

Mass Transport Analysis of a High Temperature PEM Fuel Cell

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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.

Model Definition



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 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

$$H_2 \Rightarrow 2H^+ + 2e^-$$

(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:

$$i_{a} = i_{0, \text{ ref}, a} \left(\frac{p_{\text{H}_{2}}}{p_{\text{ref}}} \exp \left(\frac{\alpha_{a, a}}{RT} F \eta_{a} \right) - \exp \left(-\frac{\alpha_{c, a}}{RT} F \eta_{a} \right) \right)$$

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

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

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

$$i_{c} = i_{0, \text{ ref}, c} \left(\left(\frac{p_{\text{H}_{2}\text{O}}}{p_{\text{ref}}} \right)^{2} \exp \left(\frac{\alpha_{a, c}}{RT} F \eta_{c} \right) - \frac{p_{\text{O}_{2}}}{p_{\text{ref}}} \exp \left(-\frac{\alpha_{c, c}}{RT} F \eta_{c} \right) \right)$$

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 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

- I In the Model Wizard window, click 间 3D.
- 2 In the Select Physics tree, select Electrochemistry>Hydrogen Fuel Cells> Proton Exchange (fc).
- 3 Click Add.
- 4 In the Select Physics tree, select Fluid Flow>Porous Media and Subsurface Flow> Free and Porous Media Flow (fp).
- 5 Click Add.
- 6 In the Velocity field text field, type ua.
- 7 In the Velocity field components table, enter the following settings:

va

wa

- 8 In the **Pressure** text field, type pa.
- 9 In the Select Physics tree, select Fluid Flow>Porous Media and Subsurface Flow> Free and Porous Media Flow (fp).
- IO Click Add.
- II In the Velocity field text field, type uc.

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

uc

vc

wc

I3 In the **Pressure** text field, type pc.

I4 Click 🔿 Study.

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

l6 Click 🗹 Done.

GLOBAL DEFINITIONS

Load the model parameters from a text file.

Parameters 1

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

ua

- 2 In the Settings window for Parameters, locate the Parameters section.
- 3 Click **b** Load from File.
- 4 Browse to the model's Application Libraries folder and double-click the file ht_pem_parameters.txt.

GEOMETRY I

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

Anode Channel

- I In the **Geometry** toolbar, click T 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** check box.
- 8 Click 🔚 Build Selected.

Anode GDL

- I 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

- I 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 틤 Build Selected.

Membrane

- I 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 틤 Build Selected.

Cathode GDE

- I 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 틤 Build Selected.

Cathode GDL

- I 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 틤 Build Selected.

Cathode Channel

- I 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

- I 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

- I In the **Definitions** toolbar, click **here 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

- I In the **Definitions** toolbar, click **here 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

- I In the Definitions toolbar, click http://www.click.ic.
- 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

- I In the **Definitions** toolbar, click **H 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 box, in the Selections to add list, choose Anode Channel, Anode GDL, and Anode GDE.
- 5 Click OK.

Cathode Compartment

- I 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 box, 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.

- I In the Model Builder window, under Component I (compl) click Free and Porous Media Flow (fp).
- 2 In the Settings window for Free and Porous Media Flow, 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

- I In the Model Builder window, under Component I (comp1) click Free and Porous Media Flow 2 (fp2).
- 2 In the Settings window for Free and Porous Media Flow, 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 An Multiphysics Couplings and choose Domain>Reacting Flow, H2 Gas Phase.

Reacting Flow, O2 Gas Phase I (rfol)

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

- **2** In the Settings window for Reacting Flow, **02** 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.

I In the Model Builder window, under Component I (compl) click Hydrogen Fuel Cell (fc).

Membrane I

- I 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 I

- I In the Physics toolbar, click 🔚 Domains and choose H2 Gas Diffusion Electrode.
- **2** In the **Settings** window for **H2 Gas Diffusion Electrode**, locate the **Domain Selection** section.
- 3 From the Selection list, choose Anode GDE.

H2 Gas Diffusion Layer I

- I 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 I

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

O2 Gas Diffusion Electrode 1

- I In the Physics toolbar, click 🔚 Domains and choose 02 Gas Diffusion Electrode.
- **2** In the **Settings** window for **02 Gas Diffusion Electrode**, locate the **Domain Selection** section.
- 3 From the Selection list, choose Cathode GDE.

O2 Gas Diffusion Layer I

- I 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 I

- I In the Physics toolbar, click 🔚 Domains and choose 02 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.

- I In the Model Builder window, click Electrolyte Phase I.
- **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 I

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

- I In the Model Builder window, click H2 Gas Diffusion Electrode I.
- 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_1_cl.
- **5** Locate the **Gas Transport** section. In the ε_g text field, type eps_gas_cl.

H2 Gas Diffusion Electrode Reaction I

- I In the Model Builder window, click H2 Gas Diffusion Electrode Reaction I.
- 2 In the Settings window for H2 Gas Diffusion Electrode Reaction, locate the Electrode Kinetics section.
- **3** In the $i_{0,\text{ref}}(T)$ 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 I

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

- In the Model Builder window, under Component I (comp1)>Hydrogen Fuel Cell (fc) click
 H2 Gas Diffusion Layer I.
- 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 I

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

- I In the Model Builder window, click O2 Gas Diffusion Electrode I.
- 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_1_cl.
- **5** Locate the **Gas Transport** section. In the ε_g text field, type eps_gas_cl.

O2 Gas Diffusion Electrode Reaction I

- I In the Model Builder window, click O2 Gas Diffusion Electrode Reaction I.
- 2 In the Settings window for O2 Gas Diffusion Electrode Reaction, locate the Electrode Kinetics section.
- **3** In the $i_{0,ref}(T)$ text field, type i0_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 I

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

In the Model Builder window, under Component I (comp1)>Hydrogen Fuel Cell (fc) click
 O2 Gas Diffusion Layer 1.

- **2** In the Settings window for **02** 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 I

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

Electric Ground 1

- I In the Physics toolbar, click 戻 Attributes and choose Electric Ground.
- **2** Select Boundaries 3 and 33 only.

Electronic Conducting Phase I

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

Electric Potential 1

- I 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

- In the Model Builder window, expand the Component I (comp1)>Hydrogen Fuel Cell (fc)>
 H2 Gas Phase I node, then 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 T_{hum} text field, type T_hum.

H2 Gas Phase I

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

H2 Inlet I

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

H2 Gas Phase I

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

H2 Outlet I

- I In the Physics toolbar, click 层 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

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

O2 Gas Phase I

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

O2 Inlet I

- I In the Physics toolbar, click 🧮 Attributes and choose 02 Inlet.
- 2 In the Settings window for O2 Inlet, locate the Boundary Selection section.
- **3** From the Selection list, choose Cathode Inlet.

O2 Gas Phase I

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

O2 Outlet I

- I In the Physics toolbar, click 📃 Attributes and choose 02 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.

- I In the Model Builder window, under Component I (comp1) click Free and Porous Media Flow- Anode (fp).
- 2 In the Settings window for Free and Porous Media Flow, 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 I

- I 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 I

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

Porous Medium 2

- I 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 I

- I In the Model Builder window, click Porous Matrix I.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- 3 From the ε_p list, choose User defined. In the associated text field, type eps_gas_cl.
- **4** From the κ list, choose **User defined**. In the associated text field, type kappa_c1.

Wall I

- I Click the 🐱 Show More Options button in the Model Builder toolbar.
- 2 In the Show More Options dialog box, in the tree, select the check box for the node Physics>Advanced Physics Options.
- 3 Click OK.
- 4 In the Model Builder window, under Component I (comp1)>Free and Porous Media Flow-Anode (fp) click Wall I.
- 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.

- I In the Physics toolbar, click 🔚 Boundaries and choose Inlet.
- 2 In the Settings window for Inlet, locate the Boundary Selection section.
- 3 From the Selection list, choose 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 I

- I In the Physics toolbar, click 🔚 Boundaries and choose Outlet.
- 2 In the Settings window for Outlet, locate the Boundary Selection section.
- **3** From the **Selection** list, choose **Anode Outlet**.
- 4 Locate the Pressure Conditions section. Select the Normal flow check box.
- 5 Click to expand the Constraint Settings section.

Symmetry I

- I 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.

- I In the Model Builder window, under Component I (compl) click Free and Porous Media Flow - Cathode (fp2).
- 2 In the Settings window for Free and Porous Media Flow, 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 I

- I 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 I

- I In the Model Builder window, click Porous Matrix I.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.

- **3** From the ε_p list, choose **User defined**. In the associated text field, type eps_gas_gdl.
- **4** From the κ list, choose **User defined**. In the associated text field, type kappa_gdl.

Porous Medium 2

- I 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 I

- I In the Model Builder window, click Porous Matrix I.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- 3 From the ε_p list, choose User defined. In the associated text field, type eps_gas_cl.
- **4** From the κ list, choose **User defined**. In the associated text field, type kappa_c1.

Wall I

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

- I In the Physics toolbar, click 🔚 Boundaries and choose Symmetry.
- **2** Select Boundaries 10, 13, 39, and 40 only.

Inlet 1

- I In the Physics toolbar, click 🔚 Boundaries and choose Inlet.
- 2 In the Settings window for Inlet, locate the Boundary Selection section.
- **3** From the Selection list, choose 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 I

- I In the Physics toolbar, click 📄 Boundaries and choose Outlet.
- 2 In the Settings window for Outlet, locate the Boundary Selection section.
- **3** From the Selection list, choose Cathode Outlet.
- 4 Locate the Pressure Conditions section. Select the Normal flow check box.

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.

- I In the Model Builder window, under Global Definitions click Default Model Inputs.
- 2 In the Settings window for Default Model Inputs, locate the Browse Model Inputs section.
- 3 In the tree, select General>Temperature (K) minput.T.
- Find the Expression for remaining selection subsection. In the Temperature text field, type T.

MESH I

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

Edge I

- I In the Mesh toolbar, click \bigwedge Boundary and choose Edge.
- 2 Select Edges 3, 17, 33, 36, 48, and 51 only.

Size 1

- I Right-click Edge I and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** Click the **Custom** button.
- 4 Locate the Element Size Parameters section.
- 5 Select the Maximum element size check box. In the associated text field, type W_Ch/8.

Edge 2

- I In the Mesh toolbar, click \bigwedge Boundary and choose Edge.
- 2 Select Edges 13 and 65 only.

Distribution I

- I 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

- I In the Model Builder window, under Component I (compl)>Mesh I 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 I

- I In the Model Builder window, expand the Edge 3 node, then click Distribution I.
- 2 In the Settings window for Distribution, locate the Distribution section.
- **3** Select the **Reverse direction** check box.

Edge 4

- I In the Mesh toolbar, click \bigwedge Boundary and choose Edge.
- 2 Select Edges 4 and 59 only.

Distribution I

- I Right-click Edge 4 and choose Distribution.
- 2 In the Settings window for Distribution, locate the Distribution section.
- 3 In the Number of elements text field, type 6.

Edge 5

- I In the Mesh toolbar, click \bigwedge Boundary and choose Edge.
- 2 Select Edges 10 and 63 only.

Distribution I

I 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 Distribution, locate the Distribution section.
- 3 In the Number of elements text field, type 10.

Edge 6

- I In the Mesh toolbar, click \bigwedge Boundary and choose Edge.
- **2** Select Edges 7 and 61 only.

Distribution I

I 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

- I In the Mesh toolbar, click \bigwedge Boundary and choose Edge.
- 2 Select Edges 29, 34, 45, and 49 only.

Distribution I

- I 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 check box.

Mapped I

- I In the Mesh toolbar, click \bigwedge Boundary and choose Mapped.
- **2** Select Boundaries 2, 5, 8, 11, 14, 23, and 27 only.

Swept I

In the Mesh toolbar, click As Swept.

Size 1

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

- I 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 I

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

- I In the Model Builder window, under Study I click Step I: Current Distribution Initialization.
- **2** In the Settings window for Current Distribution Initialization, locate the **Physics and Variables Selection** section.
- 3 In the table, clear the Solve for check boxes for Reacting Flow, H2 Gas Phase I (rfh1) and Reacting Flow, O2 Gas Phase I (rfo1).

Current Distribution Initialization 2

- I In the Study toolbar, click 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 table, clear the Solve for check boxes for Reacting Flow, H2 Gas Phase I (rfh1) and Reacting Flow, O2 Gas Phase I (rfo1).

Step 3: Stationary

- I 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 table, clear the **Solve for** check boxes for **Hydrogen Fuel Cell (fc)** and **Free and Porous Media Flow Cathode (fp2)**.
- 4 In the table, clear the Solve for check boxes for Reacting Flow, H2 Gas Phase I (rfh1) and Reacting Flow, O2 Gas Phase I (rfo1).

Stationary 2

- I In the Study toolbar, click *C* Study Steps and choose Stationary>Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- **3** In the table, clear the **Solve for** check boxes for **Hydrogen Fuel Cell (fc)** and **Free and Porous Media Flow- Anode (fp)**.
- 4 In the table, clear the Solve for check boxes for Reacting Flow, H2 Gas Phase I (rfh1) and Reacting Flow, O2 Gas Phase I (rfo1).

Stationary 3

- I In the Study toolbar, click *C* Study Steps and choose Stationary>Stationary.
- 2 In the Settings window for Stationary, click to expand the Study Extensions section.
- 3 Select the Auxiliary sweep check box.
- 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.

Polarization Plot

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

- I In the Model Builder window, expand the Results>Probe Plot Group 15 node, then click Probe Plot Group 15.
- 2 In the Settings window for ID 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 check box. In the associated text field, type Cell average current density (A/cm²).

- 6 Select the y-axis label check box. In the associated text field, type Cell voltage (V).
- 7 Select the Flip the x- and y-axes check box.
- 8 Locate the Legend section. Clear the Show legends check box.
- 9 In the Polarization Plot toolbar, click **I** Plot.
- IO Click the \longleftrightarrow 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.

- I 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.

2D Plot Group 16

- I In the **Results** toolbar, click **2D Plot Group**.
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Dataset list, choose Cut Plane I.

Contour I

- I Right-click 2D Plot Group 16 and choose Contour.
- In the Settings window for Contour, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
 Hydrogen Fuel Cell>Electrolyte current density vector A/m²>fc.llz Electrolyte current density vector, z-component.
- 3 Locate the Levels section. In the Total levels text field, type 10.

Membrane Current Density

- I In the Model Builder window, click 2D Plot Group 16.
- 2 In the 2D Plot Group 16 toolbar, click 💽 Plot.
- **3** Click the **Com Extents** button in the **Graphics** toolbar.
- 4 In the Settings window for 2D Plot Group, type Membrane Current Density in the Label text field.

28 | MASS TRANSPORT ANALYSIS OF A HIGH TEMPERATURE PEM FUEL CELL