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. 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 a 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.

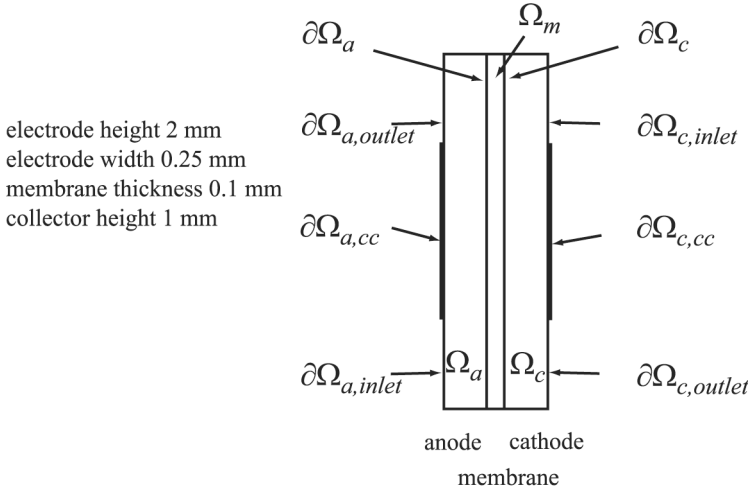

Figure 1: Model geometry with domain and boundary labels.

Each of the electrodes (gas diffusion layers) is in contact with an interdigitated gas distributor, which has an inlet channel ($\partial\Omega_{a,inlet}$), a current collector ($\partial\Omega_{a,cc}$), and an outlet channel ($\partial\Omega_{a,outlet}$). The same notation is used for the cathode side.

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. Each proton is assumed to drag three molecules of water from the anode to the cathode, resulting in the following reaction formula for the anode:

$$H_2 + 2\lambda_{H2O}H_2O \Rightarrow 2\left(H^+ + \lambda_{H2O}H_2O\right) + 2e^- \quad (1)$$

Where λ_{H2O} is the number of water molecules that are transported per proton through the membrane by water-proton interaction.

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

$$O_2 + 4\left(H^+ + \lambda_{H2O}H_2O\right) + 4e^- \Rightarrow (2 + 4\lambda_{H2O})H_2O \quad (2)$$

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 diffusion 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 Secondary Current Distribution interface is used for modeling the potential distributions in the three domains and this example models the active layers of the two electrodes as boundaries. This means that you treat the charge-transfer current density expression as an Electrolyte-Electrode Domain Interface internal boundary condition.

The current density expressions for the anode and cathode, i_a and i_c, are specified according to the equation

$$i_e = L_{act}(1-\varepsilon_{mac})j_{agg,e} \tag{3}$$

where the index e stands for "a" (anode) or "c" (cathode). Further, L_{act} is the active layer's thickness (m), ε_{mac} its porosity (the macroscopic porosity), and $j_{agg,a}$ and $j_{agg,c}$ are the current densities given by the agglomerate model.

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)

$$j_{agg,e} = 6n_eF\left(\frac{D_{agg}}{R_{agg}^2}\right)(1-\lambda_e\coth\lambda_e)\beta_e \tag{4}$$

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

$$\lambda_a = \sqrt{\frac{i_{0a}SR_{agg}^2}{2Fc_{H_2,ref}D_{agg}}} \qquad \lambda_c = \sqrt{\frac{i_{0c}SR_{agg}^2}{4Fc_{O_2,ref}D_{agg}}\exp\left(-\frac{F}{2RT}\eta_c\right)} \tag{5}$$

$$\beta_a = \left[c_{H_2,ref} - c_{H_2,ref}\exp\left(\frac{-2F}{RT}\eta_a\right)\right] \qquad \beta_c = c_{O_2,agg} \tag{6}$$

In these equations, D_{agg} is the agglomerate gas diffusivity (m^2/s), R_{agg} is the agglomerate radius (m), 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 ($1/m$), and F is Faraday's constant (C/mol). Furthermore, $c_{i,ref}$ are the reference concentrations of the species (mol/m^3), $c_{i,agg}$ are the corresponding concentrations in the agglomerate surface (mol/m^3), i_{0a} and i_{0c} are the exchange current densities (A/m^2), R is the gas constant, T is the temperature (K), and the overvoltages at the anode and the cathode are given by

$$\eta_a = \phi_s - \phi_l - E_{eq,a} \qquad \eta_c = \phi_s - \phi_l - E_{eq,c} \tag{7}$$

where E_{eq} (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

$$\begin{aligned} c_{\text{agg, H2}} &= \frac{p_{\text{H}} x_{\text{H}}}{K_{\text{H}}} \\ c_{\text{agg, O2}} &= \frac{p_{\text{O}} x_{\text{O}}}{K_{\text{O}}} \end{aligned} \tag{8}$$

where K is Henry's constant (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:

$$\begin{aligned} \phi_s &= 0 \quad \text{at } \partial\Omega_{\text{a, cc}} \\ \phi_s &= V_{\text{cell}} \text{ at } \partial\Omega_{\text{c, cc}} \end{aligned} \tag{9}$$

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 interface. The gas velocity is given by the continuity equation according to

$$\nabla \cdot (\rho \mathbf{u}) = 0 \qquad \text{in } \Omega_{\text{a}} \text{ and } \Omega_{\text{c}}. \tag{10}$$

where ρ is the mixture density of the gas phase (kg/m^3) and $\mathbf{u}$ denotes the gas velocity (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:

$$\mathbf{u} = -\frac{k_p}{\eta} \nabla p \tag{11}$$

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

$$\rho = \frac{p}{RT}\sum_i M_i x_i \tag{12}$$

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

At the inlets and outlets you specify the pressure:

$$\begin{aligned} p &= p_{\mathrm{a,\,in}} \text{ at } \partial\Omega_{\mathrm{a,\,inlet}} \\ p &= p_{\mathrm{ref}} \text{ at } \partial\Omega_{\mathrm{a,\,outlet}} \\ p &= p_{\mathrm{c,\,in}} \text{ at } \partial\Omega_{\mathrm{c,\,inlet}} \\ p &= p_{\mathrm{ref}} \text{ at } \partial\Omega_{\mathrm{c,\,outlet}} \end{aligned} \tag{13}$$

At the electrode boundary for the anode and cathode, the gas velocity is calculated from the total mass flow given by the stoichiometric coefficients of Equation 1 and 2 using Faraday's law, resulting in:

$$-\mathbf{n}\cdot\mathbf{u}\big|_{\mathrm{anode}} = \frac{j_{\mathrm{anode}}}{\rho F}\left(\frac{M_{\mathrm{H2}}}{2} + \lambda_{\mathrm{H2O}} M_{\mathrm{H2O}}\right) \tag{14}$$

$$-\mathbf{n}\cdot\mathbf{u}\big|_{\mathrm{cathode}} = \frac{j_{\mathrm{cathode}}}{\rho F}\left[\frac{M_{\mathrm{O2}}}{4} + \left(\frac{1}{2} + \lambda_{\mathrm{H2O}}\right) M_{\mathrm{H2O}}\right]. \tag{15}$$

Combined with these boundary conditions, Darcy's law determines the gas flow velocity and preserves the total mass conservation in the anode and cathode gas diffusion layers.

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 model uses one instance of the Transport of Concentrated Species interface for each electrode side. This physics interface uses Maxwell-Stefan multicomponent diffusion, governed by the following equations

$$\frac{\partial}{\partial t}\rho w_i + \nabla\cdot\left[-\rho w_i \sum_{j=1}^{N} \mathrm{D}_{ij}\left\{\frac{M}{M_j}\left(\nabla w_j + w_j\frac{\nabla M}{M}\right) + (x_j - w_j)\frac{\nabla p}{p}\right\} + w_i\rho\mathbf{u} + D_i^T\frac{\nabla T}{T}\right] = R_i \tag{16}$$

which the software solves 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. For the cathode gas, with three species (oxygen = 1, water = 2, nitrogen = 3), the mass transport is described by the following three equations together with Darcy's law, describing the flow rate:

$$\nabla \cdot \left\{ -\rho w_1 \sum_j [D_{1j}(\nabla x_j + (x_j - w_j)(\nabla p / p))] \right\} = -(\rho \mathbf{u} \cdot \nabla w_1) \tag{17}$$

$$\nabla \cdot \left\{ -\rho w_2 \sum_j [D_{2j}(\nabla x_j + (x_j - w_j)(\nabla p / p))] \right\} = -(\rho \mathbf{u} \cdot \nabla w_2) \tag{18}$$

$$w_3 = 1 - w_1 - w_2 \tag{19}$$

Here p is the pressure (Pa), T is the temperature (K), and $\mathbf{u}$ is the velocity (m/s). The density of the mixture is given by Equation 12. The Maxwell-Stefan diffusivity matrix, D_{ij} (m^2/s), is calculated from the binary diffusivities you specify in the physics interface.

The feed-gas mass fractions are specified at the inlets. At the outlets, convective flux boundary conditions are applied, meaning that the flux is convection dominated. At the electrode-membrane boundary, the mass fluxes of hydrogen in the cathode, and of oxygen and water in the cathode, are determined by the electrochemical reaction rate:

$$-\mathbf{n} \cdot \mathbf{N}_{\mathrm{H2}}\big|_{\mathrm{anode}} = \frac{j_{\mathrm{anode}}}{2F} M_{\mathrm{H2}} \tag{20}$$

$$-\mathbf{n} \cdot \mathbf{N}_{\mathrm{O2}}\big|_{\mathrm{cathode}} = \frac{j_{\mathrm{cathode}}}{4F} M_{\mathrm{O2}} \tag{21}$$

$$-\mathbf{n} \cdot \mathbf{N}_{\mathrm{H2O}}\big|_{\mathrm{cathode}} = \frac{j_{\mathrm{cathode}}}{F}\left(\frac{1}{2} + \lambda_{\mathrm{H2O}}\right) M_{\mathrm{H2O}} \tag{22}$$

Results and Discussion

Figure 2 shows the current distribution in the PEM fuel cell. There are significant current spikes present at the corners of the current collectors.

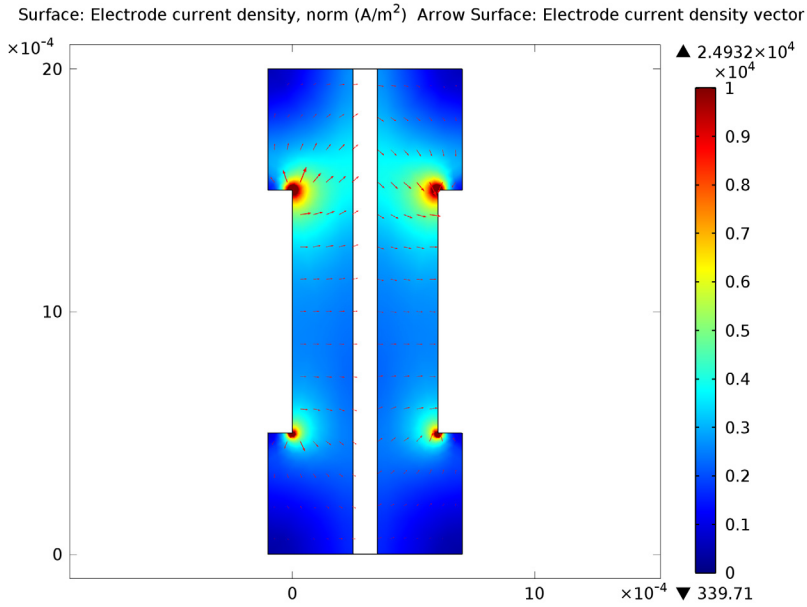

Figure 2: Current density (surface plot) and current vector field (arrow plot) in the fuel cell operating at 0.7 V. The anode is on the left and the cathode is on the right

To further analyze the cell's behavior, plot the current density at the active layer as a function of cell height (y) as in Figure 3.

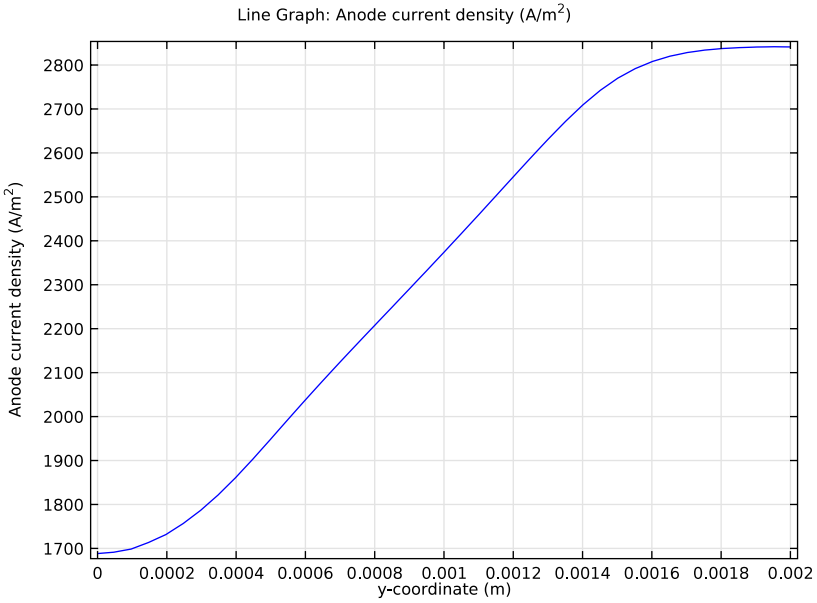

Figure 3: Current-density distribution at the active layer at the anode.

The current density is uneven with the highest density in the cell's upper region. This means that the oxygen-reduction reaction rate in the cathode determines the current-density distribution. The maximum current density arises close to the air inlet.

The convective fluxes generally dominate mass transport in the cell. To study the convective effects, plot the velocity field as in Figure 4.

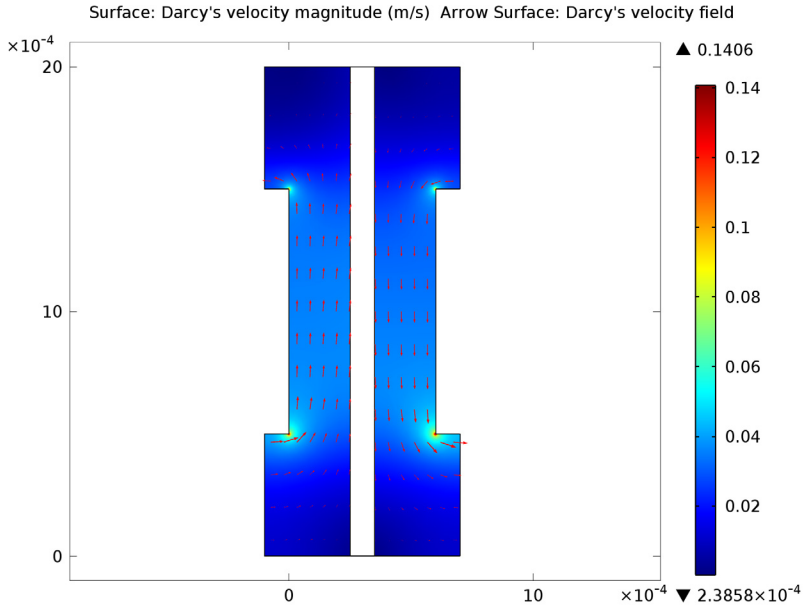

Figure 4: Gas velocity field in the anode and cathode compartments.

The flow-velocity magnitude attains its highest values at the current collector corners.

Figure 5 shows the reactant (oxygen and hydrogen) weight fractions in the cathode and anode gases. Surprisingly, the hydrogen fraction increases as the anode gas flows from the inlet (at the bottom) to the outlet (at the top). This is the result of the electroosmotic drag of water through the membrane, which results in a higher flux than the consumption of hydrogen. This means that the resulting convective flux of anode gas towards the membrane causes the weight fraction of hydrogen to go up. In the cathode gas, there is an expected decrease in oxygen content along the flow direction.

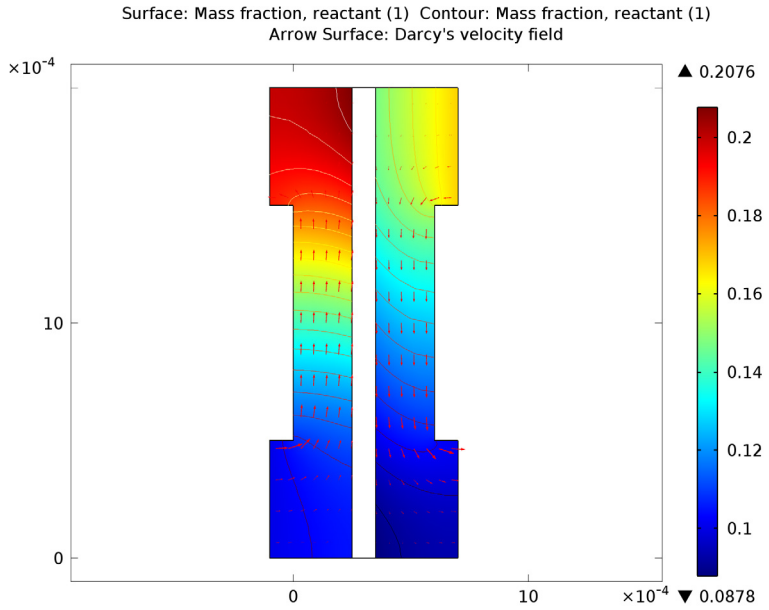

Figure 5: Reactant mass fractions, normalized by their inlet values, on the anode side (left) and cathode side (right). The reactant in the anode is hydrogen and that in the cathode is oxygen.

Although oxygen consumption is small, the concentration overvoltage in the agglomerates gives a substantial contribution to the concentration overvoltage. A small change in the oxygen flow gives a substantial change in cell polarization.

Figure 6 depicts the water mass fraction in the anode and cathode gases as well as the diffusive flux of water in the anode. It is apparent that water is transported through both diffusion and convection to the membrane on the anode side. The results show a minimum occurring in the upper corner of the membrane on the anode side. This is known to limit fuel cell performance. If the anode gas becomes too dry, the membrane dries out, resulting in decreasing ionic conductivity and the cell subsequently fails.

On the other hand, on the cathode side water levels increase with the direction of flow, and a local maximum in water current occurs in the lower corner to the membrane. This might also be critical because water droplets can clog the pores and effectively hinder gas transport to the active layer.

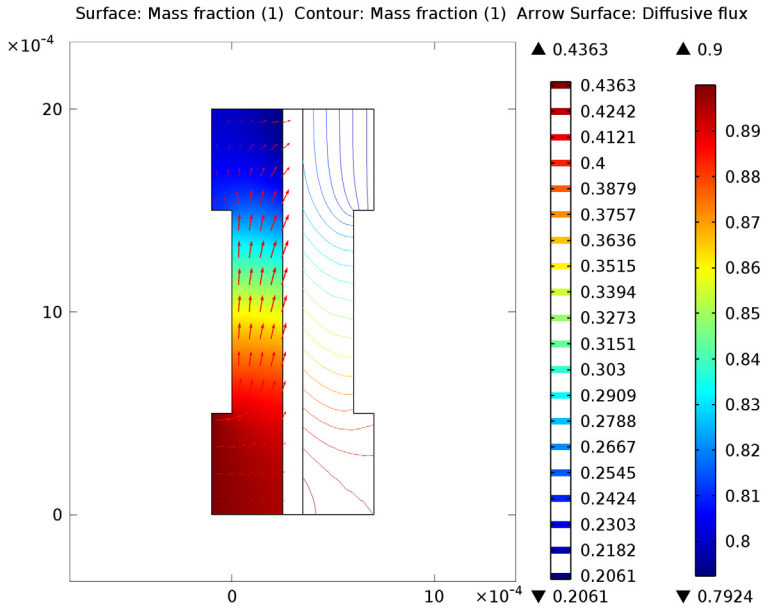

Figure 6: Water mass fraction in the anode (left, surface plot) and the cathode (right, contour plot). The arrows visualize the diffusive flux vector field on the anode side.

References

1. W. He, J.S. Yi, and T.V. Nguyen, "Two-Phase Flow Model of the Cathode of PEM Fuel Cells Using Interdigitated Flow Fields," *AIChe J.*, vol. 46, pp. 2053–2063, 2000.

2. C. Marr and X. Li, "Composition and Performance Modelling of Catalyst Layer in a Proton Exchange Membrane Fuel Cell," *J. Power Sources*, vol. 77, pp. 17–27, 1999.

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.

5. H. Scott Fogler, *Elements of Chemical Reaction Engineering*, 3rd ed., Prentice Hall, 1999.

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

7. K. Broka and P. Ekdunge, *J. Appl. Electrochem.*, vol. 27, p. 281, 1997.

8. K. Dannenberg, P. Ekdunge, and G. Lindbergh, *J. Appl. Electrochem.*, vol. 30, p. 1377, 2000.

Model Library path: `Batteries_and_Fuel_Cells_Module/PEMFC/pem_gdl_species_transport_2d`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

1 In the **New** window, click the **Model Wizard** button.

MODEL WIZARD

1 In the **Model Wizard** window, click the **2D** button.

2 In the **Select physics** tree, select **Electrochemistry>Secondary Current Distribution (siec)**.

3 Click the **Add** button.

4 In the **Select physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow>Darcy's Law (dl)**.

5 Click the **Add** button.

6 In the **Select physics** tree, select **Chemical Species Transport>Transport of Concentrated Species (chcs)**.

7 Click the **Add** button.

8 In the **Added physics** tree, select **Transport of Concentrated Species (chcs)**.

9 In the **Mass fractions** table, enter the following settings:

wH2
wH20a

10 In the **Select physics** tree, select **Chemical Species Transport>Transport of Concentrated Species (chcs)**.

11 Click the **Add** button.

12 In the **Added physics** tree, select **Transport of Concentrated Species (chcs2)**.

13 In the **Number of species** edit field, type 3.

14 In the **Mass fractions** table, enter the following settings:

w02
wH20c
wN2

15 Click the **Study** button.

16 In the tree, select **Preset Studies for Selected Physics>Stationary**.

17 Click the **Done** button.

GEOMETRY 1

Create the geometry using rectangles.

Rectangle 1

1 In the **Model Builder** window, under **Component 1** right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

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

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

Rectangle 2

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

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

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

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

Rectangle 3

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

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

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

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

Rectangle 4

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

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

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

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

Array 1

1 On the **Geometry** toolbar, click **Array**.

2 Select the object **r4** only.

3 In the **Array** settings window, locate the **Size** section.

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

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

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

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

Union 1

1 On the **Geometry** toolbar, click **Union**.

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

3 In the **Union** settings window, locate the **Union** section.

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

Union 2

1 On the **Geometry** toolbar, click **Union**.

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

3 In the **Union** settings window, locate the **Union** section.

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

5 Right-click **Geometry 1** and choose **Build All Objects**.

GLOBAL DEFINITIONS

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

Parameters

1 On the **Home** toolbar, click **Parameters**.

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Model Library 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.

Explicit 1

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

2 Select Domain 1 only.

3 Right-click **Component 1>Definitions>Explicit 1** and choose **Rename**.

4 Go to the **Rename Explicit** dialog box and type `Anode GDL` in the **New name** edit field.

5 Click **OK**.

Explicit 2

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

2 Select Domain 2 only.

3 Right-click **Component 1>Definitions>Explicit 2** and choose **Rename**.

4 Go to the **Rename Explicit** dialog box and type `Membrane` in the **New name** edit field.

5 Click **OK**.

Explicit 3

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

2 Select Domain 3 only.

3 Right-click **Component 1>Definitions>Explicit 3** and choose **Rename**.

4 Go to the **Rename Explicit** dialog box and type `Cathode GDL` in the **New name** edit field.

5 Click **OK**.

Explicit 4

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

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

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

4 Select Boundary 10 only.

5 Right-click **Component 1>Definitions>Explicit 4** and choose **Rename**.

6 Go to the **Rename Explicit** dialog box and type `Anode Electrode` in the **New name** edit field.

7 Click **OK**.

Explicit 5

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

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

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

4 Select Boundary 13 only.

5 Right-click **Component 1>Definitions>Explicit 5** and choose **Rename**.

6 Go to the **Rename Explicit** dialog box and type `Cathode Electrode` in the **New name** edit field.

7 Click **OK**.

Variables 1

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

1 Right-click **Definitions** and choose **Variables**.

2 In the **Model Builder** window, under **Component 1>Definitions** right-click **Variables 1** and choose **Rename**.

3 Go to the **Rename Variables** dialog box and type `Anode GDL Variables` in the **New name** edit field.

4 Click **OK**.

5 In the **Variables** settings window, locate the **Geometric Entity Selection** section.

6 From the **Geometric entity level** list, choose **Domain**.

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

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

Name	Expression	Unit	Description
`rho_mix`	`(chcs.x_wH2*MH2+chcs.x_wH2Oa*MH2O)*p/(R_const*T)`	kg/m³	`Fluid density`
`E`	`phis`		`Potential`
`xH2`	`chcs.x_wH2`		`Molar fraction, H2`

Name	Expression	Unit	Description
wH2O	wH2Oa		Mass fraction, H2O
wReact	wH2		Mass fraction, reactant

Variables 2

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 Right-click **Variables 2** and choose **Rename**.

3 Go to the **Rename Variables** dialog box and type `Membrane Variables` in the **New name** edit field.

4 Click **OK**.

5 In the **Variables** settings window, locate the **Geometric Entity Selection** section.

6 From the **Geometric entity level** list, choose **Domain**.

7 From the **Selection** list, choose **Membrane**.

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

Name	Expression	Unit	Description
E	phil	V	Potential

Variables 3

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 Right-click **Variables 3** and choose **Rename**.

3 Go to the **Rename Variables** dialog box and type `Cathode GDL Variables` in the **New name** edit field.

4 Click **OK**.

5 In the **Variables** settings window, locate the **Geometric Entity Selection** section.

6 From the **Geometric entity level** list, choose **Domain**.

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

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

Name	Expression	Unit	Description
rho_mix	(chcs2.x_wO2*MO2+chcs2.x_wH2Oc*MH2O+chcs2.x_wN2*MN2)*p/(R_const*T)	kg/m³	Fluid density
E	phis		Potential
xO2	chcs2.x_wO2		Molar fraction, O2

Name	Expression	Unit	Description
wReact	wO2		Mass fraction, reactant
wH2O	wH2Oc		Mass fraction, H2O

Variables 4

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 Right-click **Variables 4** and choose **Rename**.

3 Go to the **Rename Variables** dialog box and type `Anode Electrode Variables` in the **New name** edit field.

4 Click **OK**.

5 In the **Variables** settings window, locate the **Geometric Entity Selection** section.

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

7 From the **Selection** list, choose **Anode Electrode**.

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

Name	Expression	Unit	Description
cH2_agg	p*xH2/KH2	mol/m³	Henry's law hydrogen agglomerate concentration
eta_a	phis-phil-E_eq_a		Anodic overpotential
beta_a	cH2_agg*(1-exp(-2*F_const*eta_a/(R_const*T)))		
lda_a	sqrt(iO_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		Anode current density

Variables 5

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 Right-click **Variables 5** and choose **Rename**.

3 Go to the **Rename Variables** dialog box and type `Cathode Electrode Variables` in the **New name** edit field.

4 Click **OK**.

5 In the **Variables** settings window, locate the **Geometric Entity Selection** section.

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

7 From the **Selection** list, choose **Cathode Electrode**.

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

Name	Expression	Unit	Description
eta_c	phis-phil-E_eq_c		Cathodic over voltage
cO2_agg	p*xO2/KO2	mol/m³	Henry's law oxygen agglomerate concentration
lda_c	sqrt(iO_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		Cathode current density

SECONDARY CURRENT DISTRIBUTION

Now start setting up the physics. Start with the model for the electrochemical reactions and the current distribution.

Electrode 1

1 On the **Physics** toolbar, click **Domains** and choose **Electrode**.

2 Select Domains 1 and 3 only.

3 In the **Electrode** settings window, locate the **Electrode** section.

4 From the σ_s list, choose **User defined**. In the associated edit field, type `kappa_s`.

Electrolyte 1

1 In the **Model Builder** window, under **Component 1>Secondary Current Distribution** click **Electrolyte 1**.

2 In the **Electrolyte** settings window, locate the **Electrolyte** section.

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

Electric Ground 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Electric Ground**.

2 Select Boundary 8 only.

Electric Potential 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Electric Potential**.

2 Select Boundary 17 only.

3 In the **Electric Potential** settings window, locate the **Electric Potential** section.

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

Electrolyte-Electrode Domain Interface 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Electrolyte-Electrode Domain Interface**.

2 In the **Electrolyte-Electrode Domain Interface** settings window, locate the **Boundary Selection** section.

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

Electrode Reaction 1

1 In the **Model Builder** window, expand the **Electrolyte-Electrode Domain Interface 1** node, then click **Electrode Reaction 1**.

2 In the **Electrode Reaction** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **User defined**. In the i_{loc} edit field, type `i_a`.

Electrolyte-Electrode Domain Interface 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Electrolyte-Electrode Domain Interface**.

2 In the **Electrolyte-Electrode Domain Interface** settings window, locate the **Boundary Selection** section.

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

Electrode Reaction 1

1 In the **Model Builder** window, expand the **Electrolyte-Electrode Domain Interface 2** node, then click **Electrode Reaction 1**.

2 In the **Electrode Reaction** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **User defined**. In the i_{loc} edit field, type `i_c`.

Initial Values 2

Set the initial value for phis 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 On the **Physics** toolbar, click **Domains** and choose **Initial Values**.

2 Select Domain 3 only.

3 In the **Initial Values** settings window, locate the **Initial Values** section.

4 In the *phis* edit field, type `V_cell`.

DARCY'S LAW

Now define the model for the convective flow.

1 In the **Model Builder** window, under **Component 1** click **Darcy's Law**.

2 In the **Darcy's Law** settings window, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Manual**.

4 Select Domains 1 and 3 only.

Fluid and Matrix Properties 1

1 In the **Model Builder** window, under **Component 1>Darcy's Law** click **Fluid and Matrix Properties 1**.

2 In the **Fluid and Matrix Properties** settings window, locate the **Fluid Properties** section.

3 From the ρ list, choose **User defined**. In the associated edit field, type `rho_mix`.

4 Locate the **Matrix Properties** section. From the κ list, choose **User defined**. In the associated edit field, type `kappa_p`.

5 Locate the **Fluid Properties** section. From the μ list, choose **User defined**. In the associated edit field, type `eta`.

6 Locate the **Matrix Properties** section. From the ε_p list, choose **User defined**. In the associated edit field, type `1`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1>Darcy's Law** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the *p* edit field, type `p_ref`.

Pressure 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Pressure**.

2 Select Boundary 1 only.

3 In the **Pressure** settings window, locate the **Pressure** section.

4 In the p_0 edit field, type `p_a_in`.

Pressure 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Pressure**.

2 Select Boundary 22 only.

3 In the **Pressure** settings window, locate the **Pressure** section.

4 In the p_0 edit field, type `p_c_in`.

Pressure 3

1 On the **Physics** toolbar, click **Boundaries** and choose **Pressure**.

2 Select Boundaries 4 and 21 only.

3 In the **Pressure** settings window, locate the **Pressure** section.

4 In the p_0 edit field, type `p_ref`.

Electrode-Electrolyte Interface Coupling 1

The Electrode-Electrolyte Interface Couplings are used to create a boundary condition for the flow that is coupled to the electrochemical reactions. Create one coupling for each electrode.

1 On the **Physics** toolbar, click **Boundaries** and choose **Electrode-Electrolyte Interface Coupling**.

2 In the **Electrode-Electrolyte Interface Coupling** settings window, locate the **Boundary Selection** section.

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

4 Locate the **Species** section. Click **Add**.

5 In the **Species** table, enter the following settings:

Species	Molar mass (kg/mol)
1	MH2
2	MH2O

Reaction Coefficients 1

1 In the **Model Builder** window, under **Component 1>Darcy's Law>Electrode-Electrolyte Interface Coupling 1** click **Reaction Coefficients 1**.

2 In the **Reaction Coefficients** settings window, locate the **Model Inputs** section.

3 From the i_{loc} list, choose **Local current density (siec/bei1/er1)**.

4 Locate the **Stoichiometric Coefficients** section. In the n_m edit field, type `2`.

5 In the ν_1 edit field, type `1`.

6 In the ν_2 edit field, type `2*drag`.

Electrode-Electrolyte Interface Coupling 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Electrode-Electrolyte Interface Coupling**.

2 Select Boundary 13 only.

3 In the **Electrode-Electrolyte Interface Coupling** settings window, locate the **Species** section.

4 Click **Add**.

5 Click **Add**.

6 In the **Species** table, enter the following settings:

Species	Molar mass (kg/mol)
1	MO2
2	MH2O
3	MN2

Reaction Coefficients 1

1 In the **Model Builder** window, under **Component 1>Darcy's Law>Electrode-Electrolyte Interface Coupling 2** click **Reaction Coefficients 1**.

2 In the **Reaction Coefficients** settings window, locate the **Model Inputs** section.

3 From the i_{loc} list, choose **Local current density (siec/bei2/er1)**.

4 Locate the **Stoichiometric Coefficients** section. In the n_m edit field, type `4`.

5 In the ν_1 edit field, type `-1`.

6 In the ν_2 edit field, type `2+drag*4`.

TRANSPORT OF CONCENTRATED SPECIES

Now set up the model for the mass transport of hydrogen and water in the anode compartment.

1 In the **Model Builder** window, under **Component 1** right-click **Transport of Concentrated Species** and choose **Rename**.

2 Go to the **Rename Transport of Concentrated Species** dialog box and type `Transport of Concentrated Species (Anode)` in the **New name** edit field.

3 Click **OK**.

4 In the **Transport of Concentrated Species** settings window, locate the **Domain Selection** section.

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

6 Locate the **Transport Mechanisms** section. From the **Diffusion model** list, choose **Maxwell-Stefan**.

7 Locate the **Species** section. From the **From mass constraint** list, choose **wH2Oa**.

TRANSPORT OF CONCENTRATED SPECIES (ANODE)

Convection and Diffusion 1

1 In the **Convection and Diffusion** settings window, locate the **Density** section.

2 From the **Mixture density** list, choose **User defined**.

3 In the ρ edit field, type `rho_mix`.

4 In the M_{wH2} edit field, type `MH2`.

5 In the $M_{\mathrm{wH2}Oa}$ edit field, type `MH2O`.

6 Locate the **Diffusion** section. In the D_{ik} table, enter the following settings:

I	`D_effH2_H2O`
D_effH2_H2O	I

7 Locate the **Model Inputs** section. From the **u** list, choose **Darcy's velocity field (dl/dlm1)**.

8 In the T edit field, type `T`.

9 From the p list, choose **Pressure (dl/dlm1)**.

10 Clear the **Reference pressure** check box.

Initial Values 1

1 In the **Model Builder** window, under **Component 1>Transport of Concentrated Species (Anode)** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the $w_{0,wH2}$ edit field, type `wH2_in`.

Mass Fraction 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Mass Fraction**.

2 Select Boundary 1 only.

3 In the **Mass Fraction** settings window, locate the **Mass Fraction** section.

4 Select the **Species wH2** check box.

5 In the $\omega_{0,\mathrm{wH2}}$ edit field, type `wH2_in`.

Outflow 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 4 only.

Electrode-Electrolyte Interface Coupling 1

Use an Electrode-Electrolyte Interface Coupling to create a flux boundary condition that is coupled to the electrode reactions.

1. On the **Physics** toolbar, click **Boundaries** and choose **Electrode-Electrolyte Interface Coupling**.
2. In the **Electrode-Electrolyte Interface Coupling** settings window, locate the **Boundary Selection** section.
3. From the **Selection** list, choose **Anode Electrode**.

Reaction Coefficients 1

1. In the **Model Builder** window, under **Component 1>Transport of Concentrated Species (Anode)>Electrode-Electrolyte Interface Coupling 1** click **Reaction Coefficients 1**.
2. In the **Reaction Coefficients** settings window, locate the **Model Inputs** section.
3. From the i_{loc} list, choose **Local current density (siec/bei1/er1)**.
4. Locate the **Stoichiometric Coefficients** section. In the n_m edit field, type `2`.
5. In the ν_{wH2} edit field, type `1`.
6. In the $\nu_{\text{wH2}Oa}$ edit field, type `2*drag`.

TRANSPORT OF CONCENTRATED SPECIES 2

Now set up a corresponding model for the mass transport of oxygen, nitrogen and water in the cathode.

1. In the **Model Builder** window, under **Component 1** right-click **Transport of Concentrated Species 2** and choose **Rename**.
2. Go to the **Rename Transport of Concentrated Species** dialog box and type `Transport of Concentrated Species (Cathode)` in the **New name** edit field.
3. Click **OK**.
4. In the **Transport of Concentrated Species** settings window, locate the **Domain Selection** section.
5. From the **Selection** list, choose **Cathode GDL**.
6. Locate the **Transport Mechanisms** section. From the **Diffusion model** list, choose **Maxwell-Stefan**.
7. Locate the **Species** section. From the **From mass constraint** list, choose **wN2**.

TRANSPORT OF CONCENTRATED SPECIES (CATHODE)

Convection and Diffusion 1

1 In the **Convection and Diffusion** settings window, locate the **Density** section.

2 From the **Mixture density** list, choose **User defined**.

3 In the ρ edit field, type `rho_mix`.

4 In the M_{wO2} edit field, type `M02`.

5 In the M_{wH2Oc} edit field, type `MH20`.

6 In the M_{wN2} edit field, type `MN2`.

7 Locate the **Diffusion** section. In the D_{ik} table, enter the following settings:

1	`D_eff02_H20`	`D_eff02_N2`
D_effO2_H2O	1	`D_effH20_N2`
D_effO2_N2	D_effH2O_N2	1

8 Locate the **Model Inputs** section. From the **u** list, choose **Darcy's velocity field (dl/dlm1)**.

9 In the T edit field, type `T`.

10 From the p list, choose **Pressure (dl/dlm1)**.

11 Clear the **Reference pressure** check box.

Initial Values 1

1 In the **Model Builder** window, under **Component 1>Transport of Concentrated Species (Cathode)** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the $w_{0,wO2}$ edit field, type `w02_in`.

4 In the $w_{0,wH2Oc}$ edit field, type `wH20c_in`.

Inflow 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundary 22 only.

3 In the **Inflow** settings window, locate the **Inflow** section.

4 In the $w_{0,wO2}$ edit field, type `w02_in`.

5 In the $w_{0,wH2Oc}$ edit field, type `wH20c_in`.

Outflow 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 21 only.

Electrode-Electrolyte Interface Coupling 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Electrode-Electrolyte Interface Coupling**.

2 In the **Electrode-Electrolyte Interface Coupling** settings window, locate the **Boundary Selection** section.

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

Reaction Coefficients 1

1 In the **Model Builder** window, under **Component 1>Transport of Concentrated Species (Cathode)>Electrode-Electrolyte Interface Coupling 1** click **Reaction Coefficients 1**.

2 In the **Reaction Coefficients** settings window, locate the **Model Inputs** section.

3 From the i_{loc} list, choose **Local current density (siec/bei2/er1)**.

4 Locate the **Stoichiometric Coefficients** section. In the n_m edit field, type `4`.

5 In the ν_{wO2} edit field, type `-1`.

6 In the ν_{wH2Oc} edit field, type `2+4*drag`.

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** right-click **Mesh 1** and choose **Size**.

2 In the **Size** settings window, 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. Select the **Maximum element size** check box.

7 In the associated edit field, type `5e-5`.

Size 2

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

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

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

4 Select Points 6, 7, 14, and 15 only.

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

6 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

7 In the associated edit field, type `1e-5`.

8 Right-click **Mesh 1** and choose **Free Triangular**.

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

STUDY 1

Solve the model using two stationary steps. The first step solves for the flow and currents only, and the second step for the full model.

Step 1: Stationary

1 On the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

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

3 In the table, enter the following settings:

Physics	Solve for	Discretization
Transport of Concentrated Species (Anode)	×	physics
Transport of Concentrated Species (Cathode)	×	physics

4 On the **Home** toolbar, click **Compute**.

RESULTS

Electrolyte Potential (siec)

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

2D Plot Group 5

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

2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 5** and choose **Surface**.

3 In the **Surface** settings window, locate the **Expression** section.

4 Click **Electrode current density, norm (siec.NormIs)** in the upper-right corner of the section. Click to expand the **Range** section. Select the **Manual color range** check box.

5 In the **Minimum** edit field, type `0`.

6 In the **Maximum** edit field, type `1e4`.

7 In the **Model Builder** window, expand the **2D Plot Group 5** node.

8 Right-click **2D Plot Group 5** and choose **Arrow Surface**.

9 In the **Arrow Surface** settings window, locate the **Expression** section.

10 Click **Electrode current density vector (siec.lsx,...,siec.lsy)** in the upper-right corner of the section. On the **2D plot group** toolbar, click **Plot**.

11 Click the **Zoom Extents** button on the Graphics toolbar.

1D Plot Group 6

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

2 On the **1D plot group** toolbar, click **Line Graph**.

3 In the **Line Graph** settings window, locate the **Selection** section.

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

5 Locate the **y-axis data** section. Click **Anode current density (i_a)** in the upper-right corner of the section. Locate the **x-axis data** section. Click **y-coordinate (y)** in the upper-right corner of the section. On the **1D plot group** toolbar, click **Plot**.

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

2D Plot Group 7

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

2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 7** and choose **Surface**.

3 In the **Surface** settings window, locate the **Expression** section.

4 Click **Darcy's velocity magnitude (dl.U)** in the upper-right corner of the section. In the **Model Builder** window, right-click **2D Plot Group 7** and choose **Arrow Surface**.

5 In the **Arrow Surface** settings window, locate the **Expression** section.

6 Click **Darcy's velocity field (dl.u,dl.v)** in the upper-right corner of the section. On the **2D plot group** toolbar, click **Plot**.

7 Click the **Zoom Extents** button on the Graphics toolbar.

2D Plot Group 8

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

2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 8** and choose **Surface**.

3 In the **Surface** settings window, locate the **Expression** section.

4 In the **Expression** edit field, type `wReact`.

5 In the **Model Builder** window, right-click **2D Plot Group 8** and choose **Contour**.

6 In the **Contour** settings window, locate the **Expression** section.

7 In the **Expression** edit field, type `wReact`.

8 Locate the **Coloring and Style** section. From the **Color table** list, choose **Thermal**.

9 Clear the **Color legend** check box.

10 Right-click **2D Plot Group 8** and choose **Arrow Surface**.

11 In the **Arrow Surface** settings window, locate the **Expression** section.

12 Click **Darcy's velocity field (dl.u,dl.v)** in the upper-right corner of the section. On the **2D plot group** toolbar, click **Plot**.

13 Click the **Zoom Extents** button on the Graphics toolbar.

2D Plot Group 9

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

2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 9** and choose **Surface**.

3 In the **Surface** settings window, locate the **Expression** section.

4 Click **Mass fraction (wH2Oa)** in the upper-right corner of the section. In the **Model Builder** window, right-click **2D Plot Group 9** and choose **Contour**.

5 In the **Contour** settings window, locate the **Expression** section.

6 In the **Expression** edit field, type `wH2Oc`.

7 Right-click **2D Plot Group 9** and choose **Arrow Surface**.

8 In the **Arrow Surface** settings window, locate the **Expression** section.

9 Click **Diffusive flux (chcs.dfluxx_wH2Oa,...,chcs.dfluxy_wH2Oa)** in the upper-right corner of the section. On the **2D plot group** toolbar, click **Plot**.

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