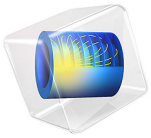

Model created in COMSOL Multiphysics 6.4

Mass Transport Analysis of a High Temperature PEM Fuel Cell

Introduction

A high-temperature PEM based on phosphoric acid doped polymer membranes typically operates in a temperature window between 100°C and 200°C.

Water is produced on the cathode side due to the electrochemical reactions, but water may also be present on the anode side if the hydrogen fuel stream contains water. The latter may be the case if the hydrogen fuel stems from reforming of hydrocarbon fuels such as natural gas, alcohols or diesel.

Water build-up in the cell results in lower partial pressures of hydrogen and oxygen on the anode and cathode, respectively, and thereby also lowers the rate of the cell reactions.

The local water concentration in the cell may have a beneficial impact on the ion conductivity of the membrane, but if water condenses in the cell it may result in leaching of phosphoric acid out from the polymer matrix, irreversibly reducing the ion conducting capabilities of the membrane and the performance of the whole cell.

During normal operation above 100°C, water normally does not condensate in the cell, but knowledge about the water content in the porous electrodes during operation may also be desired in order to optimize shut-down procedures, since water may condensate when the temperature is lowered below 100°C.

This model example investigates the steady-state transport of reactants and water in a cell including both anode and cathode mass and momentum transport phenomena in the flow channels, gas diffusion layers (GDLs) and gas diffusion electrodes (GDEs), as well as electrochemical currents in the GDLs, the GDEs and the polymer membrane.

The geometry is shown in Figure 1.

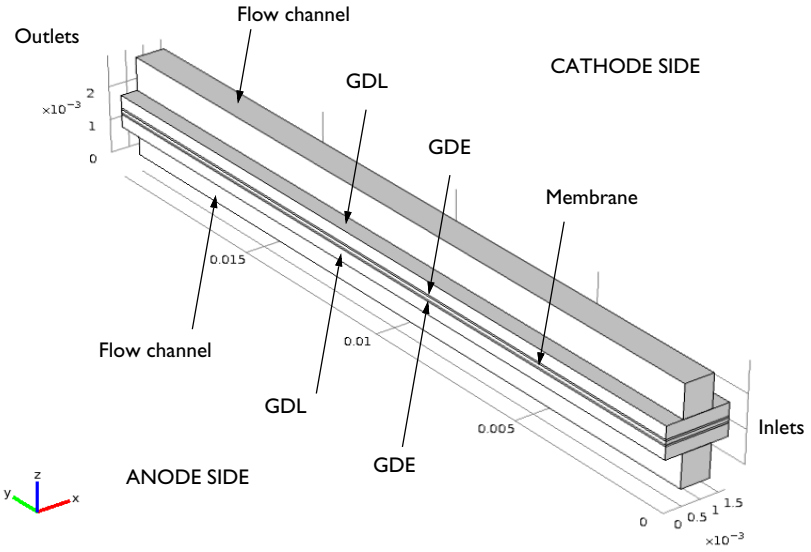

Figure 1: Modeled geometry.

The following unknown variables are solved for in the model:

- electronic potential
- ionic potential
- hydrogen mass fraction in the anode compartment
- water mass fraction in the anode compartment
- oxygen mass fraction in the cathode compartment
- water mass fraction in the cathode compartment
- nitrogen mass fraction in the cathode compartment
- velocity field vectors in the anode and cathode compartments
- pressure in the anode and cathode compartments

This is done by using a Hydrogen Fuel Cell interface, two Free and Porous Media Flow, Brinkman interfaces, along with Reacting Flow, H2 Gas Phase, and Reacting Flow, O2 Gas Phase multiphysics nodes.

ELECTROCHEMICAL CURRENTS

The Hydrogen Fuel Cell interface models the electrochemical currents using Ohm's law, solving for ϕ_s in the GDLs, ϕ_s and ϕ_l in the GDEs, and ϕ_l in the membrane. In the GDEs the local current densities depend on the ionic and electronic potentials, but also on local reactant concentrations.

On the anode, hydrogen oxidation occurs according to

$$\mathrm{H_2} \Rightarrow 2\mathrm{H^+} + 2e^-$$

(no water molecules are assumed to be involved in the proton transport), and the following local current density expression is used for the hydrogen oxidation reaction:

$$i_a = i_{0,\,\mathrm{ref},\,a}\left(\frac{p_{\mathrm{H_2}}}{p_{\mathrm{ref}}}\exp\left(\frac{\alpha_{a,\,a}}{RT}F\eta_a\right) - \exp\left(-\frac{\alpha_{c,\,a}}{RT}F\eta_a\right)\right)$$

where p_{H2} is the local hydrogen partial pressure and p_{ref} the reference pressure of 1 atm. η_a is the overpotential with respect to the equilibrium potential of the reaction at atmospheric pressures of the reacting gases.

At the cathode, oxygen reacts together with the protons to form water according to

$$\mathrm{O_2} + 4\mathrm{H^+} + 4e^- \Rightarrow 2\mathrm{H_2O}$$

and the following current density expression is used for the oxygen reduction reaction:

$$i_c = i_{0,\,\mathrm{ref},\,c}\left(\left(\frac{p_{\mathrm{H_2O}}}{p_{\mathrm{ref}}}\right)^2\exp\left(\frac{\alpha_{a,\,c}}{RT}F\eta_c\right) - \frac{p_{\mathrm{O_2}}}{p_{\mathrm{ref}}}\exp\left(-\frac{\alpha_{c,\,c}}{RT}F\eta_c\right)\right)$$

where p_{O2} and p_{H2O} are the local partial pressures of oxygen and water vapor, respectively.

The anode GDL boundaries facing the flow pattern ribs are set to zero electronic potential, and the corresponding boundaries at the cathode side are set to the cell potential. All other external boundaries are electrically isolating.

MASS TRANSFER

The Hydrogen Fuel Cells interface also solves for the species mass fractions in the flow channels, the GDLs and the GDEs using the Maxwell-Stefan equations. Note that hydrogen and water species are present on the anode side whereas oxygen, water and nitrogen are present on the cathode side.

At the channel inlets mole fractions are specified, and outlet conditions are used at the channel outlets. All other external boundaries use zero flux conditions.

MOMENTUM TRANSFER

u and p are modeled by the compressible Navier-Stokes equations in the flow channels, and by the Brinkman equations in the GDLs and the GDEs, by using two Free and Porous Media Flow, Brinkman interfaces.

Couplings for the density, viscosity, velocity, pressure and net mass sources and sinks are made to the Hydrogen Fuel Cell interface by using Reacting Flow, H2 Gas Phase and Reacting Flow, O2 Gas Phase multiphysics nodes.

At the flow channel inlet boundaries, laminar inlet flow velocity profiles are specified, whereas a pressure is specified at the flow channel outlet boundaries. To model a multiple parallel channel configuration, symmetry boundary conditions are applied along the long sides of the GDLs and the GDEs. All other wall boundaries use no slip conditions.

Results and Discussion

Figure 2 shows the polarization plot of the cell.

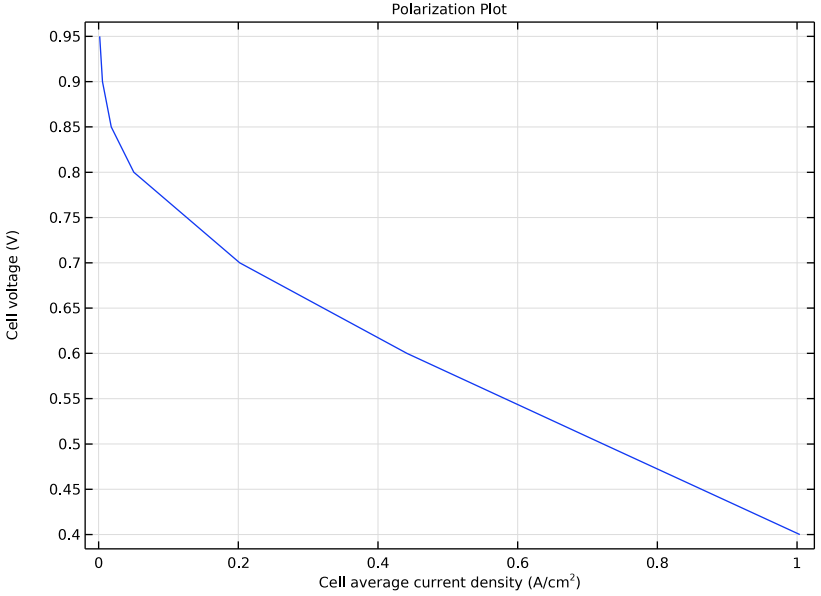

Figure 2: Polarization plot.

Figure 3 shows the ionic current in the z direction at the center of the membrane for 0.4 V. In the y direction the current density is lower toward the outlet (due to lower reactant concentrations).In the x direction the currents density is highest in the region close to the channel, where the reactant concentrations are higher, but the current density is reduced toward the very center of the channel. This is due to ohmic drops in the GDLs.

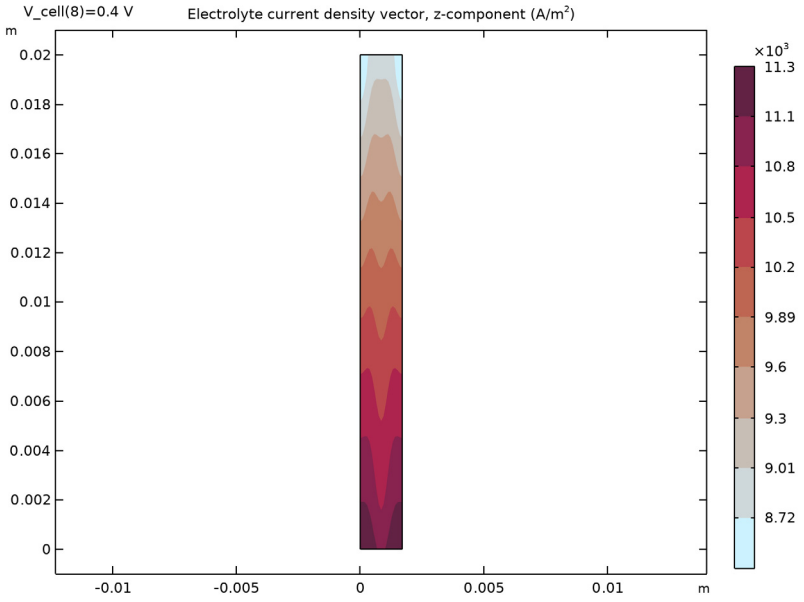

Figure 3: Ionic current in the polymer membrane at 0.4 V.

Figure 4 shows the hydrogen and oxygen mole fractions for the same voltage level. The oxygen mole fraction is significantly lower in the porous electrode and toward the end of the flow channel compared to the inlet level. For the anode the trend is the same but the hydrogen mole fraction level is more uniform.

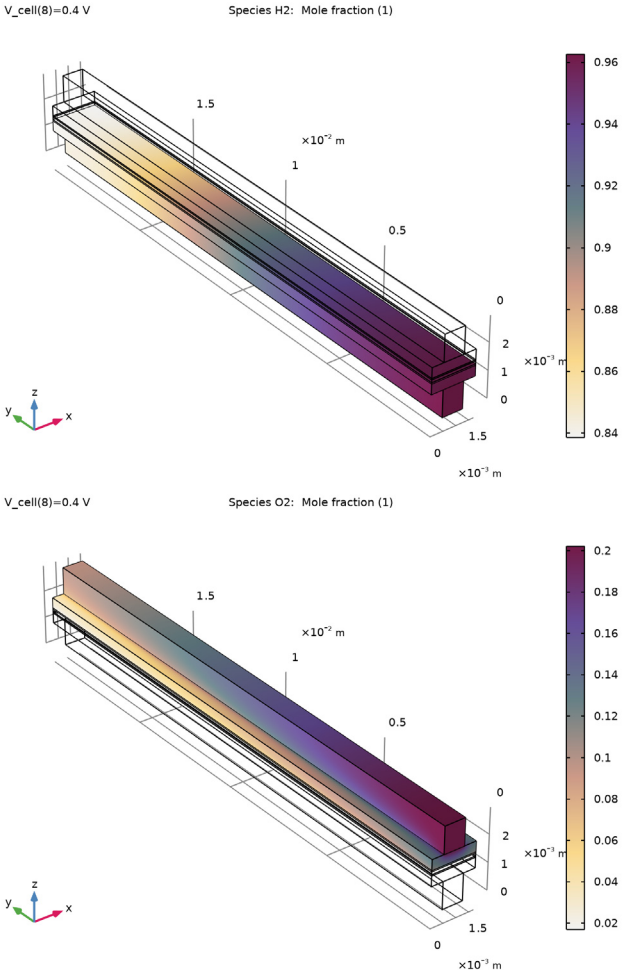

Figure 4: Hydrogen mole fraction at the anode (top) and oxygen mole fraction at the cathode (bottom) in the cell at 0.4 V.

Figure 5 shows the water mole fraction in the cell for the same voltage level. The mole fraction increase due to water production at the cathode is much larger than the effect of removing hydrogen from the gas stream at the anode for these flow and current levels.

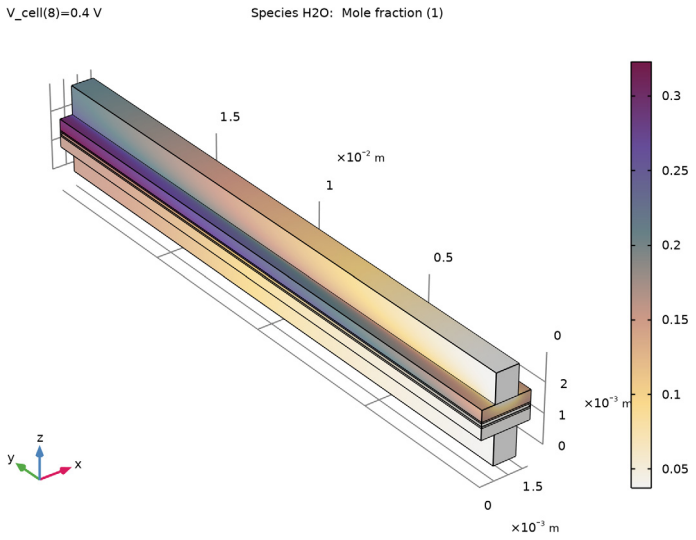

Figure 5: Water mole fraction on the anode and cathode side in the cell at 0.4 V.

Reference

1. E.U. Ubong, Z. Shi, and X. Wang, "Three-Dimensional Modeling and Experimental Study of a High Temperature PBI-Based PEM Fuel Cell," *J. Electrochemical Soc.*, vol. 156, no. 10, pp. B1276–B1282, 2009.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/ht_pem`

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** > **Free and Porous Media Flow, Brinkman (fp)**.

5 Click **Add**.

6 In the **Velocity field (m/s)** text field, type ua.

7 In the **Velocity field components** table, enter the following settings:

ua
va
wa

8 In the **Pressure (Pa)** text field, type pa.

9 In the **Select Physics** tree, select **Fluid Flow** > **Porous Media and Subsurface Flow** > **Free and Porous Media Flow, Brinkman (fp)**.

10 Click **Add**.

11 In the **Velocity field (m/s)** text field, type uc.

12 In the **Velocity field components** table, enter the following settings:

uc
vc
wc

13 In the **Pressure (Pa)** text field, type pc.

14 Click **Study**.

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

16 Click **Done**.

GLOBAL DEFINITIONS

Load the model parameters from a text file.

Parameters 1

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

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

3 Click **Load from File**.

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

GEOMETRY 1

Draw the channels, gas diffusion layers, porous gas diffusion electrodes and membrane using rectangular blocks.

Anode Channel

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

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

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

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

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

6 Locate the **Position** section. In the **x** text field, type `W_rib/2`.

7 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

8 Click **Build Selected**.

Anode GDL

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

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

3 Locate the **Size and Shape** section. In the **Width** text field, type `(W_ch+W_rib)`.

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

5 Locate the **Position** section. In the **x** text field, type `0`.

6 In the **z** text field, type `H_ch`.

7 Click **Build Selected**.

Anode GDE

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

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

3 Locate the **Size and Shape** section. In the **Height** text field, type `H_electrode`.

4 Locate the **Position** section. In the **z** text field, type `H_ch+H_gdl`.

5 Click **Build Selected**.

Membrane

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

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

3 Locate the **Size and Shape** section. In the **Height** text field, type `H_membrane`.

4 Locate the **Position** section. In the **z** text field, type `H_ch+H_gdl+H_electrode`.

5 Click  **Build Selected**.

Cathode GDE

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

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

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

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

5 Locate the **Position** section. In the **z** text field, type `H_ch+H_gdl+H_electrode+H_membrane`.

6 Click  **Build Selected**.

Cathode GDL

1 Right-click **Cathode GDE** and choose **Duplicate**.

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

3 Locate the **Size and Shape** section. In the **Height** text field, type `H_gdl`.

4 Locate the **Position** section. In the **z** text field, type `H_ch+H_gdl+H_electrode+H_membrane+H_electrode`.

5 Click  **Build Selected**.

Cathode Channel

1 Right-click **Cathode GDL** and choose **Duplicate**.

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

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

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

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

6 In the **z** text field, type `H_ch+H_gdl+H_electrode+H_membrane+H_electrode+H_gdl`.

7 Click  **Build All Objects**.

DEFINITIONS

Now create some additional selections of certain parts of the geometry to facilitate setting up the physics later on.

Anode Inlet

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundary 23 only.

Cathode Inlet

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundary 27 only.

Anode Outlet

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundary 30 only.

Cathode Outlet

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundary 31 only.

Anode Compartment

1 In the **Definitions** toolbar, click **Union**.

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

3 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

4 In the **Add** dialog, in the **Selections to add** list, choose **Anode Channel**, **Anode GDL**, and **Anode GDE**.

5 Click **OK**.

Cathode Compartment

1 In the **Definitions** toolbar, click  **Union**.

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

3 Locate the **Input Entities** section. Under **Selections to add**, click + **Add**.

4 In the **Add** dialog, in the **Selections to add** list, choose **Cathode GDE**, **Cathode GDL**, and **Cathode Channel**.

5 Click **OK**.

FREE AND POROUS MEDIA FLOW- ANODE

Set up the domains applicable for the flow interfaces.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free and Porous Media Flow, Brinkman (fp)**.

2 In the **Settings** window for **Free and Porous Media Flow, Brinkman**, type `Free and Porous Media Flow- Anode` in the **Label** text field.

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

FREE AND POROUS MEDIA FLOW - CATHODE

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free and Porous Media Flow, Brinkman 2 (fp2)**.

2 In the **Settings** window for **Free and Porous Media Flow, Brinkman**, type `Free and Porous Media Flow - Cathode` in the **Label** text field.

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

MULTIPHYSICS

Next, couple the interfaces appropriately using the reacting flow multiphysics coupling nodes. Note that currently, the multiphysics nodes may not be applicable to any domain selections, but the selections will be automatically updated when the **Hydrogen Fuel Cell** interface is set up.

Reacting Flow, H2 Gas Phase 1 (rfh1)

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

Reacting Flow, O2 Gas Phase 1 (rfo1)

1 In the **Physics** toolbar, click  **Multiphysics Couplings** and choose **Domain** > **Reacting Flow, O2 Gas Phase**.

2 In the **Settings** window for **Reacting Flow, O2 Gas Phase**, locate the **Coupled Interfaces** section.

3 From the **Fluid flow** list, choose **Free and Porous Media Flow - Cathode (fp2)**.

HYDROGEN FUEL CELL (FC)

Set up the current distribution and mass transport model. The default gas species are hydrogen and water on the anode side, and oxygen, nitrogen and water on the cathode side. Start with adding the relevant domain nodes.

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**.

H2 Gas Diffusion Electrode 1

1 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 **Anode GDE**.

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 **Anode GDL**.

H2 Gas Flow Channel 1

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 **Anode Channel**.

O2 Gas Diffusion Electrode 1

1 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 **Cathode GDE**.

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 **Cathode GDL**.

O2 Gas Flow Channel 1

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 **Cathode Channel**.

Electrolyte Phase 1

Set up the electrolyte conductivity in the **Electrolyte Phase** node. Note that in the **H2 Gas Phase** and **O2 Gas Phase** nodes, the settings are either the default option or automatically set by the multiphysics coupling nodes.

1 In the **Model Builder** window, click **Electrolyte Phase 1**.

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

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

H2 Gas Diffusion Electrode 1

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

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

2 In the **Settings** window for **H2 Gas Diffusion Electrode**, locate the **Electrode Charge Transport** section.

3 In the σ_s text field, type `sigma_gdl`.

4 Locate the **Effective Electrolyte Charge Transport** section. In the ε_l text field, type `eps_l_cl`.

5 Locate the **Gas Transport** section. In the ε_g text field, type `eps_gas_cl`.

H2 Gas Diffusion Electrode Reaction 1

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

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

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_a`.

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

H2 Gas Diffusion Layer 1

Set up the properties of the **H2 Gas Diffusion Layer** node.

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Hydrogen Fuel Cell (fc)** click **H2 Gas Diffusion Layer 1**.
2. In the **Settings** window for **H2 Gas Diffusion Layer**, locate the **Electrode Charge Transport** section.
3. In the σ_s text field, type `sigma_gdl`.
4. Locate the **Gas Transport** section. In the ε_g text field, type `eps_gas_gdl`.

O2 Gas Diffusion Electrode 1

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

1. In the **Model Builder** window, click **O2 Gas Diffusion Electrode 1**.
2. In the **Settings** window for **O2 Gas Diffusion Electrode**, locate the **Electrode Charge Transport** section.
3. In the σ_s text field, type `sigma_gdl`.
4. Locate the **Effective Electrolyte Charge Transport** section. In the ε_l text field, type `eps_l_cl`.
5. Locate the **Gas Transport** section. In the ε_g text field, type `eps_gas_cl`.

O2 Gas Diffusion Electrode Reaction 1

1. In the **Model Builder** window, click **O2 Gas Diffusion Electrode Reaction 1**.
2. In the **Settings** window for **O2 Gas Diffusion Electrode Reaction**, locate the **Electrode Kinetics** section.
3. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_c`.
4. In the α_a text field, type `4-alpha_c`.
5. Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av`.

O2 Gas Diffusion Layer 1

Set up the properties of the **O2 Gas Diffusion Layer** node.

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Hydrogen Fuel Cell (fc)** click **O2 Gas Diffusion Layer 1**.
2. In the **Settings** window for **O2 Gas Diffusion Layer**, locate the **Electrode Charge Transport** section.

3 In the σ_s text field, type `sigma_gdl`.

4 Locate the **Gas Transport** section. In the ε_g text field, type `eps_gas_gdl`.

There are no settings required on the flow channel nodes, other than the domain selection. Next, set up the boundary conditions and initial values.

Electronic Conducting Phase 1

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

Electric Ground 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electric Ground**.

2 Select Boundaries 3 and 33 only.

Electronic Conducting Phase 1

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

Electric Potential 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electric Potential**.

2 Select Boundaries 16 and 35 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the $\phi_{s,bnd}$ text field, type `V_cell`.

Initial Values 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Hydrogen Fuel Cell (fc)** > **H2 Gas Phase 1** node, then 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 mixture**.

4 In the T_{hum} text field, type `T_hum`.

H2 Gas Phase 1

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

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 **Anode Inlet**.

4 Locate the **Inlet Flow Type** section. From the **Inlet flow type** list, choose **Mixture composition constraint**.

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 **Anode Outlet**.

Initial Values 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Hydrogen Fuel Cell (fc)** > **O2 Gas Phase 1** node, then 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 T_{hum} text field, type `T_hum`.

O2 Gas Phase 1

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

O2 Inlet 1

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 **Cathode Inlet**.

4 Locate the **Inlet Flow Type** section. From the **Inlet flow type** list, choose **Mixture composition constraint**.

O2 Gas Phase 1

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

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 **Cathode Outlet**.

FREE AND POROUS MEDIA FLOW- ANODE (FP)

Next, set up the fluid flow model on the anode side. Note that the flow is compressible.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free and Porous Media Flow- Anode (fp)**.

2 In the **Settings** window for **Free and Porous Media Flow, Brinkman**, locate the **Physical Model** section.

3 From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Define the pressure reference level in the interface properties.

4 In the p_{ref} text field, type `p_ref`.

Set up the properties of the porous gas diffusion electrode, gas diffusion layer and the flow channel. Note that the density and viscosity of the gas mixture are calculated by the **Hydrogen Fuel Cell** interface and automatically set by the multiphysics coupling nodes.

Porous Medium 1

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

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

3 From the **Selection** list, choose **Anode GDL**.

Porous Matrix 1

1 In the **Model Builder** window, 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 `eps_gas_gdl`.

4 From the κ list, choose **User defined**. In the associated text field, type `kappa_gdl`.

Porous Medium 2

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

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

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

Porous Matrix 1

1 In the **Model Builder** window, 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 `eps_gas_cl`.

4 From the κ list, choose **User defined**. In the associated text field, type `kappa_cl`.

Wall 1

1 Click the **Show More Options** button in the **Model Builder** toolbar.

2 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

3 Click **OK**.

4 In the **Model Builder** window, under **Component 1 (comp1)** > **Free and Porous Media Flow-Anode (fp)** click **Wall 1**.

5 In the **Settings** window for **Wall**, click to expand the **Constraint Settings** section.

6 From the **Apply reaction terms on** list, choose **All physics (symmetric)**.

Inlet 1

Now set up the inlet and outlet conditions on the corresponding boundaries.

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 **Anode Inlet**.

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

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `U_in_anode`.

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 **Anode Outlet**.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** checkbox.

Symmetry 1

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

2 Select Boundaries 1, 4, 36, and 37 only.

FREE AND POROUS MEDIA FLOW - CATHODE (FP2)

Set up the fluid flow model on the cathode side in the same way.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free and Porous Media Flow - Cathode (fp2)**.

2 In the **Settings** window for **Free and Porous Media Flow, Brinkman**, locate the **Physical Model** section.

3 From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Define the pressure reference level in the interface properties.

4 In the p_{ref} text field, type `p_ref`.

Porous Medium 1

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

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

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

Porous Matrix 1

1 In the **Model Builder** window, 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 `eps_gas_gdl`.

4 From the κ list, choose **User defined**. In the associated text field, type `kappa_gdl`.

Porous Medium 2

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

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

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

Porous Matrix 1

1 In the **Model Builder** window, 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 `eps_gas_cl`.

4 From the κ list, choose **User defined**. In the associated text field, type `kappa_cl`.

Wall 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Free and Porous Media Flow - Cathode (fp2)** click **Wall 1**.

2 In the **Settings** window for **Wall**, locate the **Constraint Settings** section.

3 From the **Apply reaction terms on** list, choose **All physics (symmetric)**.

Symmetry 1

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

2 Select Boundaries 10, 13, 39, and 40 only.

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 **Cathode Inlet**.

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

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `U_in_cathode`.

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 **Cathode Outlet**.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** checkbox.

GLOBAL DEFINITIONS

Default Model Inputs

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

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

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

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

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

MESH 1

First create a mapped 2D mesh in the plane normal to the channel direction, then sweep this mesh in the channel direction.

Edge 1

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

2 Select Edges 3, 17, 33, 36, 48, and 51 only.

Size 1

1 Right-click **Edge 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_ch/8`.

Edge 2

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

2 Select Edges 13 and 65 only.

Distribution 1

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

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

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type 8.

5 In the **Element ratio** text field, type 4.

Edge 3

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** right-click **Edge 2** and choose **Duplicate**.

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

3 Click  **Clear Selection**.

4 Select Edges 1 and 57 only.

Distribution 1

1 In the **Model Builder** window, expand the **Edge 3** node, then click **Distribution 1**.

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

3 Select the **Reverse direction** checkbox.

Edge 4

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

2 Select Edges 4 and 59 only.

Distribution 1

1 Right-click **Edge 4** and choose **Distribution**.

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

3 In the **Number of elements** text field, type 6.

Edge 5

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

2 Select Edges 10 and 63 only.

Distribution 1

1 Right-click **Edge 5** and choose **Distribution**.

Larger concentration gradients are expected in the cathode catalyst layer (due to the lower diffusion coefficient of oxygen), therefore use a higher element density in the cathode.

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

3 In the **Number of elements** text field, type 10.

Edge 6

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

2 Select Edges 7 and 61 only.

Distribution 1

1 Right-click **Edge 6** and choose **Distribution**.

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

3 In the **Number of elements** text field, type `3`.

Edge 7

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

2 Select Edges 29, 34, 45, and 49 only.

Distribution 1

1 Right-click **Edge 7** and choose **Distribution**.

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

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type `8`.

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

6 Select the **Symmetric distribution** checkbox.

Mapped 1

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

2 Select Boundaries 2, 5, 8, 11, 14, 23, and 27 only.

Swept 1

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

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_ch`.

6 Click **Build Selected**.

DEFINITIONS

Add a domain probe for the integral of the electrochemical current density to get a polarization plot automatically during the parametric solver process. You can then use this probe also for creating a polarization curve during postprocessing.

Domain Probe 1 (dom1)

1. In the **Definitions** toolbar, click  **Probes** and choose **Domain Probe**.
2. In the **Settings** window for **Domain Probe**, locate the **Probe Type** section.
3. From the **Type** list, choose **Integral**.
4. Locate the **Source Selection** section. From the **Selection** list, choose **Anode GDE**.
5. Locate the **Expression** section. In the **Expression** text field, type `fc.iv_h2gder1/((W_ch+W_rib)*L)/1e4`.

STUDY 1

The problem is now ready for solving. Firstly, solve for current distribution initialization (both primary and secondary) in two study steps, followed by flow in two subsequent study steps. Finally, solve the entire model including the multiphysics couplings in the final step, along with an auxiliary sweep to solve for a range of potentials and simulate a polarization plot.

Step 1: Current Distribution Initialization

1. In the **Model Builder** window, under **Study 1** click **Step 1: Current Distribution Initialization**.
2. In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.
3. In the **Solve for** column of the table, under **Component 1 (comp1)** > **Multiphysics**, clear the checkboxes for **Reacting Flow, H2 Gas Phase 1 (rfh1)** and **Reacting Flow, O2 Gas Phase 1 (rfo1)**.

Step 3: Current Distribution Initialization 2

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

5 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)** > **Multiphysics**, clear the checkboxes for **Reacting Flow, H2 Gas Phase 1 (rfh1)** and **Reacting Flow, O2 Gas Phase 1 (rfo1)**.

Step 3: Stationary

1 In the **Model Builder** window, click **Step 3: Stationary**.

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

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Hydrogen Fuel Cell (fc)** and **Free and Porous Media Flow - Cathode (fp2)**.

4 In the **Solve for** column of the table, under **Component 1 (comp1)** > **Multiphysics**, clear the checkboxes for **Reacting Flow, H2 Gas Phase 1 (rfh1)** and **Reacting Flow, O2 Gas Phase 1 (rfo1)**.

Step 4: Stationary 2

1 In the **Study** toolbar, click **Stationary**.

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

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Hydrogen Fuel Cell (fc)** and **Free and Porous Media Flow- Anode (fp)**.

4 In the **Solve for** column of the table, under **Component 1 (comp1)** > **Multiphysics**, clear the checkboxes for **Reacting Flow, H2 Gas Phase 1 (rfh1)** and **Reacting Flow, O2 Gas Phase 1 (rfo1)**.

Step 5: Stationary 3

1 In the **Study** toolbar, click **Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** checkbox.

4 Click **Add**.

Use the range operator to create a list of potentials from 0.95 to 0.4 V, using steps -50 mV for the first steps, and then -100 mV toward the end.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V_cell (Cell voltage)	`range(0.95,-0.05,0.85)` `range(0.8,-0.1,0.4)`	V

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

RESULTS

Several default plots are generated. Among them are the plots seen in Figure 4 and Figure 5 that show the hydrogen, oxygen and water mole fraction distributions.

Surface 1

1. In the **Model Builder** window, expand the **Mole Fraction, H2, Surface (fc)** node, then click **Surface 1**.
2. In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
3. From the **Color table** list, choose **ConopiformisZero**.

Surface 1

1. In the **Model Builder** window, expand the **Mole Fraction, O2, Surface (fc)** node, then click **Surface 1**.
2. In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
3. From the **Color table** list, choose **ConopiformisZero**.

Surface 1

1. In the **Model Builder** window, expand the **Mole Fraction, H2O, Surface (fc)** node, then click **Surface 1**.
2. In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
3. From the **Color table** list, choose **ConopiformisZero**.

Polarization Plot

Modify the probe plot as follows to reproduce the polarization plot in Figure 2.

1. In the **Model Builder** window, expand the **Results** > **Probe Plot Group 1** node, then click **Probe Plot Group 1**.
2. In the **Settings** window for **1D Plot Group**, type `Polarization Plot` in the **Label** text field.
3. Click to expand the **Title** section. From the **Title type** list, choose **Label**.
4. Locate the **Plot Settings** section.
5. Select the **x-axis label** checkbox. In the associated text field, type `Cell average current density (A/cm<sup>2</sup>)`.
6. Select the **y-axis label** checkbox. In the associated text field, type `Cell voltage (V)`.
7. Select the **Flip the x- and y-axes** checkbox.
8. Locate the **Legend** section. Clear the **Show legends** checkbox.
9. In the **Polarization Plot** toolbar, click  **Plot**.

10 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Cut Plane 1

Next, reproduce the ionic current plot of Figure 3. Begin by creating a Cut Plane dataset.

1 In the **Results** toolbar, click  **Cut Plane**.

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

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

4 In the **z-coordinate** text field, type `H_ch+H_gdl+H_electrode+H_membrane/2`.

Membrane Current Density

1 In the **Results** toolbar, click  **2D Plot Group**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Plane 1**.

Surface 1

1 In the **Membrane Current Density** toolbar, click  **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** > **Electrolyte current density vector - A/m²** > **fc.llz - Electrolyte current density vector, z-component**.

3 Locate the **Coloring and Style** section. From the **Color table** list, choose **MetasepiaBlue**.

4 From the **Color table type** list, choose **Discrete**.

5 In the **Membrane Current Density** toolbar, click  **Plot**.

Follow the commands below to improve some plot appearances and remove redundant plots.

Multislice 1

1 In the **Model Builder** window, expand the **Electrode Potential with Respect to Ground (fc)** node, then click **Multislice 1**.

2 In the **Settings** window for **Multislice**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **MetasepiaBlue**.

Arrow Volume 1

1 In the **Model Builder** window, click **Arrow Volume 1**.

2 In the **Settings** window for **Arrow Volume**, locate the **Arrow Positioning** section.

3 From the **Placement** list, choose **Element centers**.

4 In the **Maximum number of points** text field, type 100000.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Yellow**.

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

Mole Fraction, N2, Streamline (fc), Mole Fraction, N2, Surface (fc)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Mole Fraction, N2, Streamline (fc)** and **Mole Fraction, N2, Surface (fc)**.

2 Right-click and choose **Delete**.