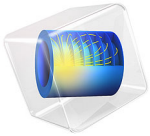

Species Transport in the Gas Diffusion Layers of a PEM

Introduction

This example focuses on the species transport within the gas diffusion layers (GDLs) of a proton exchange membrane (PEM) fuel cell. Specifically, the influence of anisotropic tortuosity on gas diffusivity in the GDLs is investigated. The geometry models a cell with two adjacent flow channels of different pressures, a situation that may occur in a cell with serpentine flow channels, or in a cell using an interdigitated flow field design. The model uses current balances, mass transport equations (Maxwell–Stefan diffusion for reactants, water and nitrogen gas), and momentum transport (Darcy's law for the gas flows) to simulate a PEM fuel cell's behavior.

Model Definition

The modeled section of the fuel cell consists of three domains: an anode (Ω_a), a proton exchange membrane (Ω_m), and a cathode (Ω_c) as indicated in Figure 1.

Electrode height: 2 mm
Electrode width:0.25 mm
Membrane thickness: 0.1 mm
Collector height: 1 mm

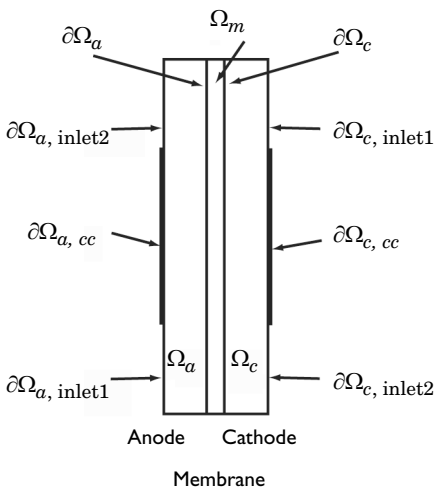

Figure 1: Model geometry with domain and boundary labels.

Each of the electrodes (gas diffusion layers) is in contact with a gas distributing flow field, featuring channels ($\partial\Omega_{a/c,\mathrm{inlet}}$) and current collector ribs ($\partial\Omega_{a/c,cc}$).

Humidified hydrogen and air are supplied to the inlet channels of the anode and cathode, respectively. Hydrogen reacts and is consumed at the anodic active layer to form protons that carry the ionic current to the cathode.

$$H_2 \Rightarrow 2H^+ + 2e^- \quad (1)$$

At the cathode, oxygen reacts together with the protons to form water at the active layer according to:

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

Both feed gases (humidified hydrogen and humidified air) are treated as ideal and are transported through diffusion and convection. The electrodes are treated as homogeneous porous media with uniform morphological properties such as porosity and permeability. The gas within each of the electrodes exists as a continuous phase so Darcy's law applies.

An agglomerate model describes the electrode reactions in the active catalyst layers. The agglomerates consist of catalyst and carbon particles embedded in polymer electrolyte. The equations for the agglomerate model originate from the analytical solution of a diffusion-reaction problem in a spherical porous particle (Ref. 5 and Ref. 6). At the anodic active catalyst layer, hydrogen is the diffusing and reacting species in the agglomerates, while oxygen is the diffusing and reacting species in the agglomerates at the cathode. An agglomerate model of the cathodic active catalyst layer of a PEM fuel cell has been presented by Broka and others (Ref. 7 and Ref. 8).

CHARGE BALANCES

The Hydrogen Fuel Cell interface is used for modeling the potential distributions in the three domains, with the charge-transfer current density of the active layers described as interior boundary conditions, using Thin H2/O2 Gas Diffusion Electrode nodes. The local current density expressions for the anode and cathode, i_a and i_c, are specified according to the equation

$$i_e = \frac{R_{agg}}{3} j_{agg,\,e}$$

where the index e stands for "a" (anode) or "c" (cathode), R_{agg} is the agglomerate radius (SI unit: m) and $j_{agg,a}$ and $j_{agg,c}$ (SI unit: A/m^3) are the current densities given by the agglomerate model. Further, L_{act} is the active layer (thin gas diffusion electrode) thickness (m) and ε_{mac} its porosity (the macroscopic porosity). The specific surface area of the thin gas diffusion electrode (SI unit: 1/m) is specified according to the following equation as

$$a_v = \frac{3}{R_{agg}}(1 - \varepsilon_{mac})$$

AGGLOMERATE MODEL FOR ANODE AND CATHODE

The agglomerate model describes the current density in an active layer consisting of agglomerates of ionic conductor material and electrically conducting particles covered partially with catalyst. The local current density can be expressed analytically by solving a combination of the diffusion equation and the Butler–Volmer electrode kinetic equation for an agglomerate with constant electric and ionic potentials. The resulting equations for the current density in the anode and cathode are (Ref. 7)

$$j_{\mathrm{agg},e} = 6n_e F\left(\frac{D_{\mathrm{agg}}}{R_{\mathrm{agg}}^2}\right)(1-\lambda_e \coth\lambda_e)\beta_e$$

where, again, the index e stands for "a" (anode) or "c" (cathode), and

$$\lambda_{\mathrm{a}} = \sqrt{\frac{i_{0\mathrm{a}} S R_{\mathrm{agg}}^2}{2F c_{\mathrm{H_2,ref}} D_{\mathrm{agg}}}} \qquad \lambda_{\mathrm{c}} = \sqrt{\frac{i_{0\mathrm{c}} S R_{\mathrm{agg}}^2}{4F c_{\mathrm{O_2,ref}} D_{\mathrm{agg}}} \exp\left(-\frac{F}{2RT}\eta_c\right)}$$

$$\beta_{\mathrm{a}} = \left[c_{\mathrm{H_2,agg}} - c_{\mathrm{H_2,ref}} \exp\left(\frac{-2F}{RT}\eta_{\mathrm{a}}\right)\right] \qquad \beta_{\mathrm{c}} = c_{\mathrm{O_2,agg}}$$

In these equations, D_{agg} is the agglomerate gas diffusivity (SI unit: m^2/s), n_e is a "charge transfer" number (1 for the anode and –2 for the cathode), S is the specific area of the catalyst inside the agglomerate (SI unit: $1/\mathrm{m}$), and F is Faraday's constant (SI unit: C/mol). Furthermore, $c_{i,\mathrm{ref}}$ are the reference concentrations of the species (SI unit: $\mathrm{mol}/\mathrm{m}^3$), $c_{i,\mathrm{agg}}$ are the corresponding concentrations in the agglomerate surface (SI unit: $\mathrm{mol}/\mathrm{m}^3$), $i_{0\mathrm{a}}$ and $i_{0\mathrm{c}}$ are the exchange current densities (SI unit: A/m^2), R is the gas constant, T is the temperature (SI unit: K), and the overvoltages at the anode and the cathode are given by

$$\eta_{\mathrm{a}} = \phi_s - \phi_l - E_{\mathrm{eq,a}} \qquad \eta_{\mathrm{c}} = \phi_s - \phi_l - E_{\mathrm{eq,c}}$$

where E_{eq} (SI unit: V) denotes the equilibrium voltage.

You set the anodic and cathodic reference states equal to the molar fractions at the inlet channels of the anode and cathode, respectively, at 1 atm. The dissolved hydrogen and oxygen concentrations at the surface of the agglomerates are related to the molar fractions of the respective species in the gas phase through Henry's law

$$c_{\text{agg, H2}} = \frac{p_{\text{H}} x_{\text{H}}}{K_{\text{H}}}$$

$$c_{\text{agg, O2}} = \frac{p_{\text{O2}} x_{\text{O2}}}{K_{\text{O2}}}$$

where K is Henry's constant (SI unit: Pa·m^3/mol).

CHARGE BALANCES, CONTINUED

The potential difference between the cathode and anode current collectors corresponds to the total cell voltage. Choose the potential at the anode current collector as the reference level by setting it to zero. Then the total cell voltage serves as the boundary condition at the cathode current collector:

$$\phi_s = 0 \quad \text{at } \partial\Omega_{\text{a, cc}}$$
$$\phi_s = V_{\text{cell}} \text{ at } \partial\Omega_{\text{c, cc}}$$

For the other boundaries you have electric insulation boundary conditions.

POROUS MEDIA FLUID FLOW

To model the gas flows in the gas backings, this example uses the Darcy's law in the Hydrogen Fuel Cell interface. The gas velocity is given by the continuity equation according to

$$\nabla \cdot (\rho \mathbf{u}) = 0 \qquad \text{in } \Omega_{\text{a}} \text{ and } \Omega_{\text{c}}$$

where ρ is the mixture density of the gas phase (SI unit: kg/m^3) and $\mathbf{u}$ denotes the gas velocity (SI unit: m/s). Darcy's law for porous media states that the gradient of pressure, the viscosity of the fluid, and the structure of the porous media determine the velocity:

$$\mathbf{u} = -\frac{k_p}{\eta} \nabla p$$

Here k_p denotes the electrode's permeability (SI unit: m^2), η represents the gas viscosity (SI unit: Pa·s), and p is the pressure (SI unit: Pa). The ideal gas law gives the gas phase's mixture density, ρ:

$$\rho = \frac{p}{RT} \sum_i M_i x_i \tag{3}$$

In this equation, R denotes the gas constant (SI unit: J/(mol·K)), T is the temperature (SI unit: K), M is the molar mass (SI unit: kg/mol), and x is the mole fraction.

At the inlets you specify the pressure as follows:

$$p = p_{\mathrm{a,\,in}} \text{ at } \partial\Omega_{\mathrm{a,\,inlet1}}$$
$$p = p_{\mathrm{ref}} \text{ at } \partial\Omega_{\mathrm{a,\,inlet2}}$$
$$p = p_{\mathrm{c,\,in}} \text{ at } \partial\Omega_{\mathrm{c,\,inlet1}}$$
$$p = p_{\mathrm{ref}} \text{ at } \partial\Omega_{\mathrm{c,\,inlet2}}$$

At the thin gas diffusion electrode boundary for the anode and cathode, the gas velocity is calculated automatically by the Hydrogen Fuel Cell interface, from the total mass flow given by the electrochemical reaction rate and the stoichiometric coefficients of Equation 1 and Equation 2, using Faraday's law.

MAXWELL-STEFAN MASS TRANSPORT

The model takes into account two species in the anode — H_2 and H_2O — and three at the cathode — O_2, H_2O, and N_2. The Hydrogen Fuel Cell interface uses Maxwell-Stefan multicomponent diffusion governed by the equations

$$\frac{\partial}{\partial t}\rho w_i + \nabla\cdot\left[-\rho w_i\sum_{j=1}^{N} D_{ij}\left\{\frac{M}{M_j}\left(\nabla w_j + w_j\frac{\nabla M}{M}\right) + (x_j - w_j)\frac{\nabla p}{p}\right\} + w_i\rho\mathbf{u} + D_i^T\frac{\nabla T}{T}\right] = R_i$$

to solve for the mass fractions, w_i. This particular PEM fuel cell model assumes that the temperature-driven diffusion is insignificant and sets the source term, R, to zero. The Maxwell-Stefan binary diffusion coefficients, D_{ij} (SI unit: m^2/s), are calculated automatically by the interface. In the porous GDLs, effective binary diffusion coefficients, $D_{ij,\mathrm{eff}}$, need to be considered using a porous media diffusivity correction. This correction is based on the porosity, ε_g, and tortuosity, τ_g, giving the following binary diffusion coefficient definition

$$D_{ij,\mathrm{eff}} = \varepsilon_g\tau_g^{-1}D_{ij}$$

where the tortuosity is defined as a tensor in the form of a diagonal 2 x 2 matrix

$$\tau_g = \begin{bmatrix} \tau_{g,\,xx} & 0 \\ 0 & \tau_{g,\,yy} \end{bmatrix}$$

The feed-gas mole fractions are specified at the inlets. At the thin gas diffusion electrode boundaries, the mass fluxes of the species are automatically determined from the electrochemical reaction rate and stoichiometric coefficients, using Faraday's law. The Stefan velocity contributions are also automatically calculated by the interface.

The Membrane Transport features of the Hydrogen Fuel Cell interface are used to model the transport of water in the ionomer phase in the membrane domain. The molecular flux of water depends both on chemical potential gradient driven permeation and electroosmotic drag, using experimentally estimated parameters available in the Nafion material in the Fuel Cell and Electrolyzer Material Library.

Results and Discussion

Figure 2 shows polarization curves for the PEM fuel cell. Four cases are displayed to visualize the influence of tortuosity in the GDLs on the performance. In the anisotropic cases, the tortuosity settings correspond to more diffusivity limitations either along the height (y) or the thickness (x) of each GDL.

Results indicate that the cell performance is particularly sensitive to an increased tortuosity in the x-direction and is due to the fact that reactants need to pass through the layer thickness to reach the thin electrode layer. However, the increased tortuosity in the y-

direction represents the most realistic scenario since the in-plane GDL structure, parallel to the y-direction, is usually more tortuous.

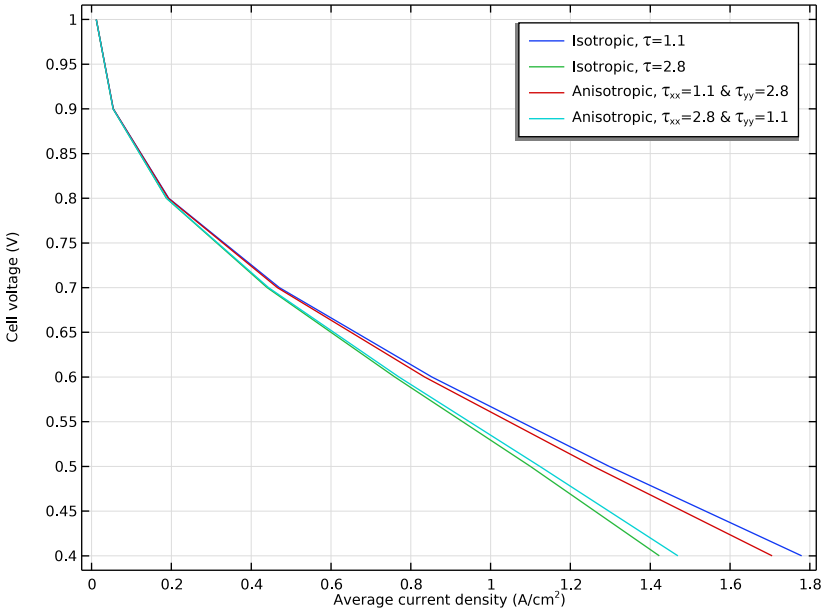

Figure 2: Polarization curves for the PEM fuel cell for different tortuosity conditions in the GDLs.

For the more realistic anisotropic tortuosity case ($\tau_{xx} = 1.1$ and $\tau_{yy} = 2.8$), a small but evident difference increasing with current density is shown compared to the corresponding isotropic tortuosity case ($\tau = 1.1$).

The current density at the active layer at the anode is displayed as a function of cell height in Figure 3. An uneven current distribution can be seen for both plotted cases, with the situation being more pronounced with anisotropic tortuosity.

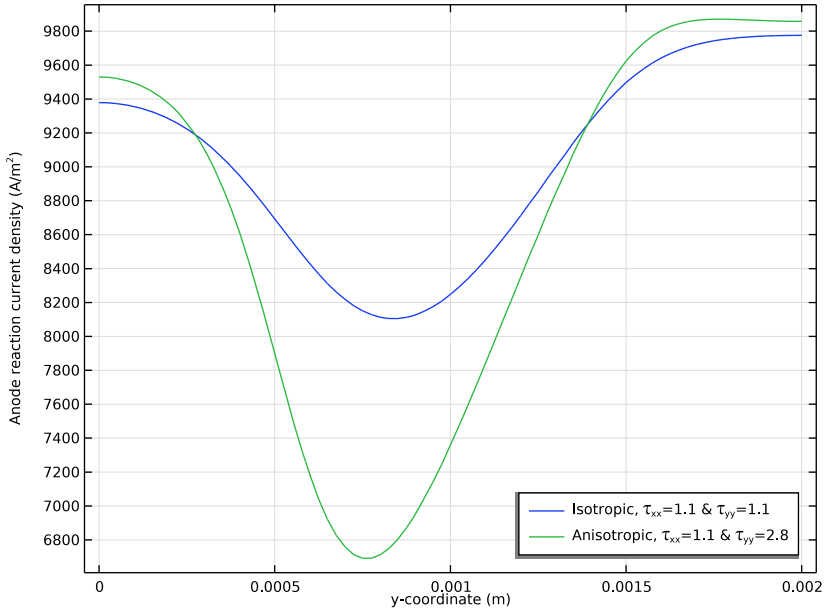

Figure 3: Current-density distribution at the anodic active layer for the PEM fuel cell operating at 0.4 V for two GDL tortuosity cases.

The current density is the highest in the cell's upper region but with even less activity in the center of the layer if anisotropic tortuosity is considered. For both cases, the oxygen-reduction reaction rate in the cathode determines the current-density distribution. The maximum current density arises close to the air inlet.

Figure 4 and Figure 5 depict the reactant (oxygen and hydrogen) weight fractions in the cathode and anode gases for the isotropic and anisotropic cases, respectively. The reactant minimum is decreasing substantially in the latter case and is consistent with the minimum in the current-density distribution.

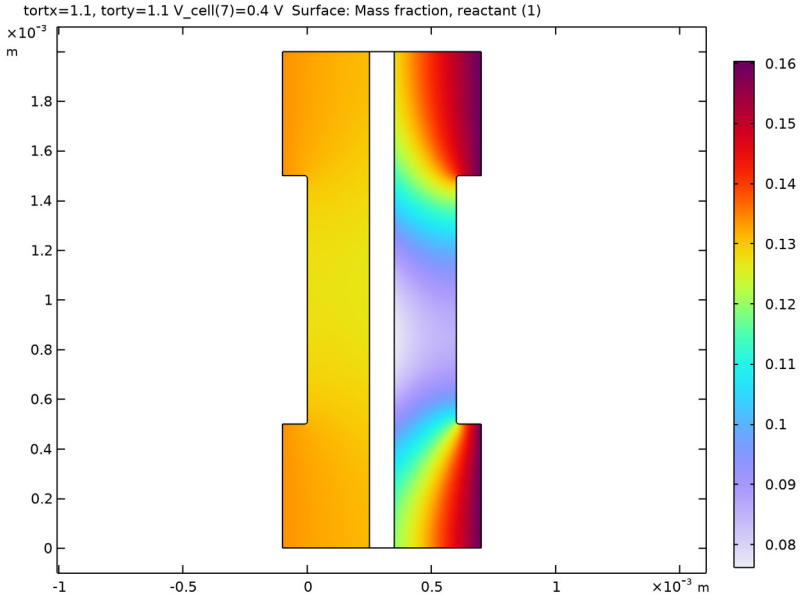

Figure 4: Reactant mass fractions on the anode side (left) and cathode side (right) at 0.4 V with isotropic GDL tortuosity. The reactant in the anode is hydrogen and that in the cathode is oxygen.

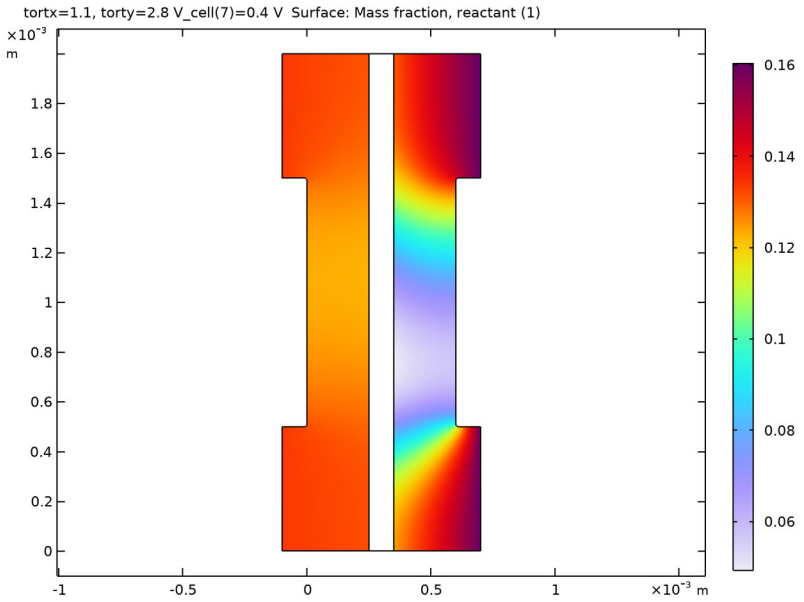

Figure 5: Reactant mass fractions on the anode side (left) and cathode side (right) at 0.4 V with anisotropic GDL tortuosity. The reactant in the anode is hydrogen and that in the cathode is oxygen.

Figure 6 and Figure 7 show the current distribution over the fuel cell for the isotropic and anisotropic cases, respectively. The minimum near the center of the cell is slightly lower in the latter case, but the difference is small and local. This displays that over the cell level, the system is not especially affected by higher in-plane tortuosity for species diffusion in the GDLs. A behavior also manifested in the small loss in performance (Figure 2).

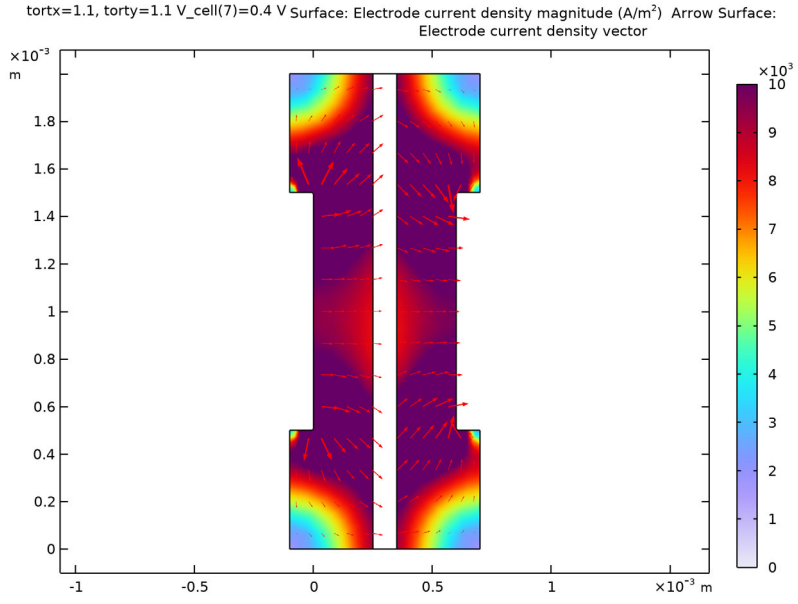

Figure 6: Current density (surface plot) and current vector field (arrow plot) in fuel cell operating at 0.4 V with isotropic GDL tortuosity. The anode is on the left and the cathode is on the right.

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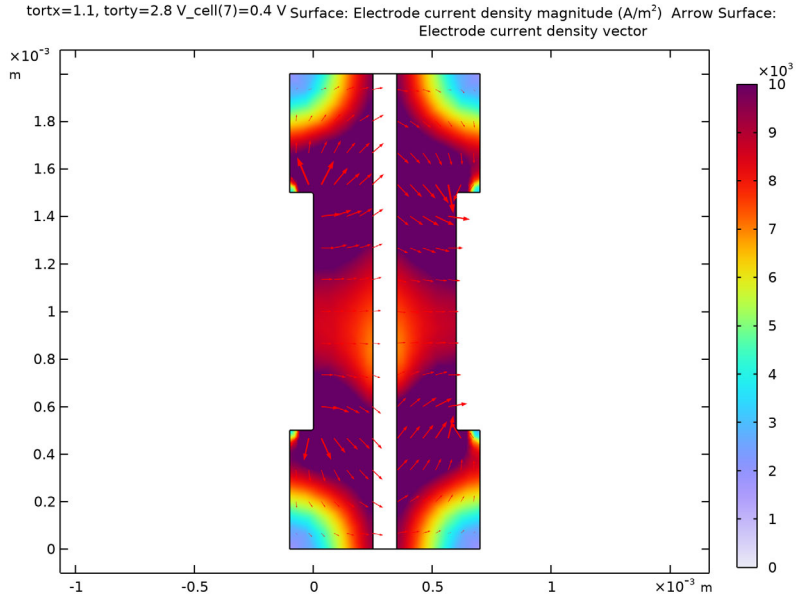

Figure 7: Current density (surface plot) and current vector field (arrow plot) in fuel cell operating at 0.4 V with anisotropic GDL tortuosity. The anode is on the left and the cathode is on the right.

Other processes accounted for in the model, mainly convective mass-transport flux, dictate the fuel cell performance. In Figure 8, the velocity field for the PEM is shown. The field

is close to identical for all investigated tortuosities. It should be noted that the gas permeability is set be tortuosity independent in this model.

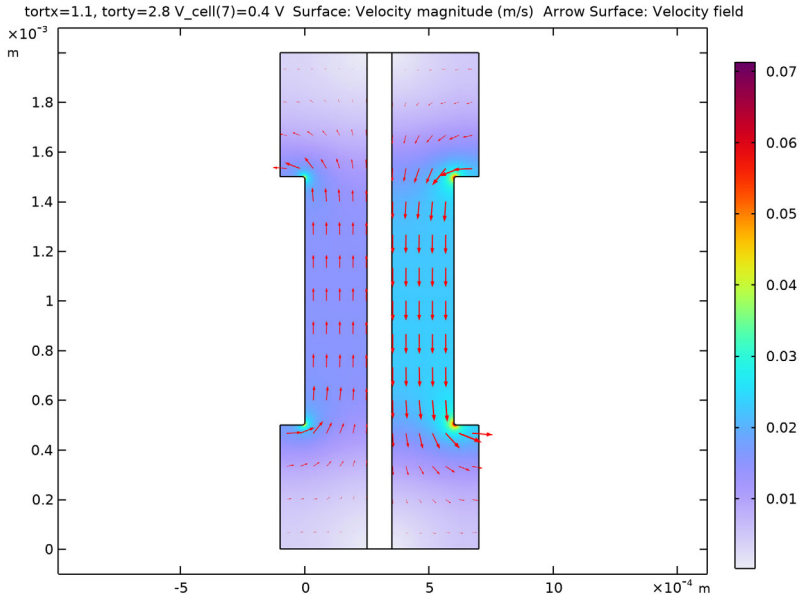

Figure 8: Gas velocity field in the anode and cathode compartments at 0.4 V.

References

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3. P. Futerko and I.-M. Hsing, "Two-Dimensional Finite Element Method Study of the Resistance of Membranes in Polymer Electrolyte Fuel Cells," *Electrochimica Acta*, vol. 45, pp. 1741–1751, 2000.

4. D.M. Bernardi and M.W. Verbrugge, "Mathematical Model of a Gas Diffusion Electrode Bonded to a Polymer Electrolyte," *AIChe J.*, vol. 37, pp. 1151–1163, 1991.

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6. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, John Wiley & Sons, 1960.

7. K. Broka and P. Ekdunge, "Modelling the PEM fuel cell cathode," *J. Appl. Electrochem.*, vol. 27, pp. 281–289, 1997.

8. K. Dannenberg, P. Ekdunge, and G. Lindbergh, "Mathematical model of the PEMFC", *J. Appl. Electrochem.*, vol. 30, pp. 1377–1387, 2000.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pem_gdl_species_transport_2d`

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 **2D**.

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

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Stationary with Initialization**.

6 Click **Done**.

GEOMETRY 1

Create the geometry using rectangles.

Rectangle 1 (r1)

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

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `2.5e-4`.

4 In the **Height** text field, type `2e-3`.

Rectangle 2 (r2)

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

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `1e-4`.

4 In the **Height** text field, type `2e-3`.

5 Locate the **Position** section. In the **x** text field, type `2.5e-4`.

Rectangle 3 (r3)

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

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `2.5e-4`.

4 In the **Height** text field, type `2e-3`.

5 Locate the **Position** section. In the **x** text field, type `3.5e-4`.

Rectangle 4 (r4)

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

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `1e-4`.

4 In the **Height** text field, type `5e-4`.

5 Locate the **Position** section. In the **x** text field, type `-1e-4`.

Array 1 (arr1)

1 In the **Geometry** toolbar, click **Transforms** and choose **Array**.

2 Select the object **r4** only.

3 In the **Settings** window for **Array**, locate the **Size** section.

4 In the **x size** text field, type `2`.

5 In the **y size** text field, type `2`.

6 Locate the **Displacement** section. In the **x** text field, type `7e-4`.

7 In the **y** text field, type `1.5e-3`.

Union 1 (uni1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

2 Select the objects **arr1(1,1)**, **arr1(1,2)**, and **r1** only.

3 In the **Settings** window for **Union**, locate the **Union** section.

4 Clear the **Keep interior boundaries** check box.

Union 2 (uni2)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

2 Select the objects **arr1(2,1)**, **arr1(2,2)**, and **r3** only.

3 In the **Settings** window for **Union**, locate the **Union** section.

4 Clear the **Keep interior boundaries** check box.

Fillet 1 (fil1)

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

2 In the **Settings** window for **Fillet**, locate the **Points** section.

3 Click to clear the **Activate Selection** toggle button for **Vertices to fillet**.

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

5 On the object **uni1**, select Points 6 and 7 only.

6 On the object **uni2**, select Points 4 and 5 only.

7 Click to select the **Activate Selection** toggle button for **Vertices to fillet**.

8 On the object **uni1**, select Points 6 and 7 only.

9 On the object **uni2**, select Points 4 and 5 only.

10 Locate the **Radius** section. In the **Radius** text field, type `1e-5`.

11 In the **Geometry** toolbar, click **Build All**.

GLOBAL DEFINITIONS

Proceed to load a set of global model parameters from a text file provided with the Application Library.

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 `pem_gdl_species_transport_2d_parameters.txt`.

DEFINITIONS

Set up a number of selections on the geometry. These will be used later when setting up the physics.

Anode GDL

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

2 Select Domain 1 only.

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

Membrane

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

2 Select Domain 2 only.

3 In the **Settings** window for **Explicit**, type `Membrane` in the **Label** text field.

Cathode GDL

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

2 Select Domain 3 only.

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

Anode GDE

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

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 10 only.

5 In the **Label** text field, type `Anode GDE`.

Cathode GDE

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

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 13 only.

5 In the **Label** text field, type `Cathode GDE`.

Anode GDL Variables

Define a number of domain- and boundary-specific variables. These will be used both for setting up the physics and in postprocessing.

1 In the **Definitions** toolbar, click **Local Variables**.

2 In the **Settings** window for **Variables**, type `Anode 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 **Anode GDL**.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
wReact	fc.wH2		Mass fraction, reactant

Cathode GDL Variables

1 In the **Definitions** toolbar, click a= **Local Variables**.

2 In the **Settings** window for **Variables**, type `Cathode 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 **Cathode GDL**.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
wReact	fc.wO2		Mass fraction, reactant

Anode GDE Variables

1 In the **Definitions** toolbar, click a= **Local Variables**.

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

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

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

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
cH2_agg	fc.p*fc.xH2/KH2		Henry's law hydrogen agglomerate concentration
eta_a	fc.phis-fc.phil-E_eq_a	V	Anodic overpotential
beta_a	cH2_agg-cH2_ref*exp(-2*F_const*eta_a/(R_const*T))		

Name	Expression	Unit	Description
lda_a	sqrt(i0_a*S*R_agg^2/(2*F_const*cH2_ref*D_agg))		Anodic current density subexpression
i_a	K*(1-lda_a*coth(lda_a))*beta_a*(R_agg/3)		Anode current density

Cathode GDE Variables

1 In the **Definitions** toolbar, click **Local Variables**.

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

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

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

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
cO2_agg	fc.p*fc.xO2/KO2		Henry's law oxygen agglomerate concentration
eta_c	fc.phis-fc.phil-E_eq_c	V	Cathodic overvoltage
lda_c	sqrt(i0_c*S*R_agg^2*exp(-F_const*eta_c/(2*R_const*T))/(4*F_const*cO2_ref*D_agg))		Cathodic current density subexpression
i_c	-2*K*(1-lda_c*coth(lda_c))*cO2_agg*(R_agg/3)		Cathode current density

Average collector

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Average**.

2 In the **Settings** window for **Average**, type `Average collector` in the **Label** text field.

3 In the **Operator name** text field, type `aveop_ca`.

4 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

5 Select Boundaries 8, 23, and 24 only.

MATERIALS

This model uses polymer electrolyte material (Nafion 1100, vapor equilibrated) that is available in the material library. Add the material twice, and assign it first to the membrane domain, and next to the membrane boundaries adjacent to the gas phase nodes.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Fuel Cell and Electrolyzer>Polymer Electrolytes>Nafion, EW 1100, Vapor Equilibrated, Protonated**.

4 Right-click and choose **Add to Component 1 (comp1)**.

MATERIALS

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

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Nafion, EW 1100, Vapor Equilibrated, Protonated (mat1)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

3 Click **Clear Selection**.

4 Select Domain 2 only.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Fuel Cell and Electrolyzer>Polymer Electrolytes>Nafion, EW 1100, Vapor Equilibrated, Protonated**.

3 Right-click and choose **Add to Component 1 (comp1)**.

4 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

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

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Geometric entity level** list, choose **Boundary**.

3 Select Boundaries 10 and 13 only.

HYDROGEN FUEL CELL (FC)

Set up the current distribution and transport model. Include mass transport using Maxwell-Stefan diffusion and momentum transport using Darcy's Law in both the anode and cathode gas mixtures, along with electroosmotic water drag in the membrane. Also, define the reference pressure level in the interface properties. Note that 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.

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 **Transport mechanisms** subsection. Select the **Use Darcy's Law for momentum transport** check box.

4 Locate the **O2 Gas Mixture** section. Select the **Use Darcy's Law for momentum transport** check box.

5 Click to expand the **Membrane Transport** section. Select the **Electroosmotic water drag** check box.

6 Click to expand the **Reference Pressure Level** section. In the p_{ref} text field, type 0.

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 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**.

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**.

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 **Anode GDE**.

Thin O2 Gas Diffusion Electrode 1

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 **Cathode GDE**.

In the **Electrolyte Phase** node, the electrolyte conductivity is set to be taken from the **Materials** node. Inspect the settings in the **H2 Gas Phase** and **O2 Gas Phase** nodes. Note that the density and viscosity of the gas mixture, and the binary diffusion coefficients are calculated automatically when the respective default settings are used.

The properties for electroosmotic water drag in the **Membrane** node and in the child nodes that added by default are automatically taken from the **Materials** node.

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 T_0 text field, type `T`.

H2 Gas Diffusion Layer 1

Set up the properties of the **H2 Gas Diffusion Layer** and **O2 Gas Diffusion Layer** nodes.

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 `kappa_s`.

4 Locate the **Gas Transport** section. From the **Effective diffusivity correction** list, choose **Tortuosity**.

5 In the ε_g text field, type `eps_mac`.

6 From the list, choose **Diagonal**.

7 In the τ_g table, enter the following settings:

`tortx`	`0`
`0`	`torty`

8 In the κ_g text field, type `kappa_p`.

O2 Gas Diffusion Layer 1

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

4 Locate the **Gas Transport** section. From the **Effective diffusivity correction** list, choose **Tortuosity**.

5 In the ε_g text field, type `eps_mac`.

6 From the list, choose **Diagonal**.

7 In the τ_g table, enter the following settings:

`tortx`	`0`
`0`	`torty`

8 In the κ_g text field, type `kappa_p`.

Thin H2 Gas Diffusion Electrode 1

Set up the properties of the **Thin H2 Gas Diffusion Electrode** node. The details of electrode kinetics are set in the child node.

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

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

3 In the d_{gde} text field, type `l_act`.

Thin H2 Gas Diffusion Electrode Reaction 1

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

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

3 From the E_{eq} list, choose **User defined**. Due to the user-defined kinetics expression, the equilibrium potential parameter is not in use in this model. Therefore keep the default value of 0 V.

4 Locate the **Electrode Kinetics** section. From the $i_{loc,expr}$ list, choose **User defined**. In the associated text field, type `i_a`.

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

Thin O2 Gas Diffusion Electrode 1

Similarly, set up the properties of the **Thin O2 Gas Diffusion Electrode** node. The details of electrode kinetics are set in the child node.

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

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

3 In the d_{gde} text field, type `l_act`.

Thin O2 Gas Diffusion Electrode Reaction 1

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

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

3 From the E_{eq} list, choose **User defined**. Also for the oxygen reduction reaction, the equilibrium potential parameter is not in use in this model. Therefore keep the default value of 0 V.

4 Locate the **Electrode Kinetics** section. From the $i_{\text{loc,expr}}$ list, choose **User defined**. In the associated text field, type `i_c`.

5 Locate the **Active Specific Surface Area** section. In the a_{v} text field, type `Av`.

Finally, set up the exterior boundary conditions and the initial values.

Electronic Conducting Phase 1

Set the initial value for electric potential in the cathode electrode to the cell potential. (The default zero initial values are used for both potentials in the rest of the geometry.)

1 In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** click **Electronic Conducting Phase 1**.

Initial Values, O2 Domains 1

1 In the **Physics** toolbar, click **Attributes** and choose **Initial Values, O2 Domains**.

2 Select Domain 3 only.

3 In the **Settings** window for **Initial Values, O2 Domains**, locate the **Initial Values** section.

4 In the ϕ_{s} text field, type `V_cell`.

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 8, 23, and 24 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 Boundary 17 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`.

H2 Gas Phase 1

In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** click **H2 Gas Phase 1**.

H2 Inlet 1

1 In the **Physics** toolbar, click **Attributes** and choose **H2 Inlet**.

2 Select Boundary 1 only.

3 In the **Settings** window for **H2 Inlet**, locate the **Flow Boundary Condition** section.

4 From the list, choose **Pressure**.

5 In the p_0 text field, type `p_a_in`.

H2 Gas Phase 1

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

H2 Inlet 2

1 In the **Physics** toolbar, click **Attributes** and choose **H2 Inlet**.

2 Select Boundary 4 only.

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 In the $x_{0,H2O}$ text field, type `xH2Oa_in`.

4 Locate the **Initial Pressure** section. In the p_0 text field, type `p_ref`.

O2 Gas Phase 1

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

O2 Inlet 1

1 In the **Physics** toolbar, click **Attributes** and choose **O2 Inlet**.

2 Select Boundary 22 only.

3 In the **Settings** window for **O2 Inlet**, locate the **Flow Boundary Condition** section.

4 From the list, choose **Pressure**.

5 In the p_0 text field, type `p_c_in`.

O2 Gas Phase 1

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

O2 Inlet 2

1 In the **Physics** toolbar, click **Attributes** and choose **O2 Inlet**.

2 Select Boundary 21 only.

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 In the $x_{0,\mathrm{H2O}}$ text field, type `xH2Oc_in`.

4 In the $x_{0,\mathrm{N2}}$ text field, type `xN2_in`.

5 Locate the **Initial Pressure** section. In the p_0 text field, type `p_ref`.

GLOBAL DEFINITIONS

Default Model Inputs

Since we will be using the same temperature everywhere in the model, we will define the temperature only once in the **Default Model Inputs** node. 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

Steep gradients are expected close to the electrodes and at the corner points where the ribs of the flow plates are suppressed into the GDL. Create a mesh with finer resolution at these parts of the geometry.

Size 1

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

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 10 and 13 only.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section.

7 Select the **Maximum element size** check box. In the associated text field, type `2.5e-5`.

Size 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Points 5, 6, 16, and 17 only.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section.

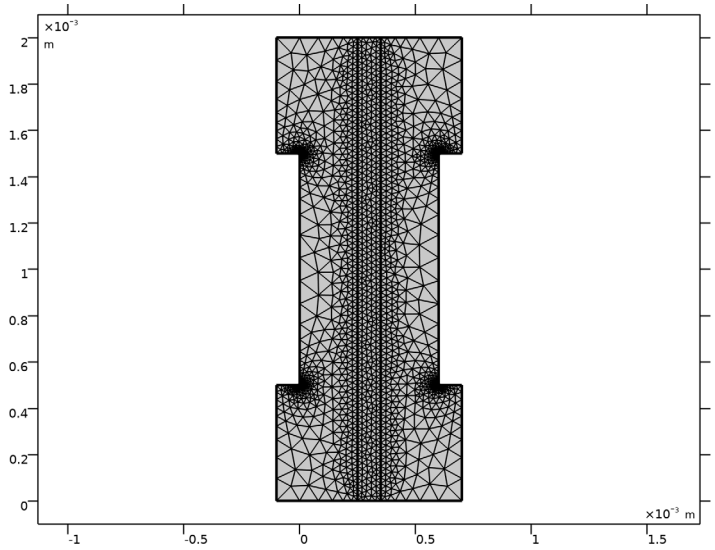
7 Select the **Maximum element size** check box. In the associated text field, type `1e-5`.

Free Triangular 1

1 In the **Mesh** toolbar, click  **Free Triangular**.

2 Right-click **Mesh 1** and choose **Build All**.

The finalized mesh should now look as follows:



STUDY 1

The problem is now ready for solving. In the first step, solve for secondary current distribution initialization.

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 **Study Settings** section.

3 From the **Current distribution type** list, choose **Secondary**.

Step 2: Stationary

1 In the **Model Builder** window, click **Step 2: 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**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V_cell (Cell voltage)	range(1,-0.1,0.4)	V

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
tortx (Tortuosity, x-direction)	1.1 2.8	

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
torty (Tortuosity, y-direction)	1.1 2.8	

7 From the **Sweep type** list, choose **All combinations**.

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

RESULTS

The following steps reproduce the figures found in the Results and Discussion section.

Polarization curves

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Polarization curves` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `Average cell current density (A/m<sup>2</sup>)`.

7 Select the **y-axis label** check box. In the associated text field, type `Cell voltage (V)`.

8 Select the **Flip the x- and y-axes** check box.

Global 1

1 Right-click **Polarization curves** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
aveop_ca(-fc.nIs)	A/cm^2	Average current density (A/cm>sup>2</sup>)

4 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

Legends
Isotropic, \tau_{xx}=1.1 & \tau_{yy}=1.1
Anisotropic, \tau_{xx}=1.1 & \tau_{yy}=2.8
Anisotropic, \tau_{xx}=2.8 & \tau_{yy}=1.1
Isotropic, \tau_{xx}=2.8 & \tau_{yy}=2.8

GDL Current Density Distribution

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 From the **Parameter value (tortx)** list, choose **1.1**.

5 From the **Parameter value (torty)** list, choose **1.1**.

Surface 1

1 Right-click **GDL Current Density Distribution** 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.IsMag - Electrode current density magnitude - A/m²**.

3 Click to expand the **Range** section. Select the **Manual color range** check box.

4 In the **Maximum** text field, type 1e4.

5 Click to expand the **Coloring and Style** section. Click **Change Color Table**.

6 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

7 Click **OK**.

Arrow Surface 1

1. In the **Model Builder** window, right-click **GDL Current Density Distribution** and choose **Arrow Surface**.
2. In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Hydrogen Fuel Cell>fc.Isx,fc.Isy - Electrode current density vector**.
3. Click to expand the **Coloring and Style** section.
4. Select the **Scale factor** check box. In the associated text field, type `5e-9`.
5. In the **GDL Current Density Distribution** toolbar, click **Plot**.
6. Click the **Zoom Extents** button in the **Graphics** toolbar.

GDL Current Density Distribution

1. In the **Model Builder** window, click **GDL Current Density Distribution**.
2. In the **Settings** window for **2D Plot Group**, locate the **Data** section.
3. From the **Parameter value (torty)** list, choose **2.8**.
4. In the **GDL Current Density Distribution** toolbar, click **Plot**.
5. Click the **Zoom Extents** button in the **Graphics** toolbar.

Anode Reaction Current Density

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Anode Reaction Current Density` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **None**.
4. Click to expand the **Title** section. From the **Title type** list, choose **None**.
5. Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Line Graph 1

1. Right-click **Anode Reaction Current Density** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Data** section.
3. From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.
4. From the **Parameter selection (tortx)** list, choose **First**.
5. From the **Parameter selection (torty)** list, choose **First**.
6. From the **Parameter selection (V_cell)** list, choose **Last**.
7. Locate the **Selection** section. From the **Selection** list, choose **Anode GDE**.

8 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>i_a - Anode current density - A/m²**.

9 Locate the **y-Axis Data** section. In the **Expression** text field, type `i_a*Av*l_act`.

10 Select the **Description** check box. In the associated text field, type `Anode reaction current density`.

11 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1)>Geometry>Coordinate>y - y-coordinate**.

12 Click to expand the **Legends** section. Select the **Show legends** check box.

13 From the **Legends** list, choose **Manual**.

14 In the table, enter the following settings:

Legends
`Isotropic, \tau<sub>xx</sub>=1.1 & \tau<sub>yy</sub>=1.1`

15 Right-click **Line Graph 1** and choose **Duplicate**.

Line Graph 2

1 In the **Model Builder** window, click **Line Graph 2**.

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 From the **Parameter selection (torty)** list, choose **Last**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Anisotropic, \tau<sub>xx</sub>=1.1 & \tau<sub>yy</sub>=2.8`

5 In the **Anode Reaction Current Density** toolbar, click **Plot**.

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

Velocity Field

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Velocity Field` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 From the **Parameter value (tortx)** list, choose **1.1**.

Surface 1

1 Right-click **Velocity Field** 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.U - Velocity magnitude - m/s**.

3 Locate the **Coloring and Style** section. Click **Change Color Table**.

4 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

5 Click **OK**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Velocity Field** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Hydrogen Fuel Cell>fc.u,fc.v - Velocity field**.

3 Locate the **Coloring and Style** section.

4 Select the **Scale factor** check box. In the associated text field, type `0.0035`.

5 In the **Velocity Field** toolbar, click **Plot**.

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

Reactant Mass Fraction

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Reactant Mass Fraction` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 From the **Parameter value (tortx)** list, choose **1.1**.

5 From the **Parameter value (torty)** list, choose **1.1**.

Surface 1

1 Right-click **Reactant Mass Fraction** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `wReact`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

6 Click **OK**.

7 In the **Reactant Mass Fraction** toolbar, click **Plot**.

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

Reactant Mass Fraction

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

2 From the **Parameter value (torty)** list, choose **2.8**.

3 In the **Model Builder** window, expand the **Reactant Mass Fraction** node.

Electrode Potential with Respect to Ground (fc), Electrolyte Potential (fc)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Electrode Potential with Respect to Ground (fc)** and **Electrolyte Potential (fc)**.

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