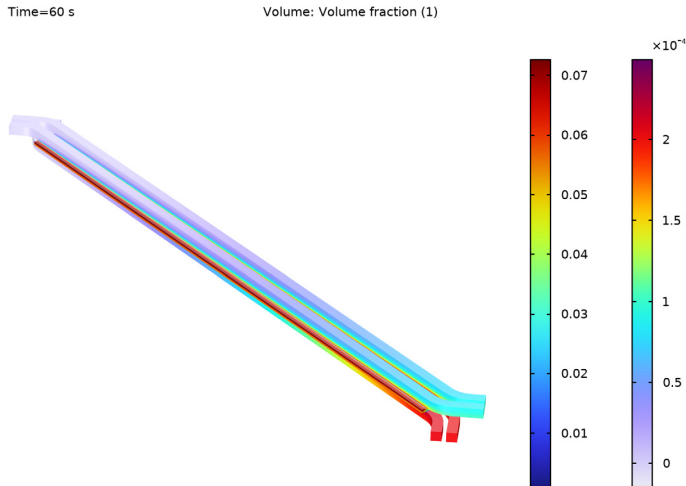
Selection 1

- 1 In the **Model Builder** window, expand the **Volume 2** node, then click **Selection 1**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Channels**.


Liquid Volume Fraction

- 1 In the **Model Builder** window, under **Results** click **Liquid Volume Fraction**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
- 3 Clear the **Plot dataset edges** checkbox.

- 4 In the **Liquid Volume Fraction** toolbar, click  **Plot**.



Cross-Membrane Current Density

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Cross-Membrane Current Density in the **Label** text field.
- 3 Click to expand the **Selection** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 From the **Selection** list, choose **Oxygen GDE**.

Surface 1

- 1 Right-click **Cross-Membrane Current 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) > Hydrogen Fuel Cell > fc.nll - Normal electrolyte current density - A/m²**.

Cross-Membrane Current Density

- 1 In the **Model Builder** window, click **Cross-Membrane Current Density**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
- 3 Clear the **Plot dataset edges** checkbox.

4 In the **Cross-Membrane Current Density** toolbar, click  **Plot**.

