Model created in COMSOL Multiphysics 6.4

Carbon Corrosion in a Polymer Electrolyte Membrane Fuel Cell

Introduction

Carbon corrosion is one of the important degradation mechanisms in polymer electrolyte membrane (PEM) fuel cells. It predominantly occurs during start up or shut down of the cell. During carbon corrosion, the noble-metal-catalyst carbon support is compromised, affecting the cell performance.

In this model, a shut-down air purging scenario is modeled by introducing air in a flow channel on the hydrogen (H_2) side, at the same as one of the channels on the H_2 side remains filled with H_2. This situation may for instance occur if a gas flow channel on the H_2 side is clogged by a water droplet during air purging.

Model Definition

Figure 1 shows the model geometry. Three computational domains are used in the model: H_2 and O_2 gas-diffusion layers (GDL), and the membrane. Thin H_2 and O_2 gas-diffusion electrodes, H_2 inlets, electrode current and electric ground boundary conditions are also shown in Figure 1.

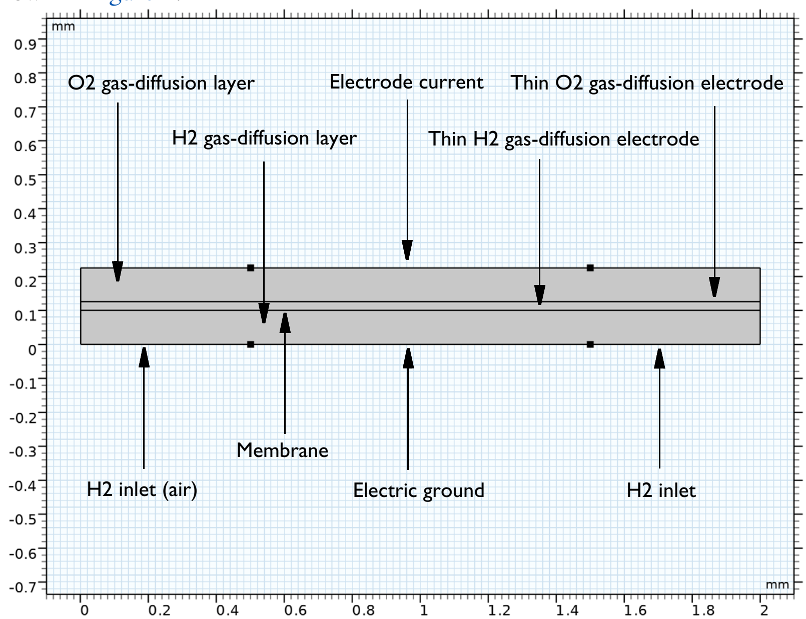

Figure 1: Model geometry. From top: O_2 gas-diffusion layer, Membrane and H_2 gas-diffusion layer. Thin O_2 gas-diffusion electrode, Thin H_2 gas-diffusion electrode, H_2 inlets, Electrode current and Electric ground boundary conditions are indicated in the figure.

The gas mixture at the anode consists of H_2, H_2O, N_2, and O_2, whereas that at the cathode consists of O_2, H_2O, N_2, and CO_2. The mass transport of the gaseous species and momentum transport using Darcy's Law is modeled for the H_2 gas mixture whereas a constant gas mixture (humidified air) is assumed for the O_2 gas mixture.

The Hydrogen Fuel Cell interface is used to define the electrode reactions, the electrolyte charge transport in the electrolyte layer, the electrode charge transport in the porous gas-diffusion layers, as well as the mass transport of the H_2 GDL.

The top boundary of the O_2 GDL in Figure 1 is facing O_2 gas channel and the bottom boundary of the H_2 GDL is facing H_2 gas channel. Note that gas channels are not explicitly defined as domains in the geometry; instead they are represented by boundary conditions. H_2 is fed from the right bottom boundary of the H_2 GDL whereas air is fed from the left bottom boundary of the H_2 GDL using a ramp function to introduce air gradually with time. A zero electrode current is set at the top middle boundary of the O_2 GDL, and the bottom middle boundary of the H_2 GDL is grounded. Although the net current of the cell is 0, internal current circulation exists in the cell due to local potential variation within the cell. The Thin H_2 and O_2 gas-diffusion electrodes define electrode kinetics for the electrochemical reactions considered in the model.

On the H_2 side (anode during normal operation), the hydrogen oxidation (HOR) and oxygen reduction (ORR) reactions are considered at the Thin H_2 gas diffusion electrode:

$$\mathrm{H_2(g)} \leftrightarrow \mathrm{2H^+} + 2e^- \tag{1}$$

$$\mathrm{O_2(g)} + \mathrm{4H^+} + 4e^- \leftrightarrow \mathrm{2H_2O(g)} \tag{2}$$

whereas on the O_2 side (cathode during normal operation), the oxygen reduction (ORR) and carbon oxidation (COR) reactions are considered at the Thin O_2 gas diffusion electrode:

$$\mathrm{O_2(g)} + \mathrm{4H^+} + 4e^- \leftrightarrow \mathrm{2H_2O(g)} \tag{3}$$

$$\mathrm{C(s)} + \mathrm{2H_2O(g)} \leftrightarrow \mathrm{CO_2(g)} + \mathrm{4H^+} + 4e^- \tag{4}$$

On the H_2 side, the electrode kinetics depends on the local concentrations of H_2 for the HOR and on the local concentrations of H_2O and O_2 for the ORR according to the Butler-Volmer kinetics (and the Nernst equation). On the O_2 side, the electrode kinetics depends on the local concentrations of H_2O and O_2 for the ORR and on H_2O and CO_2 for the COR according to the Butler-Volmer kinetics (and the Nernst equation).

The properties of the gas mixtures at both sides, as well as the equilibrium potentials of the electrode reactions (except for the COR) are automatically defined by the default built-in options of the Hydrogen Fuel Cell interface.

HYDROGEN CROSS-OVER TRANSPORT THROUGH THE MEMBRANE

Hydrogen diffusing from the anode side through the membrane is assumed to be oxidized as soon as it reaches the cathode catalytic layer according to

$$\mathrm{H_2(mem)} \rightarrow 2\mathrm{H}^+ + 2e^- \tag{5}$$

Assuming the hydrogen concentration to be zero at the membrane-cathode catalytic boundary and in equilibrium with gaseous hydrogen on the anode side, the flux of hydrogen though the membrane is defined as

$$J_{\mathrm{H2,ionomer}} = \frac{\Psi_{\mathrm{H2}} p_{\mathrm{H2,\,gas,\,anode}}}{L_{\mathrm{mem}}} \tag{6}$$

where Ψ_{H2} (SI unit: m^2/s) is the hydrogen permeation coefficient in the ionomer (incorporating the hydrogen gas-ionomer phase transfer partition constant) and L_{mem} is the membrane thickness.

The hydrogen oxidation current is added to the charge balance as a boundary electrolyte current density contribution

$$i_{\mathrm{H2}} = 2FJ_{\mathrm{H2,ionomer}} \tag{7}$$

The model uses the three study steps: Current Distribution Initialization, Stationary and Time dependent. Secondary current distribution type is used in the Current Distribution Initialization study step. The stationary study step solves for H_2 side without air and the Time dependent study solves for H_2 side with gradually introduced air.

Results and Discussion

Figure 2 shows the change in the cell voltage versus time. It can be seen that the cell voltage is almost uniform at the beginning, before suddenly dropping to its new steady-state of around 0.88 V at around 1 s. This sudden drop in the cell voltage is attributed to the carbon oxidation reaction occurring in the oxygen-side of the cell, as discussed later.

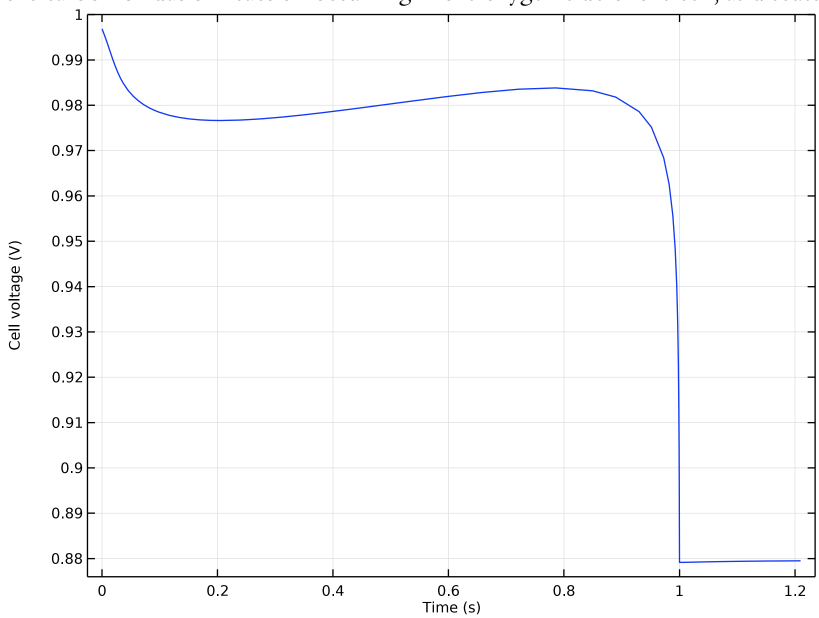

Figure 2: Cell voltage versus time.

Figure 3 shows the H_2 mole-fraction distribution in the H_2 gas-diffusion layer at t = 1.2 s.

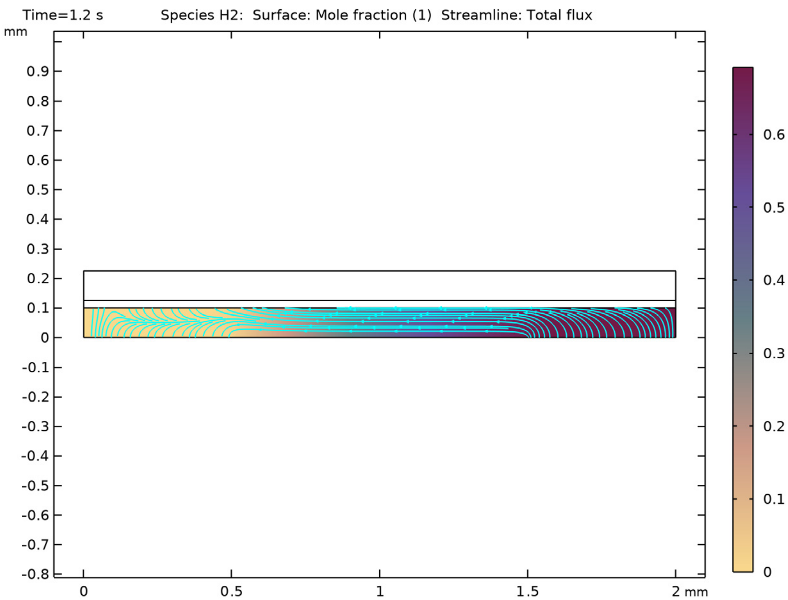

Figure 3: H_2 mole-fraction distribution in the H_2 gas-diffusion layer at t = 1.2 s.

Figure 4 shows the O_2 mole-fraction distribution in the H_2 and O_2 gas-diffusion layers at t = 1.2 s. The presence of oxygen in the anode domain is due to humidified air fed into the anode domain from one end, mimicking shut-down operation of the fuel cell.

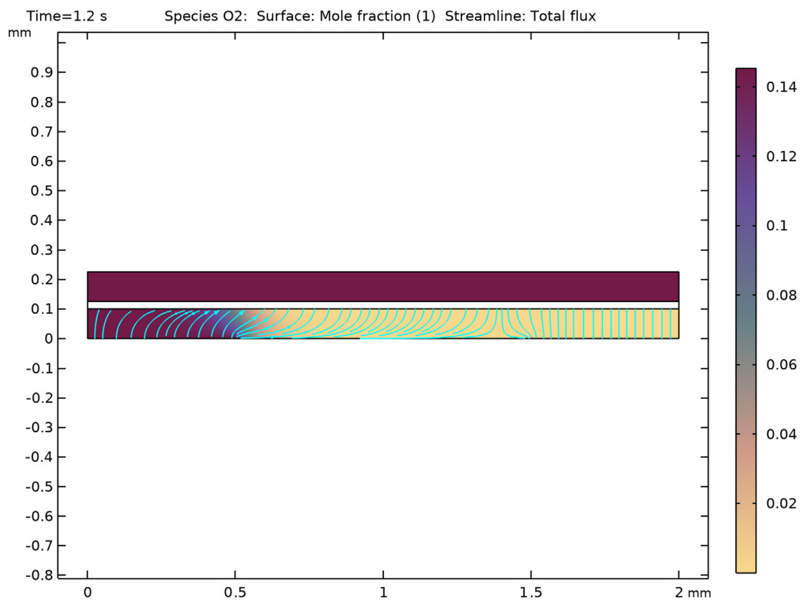

Figure 4: O_2 mole-fraction distribution in the H_2 and O_2 gas-diffusion layers at t = 1.2 s.

Figure 5 shows the change in the hydrogen-side electrode potential along the length of the fuel cell for different times. The hydrogen-side electrode potential increases with time before attaining a maximum steady-state potential of around 0.7 V at around 1 s.

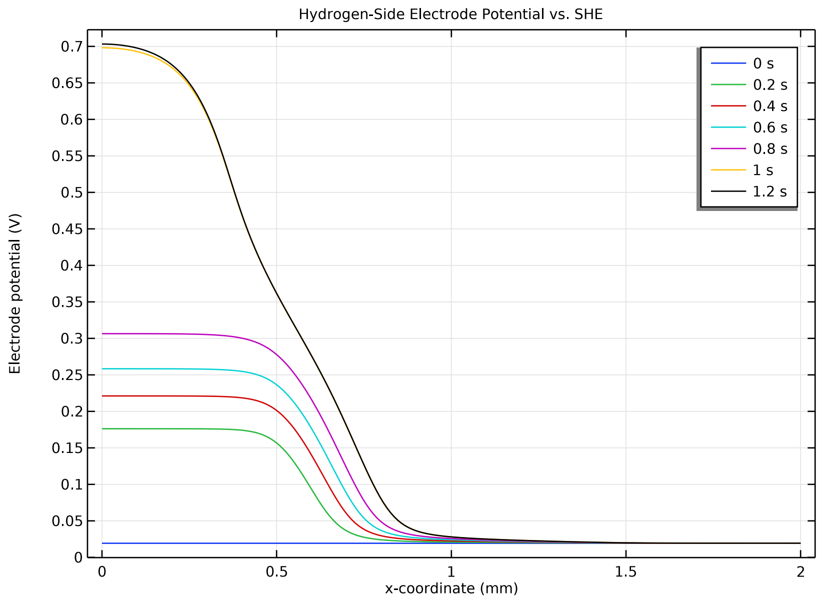

Figure 5: Change in the hydrogen-side electrode potential along the length of the fuel cell.

Figure 6 shows the change in the oxygen-side electrode potential along the length of the fuel cell for different times. The oxygen-side electrode potential increases with time before attaining a maximum steady state potential of around 1.55 V at around 1 s.

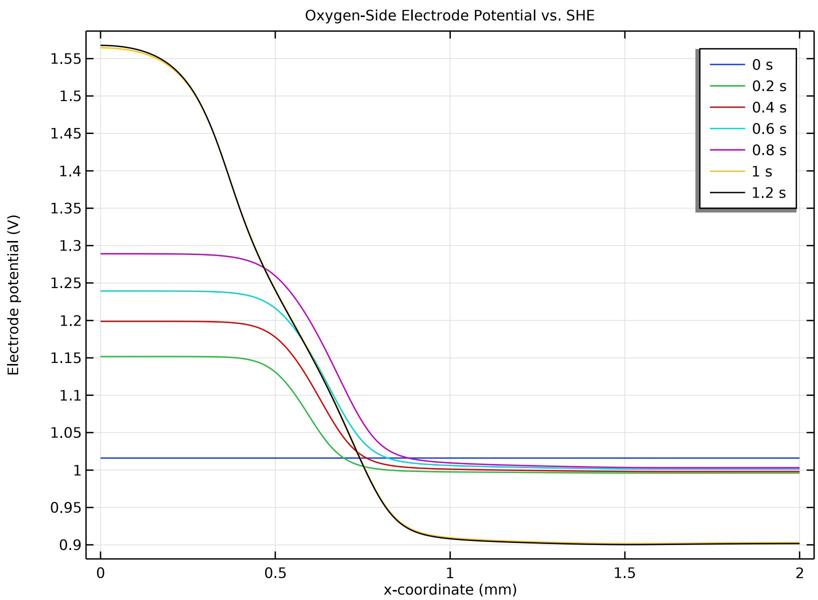

Figure 6: Change in the oxygen-side electrode potential along the length of the fuel cell.

Figure 7 shows the change in the carbon corrosion rate, which is evaluated from the local current density for the carbon oxidation reaction, along the length of the fuel cell for different times. The carbon corrosion rate increases with time and is found to be at its peak at around 1 s. The carbon corrosion is also found to occur in the region where humidified air is fed in the hydrogen-side of the fuel cell.

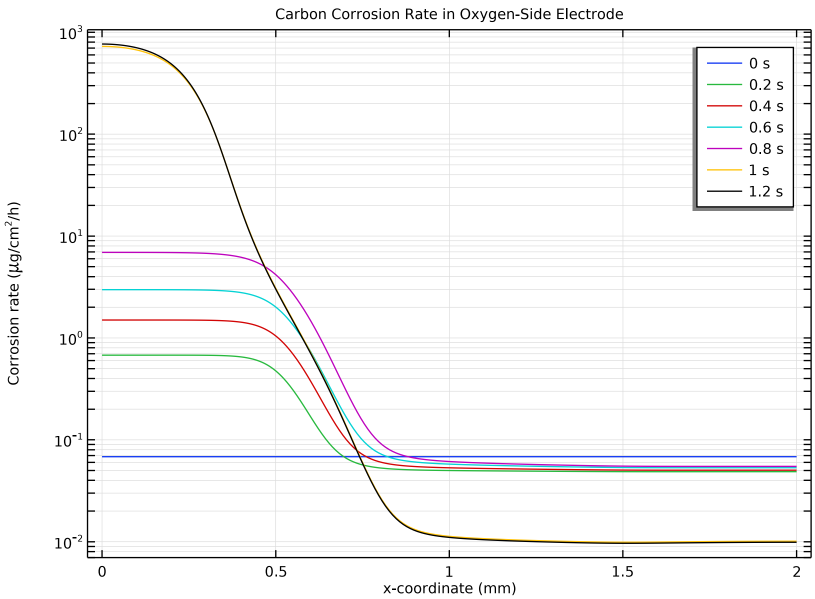

Figure 7: Change in the carbon corrosion rate along the length of the fuel cell.

Figure 8 shows the change in the hydrogen-side local current density along the length of the fuel cell at t = 1.2 s. It can be seen that both the hydrogen oxidation and oxygen reduction reactions occur, particularly at the interface between hydrogen and air, at the Thin H_2 gas-diffusion electrodes node.

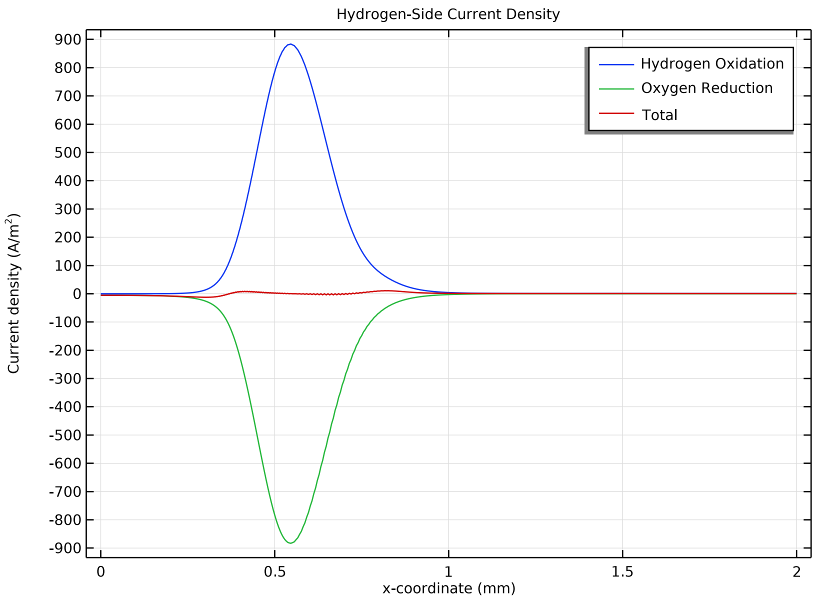

Figure 8: Change in the hydrogen-side current density along the length of the fuel cell.

Finally, Figure 9 shows the change in the oxygen-side local current density for the oxygen reduction and carbon oxidation reactions and the total current density along the length of the fuel cell at t = 1.2 s. It can be seen that the oxygen reduction reaction occurs at the Thin O_2 gas-diffusion electrodes node in the region where hydrogen is fed whereas the oxygen evolution reaction occurs in the region where humidified air is fed in the hydrogen-side of the fuel cell.

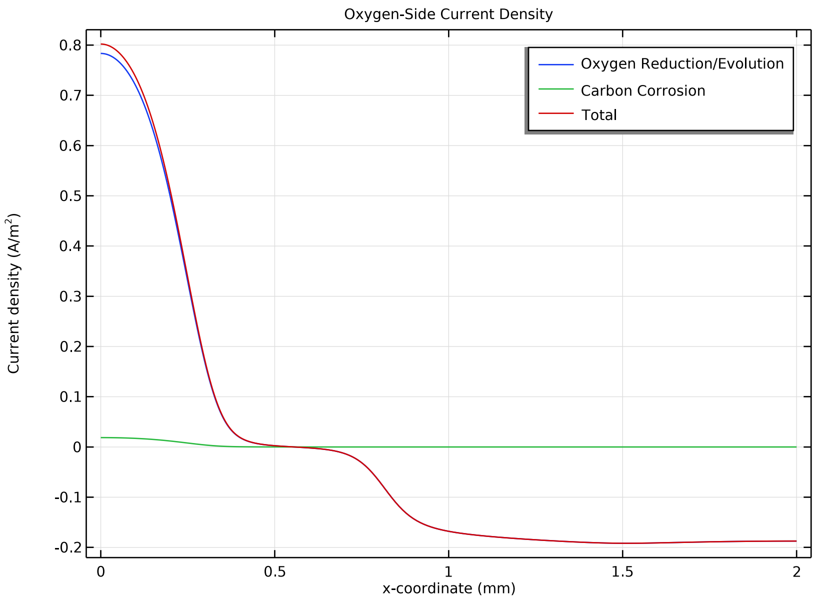

Figure 9: Change in the oxygen-side current density along the length of the fuel cell.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pemfc_carbon_corrosion`

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 Membrane (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**.

GLOBAL DEFINITIONS

Parameters 1

First load the model parameters.

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 `pemfc_carbon_corrosion_parameters.txt`.

GEOMETRY 1

The model geometry consists of three domains: the hydrogen-side gas diffusion layer (GDL), the membrane, and the oxygen-side GDL.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

4 In the **Sketch** toolbar, click **Rectangle** and choose **Rectangle**.

H2 Gas-Diffusion Layer

1 In the **Model Builder** window, expand the **Geometry 1** node.

2 Right-click **Component 1 (comp1) > Geometry 1** and choose **Rectangle**.

3 In the **Settings** window for **Rectangle**, type `H2 Gas-Diffusion Layer` in the **Label** text field.

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

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

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

Membrane

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

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

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

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

5 Locate the **Position** section. In the **y** text field, type `H_gdl`.

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

O2 Gas-Diffusion Layer

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

2 In the **Settings** window for **Rectangle**, type `O2 Gas-Diffusion Layer` in the **Label** text field.

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

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

5 Locate the **Position** section. In the **y** text field, type `H_gdl+H_mem`.

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

7 In the **Sketch** toolbar, click **Point**.

Point 1 (pt1)

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

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

3 In the **x** text field, type `W_ch/2`.

Point 2 (pt2)

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

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

3 In the **x** text field, type `W_ch/2+W_rib`.

Copy 1 (copy1)

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

2 Select the objects **pt1** and **pt2** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **y** text field, type `2*H_gdl+H_mem`.

5 Click **Build Selected**.

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

DEFINITIONS

Variables 1

Next, add variables.

1 In the **Definitions** toolbar, click **Local Variables**.
2 In the **Settings** window for **Variables**, locate the **Variables** section.
3 Click **Load from File**.
4 Browse to the model's Application Libraries folder and double-click the file `pemfc_carbon_corrosion_variables.txt`.

MATERIALS

Add the polymer electrolyte material from the material library. The material added will be used by the **Electrolyte Phase** node to define the conductivity of the electrolyte and by the **Membrane** node to define the permeation coefficient of the membrane.

ADD MATERIAL

1 In the **Materials** toolbar, click **Add Material** to open the **Add Material** window.
2 Go to the **Add Material** window.
3 In the tree, select **Fuel Cell and Electrolyzer** > **Polymer Electrolytes** > **Nafion**®, EW 1100, Vapor Equilibrated, Protonated.
4 Right-click and choose **Add to Component 1 (comp1)**.
5 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

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 the anode gas mixture. A constant gas mixture (humidified air) is assumed on the cathode side. Additionally, include crossover of hydrogen in the membrane. Note that the default gas species are hydrogen, water, nitrogen and oxygen on the anode side, and oxygen, water, nitrogen and carbon dioxide on the cathode side. Start with adding the relevant domain nodes.

1 In the **Settings** window for **Hydrogen Fuel Cell**, locate the **H2 Gas Mixture** section.
2 Select the **N2** checkbox.
3 Select the **O2** checkbox.
4 Find the **Transport mechanisms** subsection. Select the **Use Darcy's Law for momentum transport** checkbox.

5 Locate the **O2 Gas Mixture** section. Select the **CO2** checkbox.

6 Clear the **Include gas phase diffusion** checkbox.

7 Click to expand the **Electrolyte and Membrane Transport** section. Find the **Crossover species** subsection. Select the **H2** checkbox.

Membrane 1

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

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

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

4 Locate the **Electrolyte Water Activity for Material Model Input** section. In the a_w text field, type `0.95`.

H2 Gas Diffusion Layer 1

1 In the **Physics** toolbar, click **Domains** and choose **H2 Gas Diffusion Layer**.

Set up the properties of the anode gas-diffusion layer in the **H2 Gas-Diffusion Layer** node.

2 In the **Settings** window for **H2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **H2 Gas-Diffusion Layer**.

4 Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_GDL`.

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

6 In the κ_g text field, type `kappag_GDL`.

O2 Gas Diffusion Layer 1

1 In the **Physics** toolbar, click **Domains** and choose **O2 Gas Diffusion Layer**.

Set up the properties of the cathode gas-diffusion layer in the **O2 Gas-Diffusion Layer** node.

2 In the **Settings** window for **O2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **O2 Gas-Diffusion Layer**.

4 Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_GDL`.

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 nodes. Note that the reference equilibrium potential is calculated automatically when the default **Built in** option is used.

1 In the **Physics** toolbar, click **Boundaries** and choose **Thin H2 Gas Diffusion Electrode**.

2 Select Boundary 4 only.

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

4 In the d_{gde} text field, type `H_gde`.

Thin H2 Gas-Diffusion Electrode Reaction - HOR

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

2 In the **Settings** window for **Thin H2 Gas Diffusion Electrode Reaction**, type `Thin H2 Gas-Diffusion Electrode Reaction - HOR` in the **Label** text field.

3 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_HOR`.

4 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_Pt_H2_side`.

Thin H2 Gas Diffusion Electrode 1

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

Thin H2 Gas-Diffusion Electrode Reaction - ORR

1 In the **Physics** toolbar, click **Attributes** and choose **Thin H2 Gas Diffusion Electrode Reaction**.

2 In the **Settings** window for **Thin H2 Gas Diffusion Electrode Reaction**, type `Thin H2 Gas-Diffusion Electrode Reaction - ORR` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the n text field, type `4`.

4 In the ν_{O2} text field, type `-1`.

5 In the ν_{H2O} text field, type `2`.

6 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Lumped multistep**.

7 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_ORR`.

8 From the **Pressure dependence** list, choose **Cathodic reaction orders**.

9 In the $\xi_{c,O2}$ text field, type `1`.

10 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_Pt_H2_side`.

Thin O2 Gas Diffusion Electrode 1

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

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

2 Select Boundary 6 only.

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

4 In the d_{gde} text field, type `H_gde`.

Thin O2 Gas-Diffusion Electrode Reaction - ORR

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

2 In the **Settings** window for **Thin O2 Gas Diffusion Electrode Reaction**, type `Thin O2 Gas-Diffusion Electrode Reaction - ORR` in the **Label** text field.

3 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Lumped multistep**.

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

5 From the **Pressure dependence** list, choose **Cathodic reaction orders**.

6 In the $\xi_{c,O2}$ text field, type `1`.

7 In the α_a text field, type `0.5`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_Pt_O2_side`.

Thin O2 Gas Diffusion Electrode 1

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

Thin O2 Gas-Diffusion Electrode Reaction - COR

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

2 In the **Settings** window for **Thin O2 Gas Diffusion Electrode Reaction**, type `Thin O2 Gas-Diffusion Electrode Reaction - COR` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the n text field, type `4`.

4 In the ν_{H2O} text field, type `2`.

5 In the ν_{CO2} text field, type `-1`.

6 Locate the **Equilibrium Potential** section. From the $E_{eq,ref}(T)$ list, choose **User defined**. In the associated text field, type `Eeq_COR`.

7 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_ref_COR`.

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

Electronic Conducting Phase 1

Next, specify the initial values for the oxygen domain to enhance convergence and set the boundary conditions.

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.

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 Boundary 8 only.

Electronic Conducting Phase 1

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

Electrode Current 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Current**.

2 Select Boundary 9 only.

3 In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.

4 In the $I_{\mathrm{s,total}}$ text field, type `0[A]`.

Next, specify initial values, and set the hydrogen inlet boundary conditions.

Initial Values 1

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

2 In the **Settings** window for **Initial Values**, locate the **Initial Composition** section.

3 From the **Mixture specification** list, choose **Humidified mixture**.

4 In the $x_{0,\mathrm{N2,dry}}$ text field, type `xN2_min`.

5 In the $x_{0,\mathrm{O2,dry}}$ text field, type `xO2_min`.

6 In the $\mathrm{RH_{hum}}$ text field, type `RH`.

7 In the T_{hum} text field, type `T_cell`.

H2 Gas Phase 1

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

H2 Inlet 1

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

2 Select Boundary 10 only.

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

4 From the **Inlet flow type** list, choose **Mixture composition constraint**.

H2 Gas Phase 1

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

H2 Inlet 2

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

2 Select Boundary 2 only.

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

4 From the **Inlet flow type** list, choose **Mixture composition constraint**.

5 Locate the **Mixture Specification** section. From the list, choose **Humidified mixture**.

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

7 In the $x_{0,\mathrm{O2,dry}}$ text field, type `xO2_in`.

8 In the $\mathrm{RH}_{\mathrm{hum}}$ text field, type `RH`.

9 In the T_{hum} text field, type `T_cell`.

O2 Gas Phase 1

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

2 In the **Settings** window for **O2 Gas Phase**, locate the **Composition** section.

3 From the **Mixture specification** list, choose **Humidified air**.

4 In the $\mathrm{RH}_{\mathrm{hum}}$ text field, type `RH`.

5 In the T_{hum} text field, type `T_cell`.

DEFINITIONS

Ramp 1 (rm1)

Add a ramp function.

1 In the **Definitions** toolbar, click f(x) **More Functions** and choose **Ramp**.

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

3 Select the **Cutoff** checkbox.

Global Variable Probe 1 (var1)

Next, add a global variable probe to be used later in postprocessing.

1 In the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, locate the **Expression** section.

3 In the **Expression** text field, type `fc.phis0_ec1`.

4 Select the **Description** checkbox. In the associated text field, type `Cell voltage`.

GLOBAL DEFINITIONS

Default Model Inputs

Set the temperature to `T_cell` in the Default Model Inputs.

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_cell`.

MESH 1

Next, set up a user-controlled mesh.

Edge 1

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

Size

1 In the **Model Builder** window, click **Size**.

2 In the **Settings** window for **Size**, click to expand the **Element Size Parameters** section.

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

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `H_gdl/3`.

5 In the **Minimum element size** text field, type `9.0E-6`.

Edge 1

1 In the **Model Builder** window, click **Edge 1**.

2 Select Boundaries 1, 3, and 5 only.

Distribution 1

1 In the **Mesh** toolbar, click **Distribution**.

2 Select Boundary 5 only.

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

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

5 Select Boundaries 1 and 5 only.

Distribution 2

1 In the **Mesh** toolbar, click **Distribution**.

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

3 In the list box, select **1**.

4 Click **Remove from Selection**.

5 Select Boundaries 3 and 5 only.

6 In the list box, select **5**.

7 Select Boundary 3 only.

Copy Edge 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Copying Operations** > **Copy Edge**.

2 Select Boundaries 1, 3, and 5 only.

3 In the **Settings** window for **Copy Edge**, locate the **Destination Boundaries** section.

4 Click to select the **Activate Selection** toggle button.

5 Select Boundaries 12–14 only.

Edge 2

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

2 Select Boundaries 7, 9, and 11 only.

Distribution 1

1 In the **Mesh** toolbar, click **Distribution**.

2 Select Boundary 7 only.

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

4 In the **Number of elements** text field, type 100.

Distribution 2

1 In the **Mesh** toolbar, click **Distribution**.

2 Select Boundary 11 only.

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

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

5 In the **Number of elements** text field, type 25.

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

Distribution 3

1 In the **Mesh** toolbar, click **Distribution**.

2 Select Boundary 9 only.

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

4 In the **Number of elements** text field, type `100`.

Copy Edge 2

1 Right-click **Mesh 1** and choose **Copying Operations** > **Copy Edge**.

2 Select Boundaries 7, 9, and 11 only.

3 In the **Settings** window for **Copy Edge**, locate the **Destination Boundaries** section.

4 Click to select the **Activate Selection** toggle button.

5 Select Boundaries 2, 4, 6, 8, and 10 only.

Mapped 1

1 In the **Mesh** toolbar, click **Mapped**.

2 In the **Settings** window for **Mapped**, click **Build All**.

STUDY 1

Finally, set current distribution type to **Secondary** and add a **Time Dependent** study node.

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 3: Time Dependent

1 In the **Study** toolbar, click **Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,0.2,1.2)`.

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

RESULTS

Some plots are added by default. Follow the instructions below to reproduce the figures in the Results and Discussion section.

Cell Voltage vs. Time

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

2 In the **Settings** window for **1D Plot Group**, type `Cell Voltage vs. Time` in the **Label** text field.

3 Locate the **Legend** section. Clear the **Show legends** checkbox.

4 In the **Cell Voltage vs. Time** toolbar, click **Plot**.

The plot should look like Figure 2.

Surface 1

1 In the **Model Builder** window, expand the **Mole Fraction, H2 (fc)** node, then click **Surface 1**.

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

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

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.

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

3 In the **Density level** text field, type `9`.

4 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **Cyan**.

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

The plot should look like Figure 3.

Surface 1

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

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

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

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.

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

3 In the **Density level** text field, type `8`.

4 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **Cyan**.

5 In the **Mole Fraction, O2 (fc)** toolbar, click **Plot**.

The plot should look like Figure 4.

Hydrogen-Side Electrode Potential vs. SHE

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

2 In the **Settings** window for **1D Plot Group**, type `Hydrogen-Side Electrode Potential vs. SHE` in the **Label** text field.

Line Graph 1

1 In the **Hydrogen-Side Electrode Potential vs. SHE** toolbar, click **Line Graph**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `fc.Ect`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Click to expand the **Legends** section. Select the **Show legends** checkbox.

Hydrogen-Side Electrode Potential vs. SHE

1 In the **Model Builder** window, click **Hydrogen-Side Electrode Potential vs. SHE**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **Label**.

4 In the **Hydrogen-Side Electrode Potential vs. SHE** toolbar, click **Plot**.

The plot should look like Figure 5.

Hydrogen-Side Electrode Potential vs. SHE 1

Right-click **Hydrogen-Side Electrode Potential vs. SHE** and choose **Duplicate**.

Hydrogen-Side Electrode Potential vs. SHE

In the **Model Builder** window, collapse the **Results** > **Hydrogen-Side Electrode Potential vs. SHE** node.

Oxygen-Side Electrode Potential vs. SHE

1 In the **Model Builder** window, under **Results** click **Hydrogen-Side Electrode Potential vs. SHE 1**.

2 In the **Settings** window for **1D Plot Group**, type `Oxygen-Side Electrode Potential vs. SHE` in the **Label** text field.

Line Graph 1

1. In the **Model Builder** window, expand the **Oxygen-Side Electrode Potential vs. SHE** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **Selection** section.
3. Click to select the **Activate Selection** toggle button.
4. Select Boundary 6 only.

Oxygen-Side Electrode Potential vs. SHE

1. In the **Model Builder** window, click **Oxygen-Side Electrode Potential vs. SHE**.
2. In the **Oxygen-Side Electrode Potential vs. SHE** toolbar, click **Plot**.

   The plot should look like Figure 6.

Carbon Corrosion Rate in Oxygen-Side Electrode

1. Right-click **Oxygen-Side Electrode Potential vs. SHE** and choose **Duplicate**.
2. In the **Settings** window for **1D Plot Group**, type `Carbon Corrosion Rate in Oxygen-Side Electrode` in the **Label** text field.
3. Locate the **Plot Settings** section.
4. Select the **y-axis label** checkbox. In the associated text field, type `Corrosion rate (\mu g/cm<sup>2</sup>/h)`.

Line Graph 1

1. In the **Model Builder** window, expand the **Carbon Corrosion Rate in Oxygen-Side Electrode** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3. In the **Expression** text field, type `CR`.
4. In the **Unit** field, type `ug/cm^2/h`.

Carbon Corrosion Rate in Oxygen-Side Electrode

1. In the **Model Builder** window, click **Carbon Corrosion Rate in Oxygen-Side Electrode**.
2. In the **Settings** window for **1D Plot Group**, locate the **Axis** section.
3. Select the **y-axis log scale** checkbox.
4. In the **Carbon Corrosion Rate in Oxygen-Side Electrode** toolbar, click **Plot**.

   The plot should look like Figure 7.
5. In the **Model Builder** window, collapse the **Carbon Corrosion Rate in Oxygen-Side Electrode** node.

Hydrogen-Side Current Density

1 In the **Results** toolbar, click **1D Plot Group**.
2 In the **Settings** window for **1D Plot Group**, type `Hydrogen-Side Current Density` in the **Label** text field.
3 Locate the **Data** section. From the **Time selection** list, choose **Last**.
4 Locate the **Title** section. From the **Title type** list, choose **Label**.
5 Locate the **Plot Settings** section.
6 Select the **y-axis label** checkbox. In the associated text field, type `Current density (A/m<sup>2</sup>)`.

Line Graph 1

1 In the **Hydrogen-Side Current Density** toolbar, click **Line Graph**.
2 Select Boundary 4 only.
3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Hydrogen Fuel Cell** > **Electrode kinetics** > **fc.iloc_th2gder1 - Local current density - A/m²**.
4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
5 In the **Expression** text field, type `x`.
6 Locate the **Legends** section. Select the **Show legends** checkbox.
7 From the **Legends** list, choose **Manual**.
8 In the table, enter the following settings:

Legends
`Hydrogen Oxidation`

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.
2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3 In the **Expression** text field, type `fc.iloc_th2gder2`.
4 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Oxygen Reduction`

Line Graph 3

1 Right-click **Line Graph 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Hydrogen Fuel Cell** > **Electrode kinetics** > **fc.itot - Total interface current density - A/m²**.

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

Legends
Total

Hydrogen-Side Current Density

1 In the **Model Builder** window, click **Hydrogen-Side Current Density**.

2 In the **Hydrogen-Side Current Density** toolbar, click **Plot**.

The plot should look like Figure 8.

Hydrogen-Side Current Density 1

Right-click **Hydrogen-Side Current Density** and choose **Duplicate**.

Hydrogen-Side Current Density

In the **Model Builder** window, collapse the **Results** > **Hydrogen-Side Current Density** node.

Oxygen-Side Current Density

1 In the **Model Builder** window, under **Results** click **Hydrogen-Side Current Density 1**.

2 In the **Settings** window for **1D Plot Group**, type `Oxygen-Side Current Density` in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, expand the **Oxygen-Side Current Density** node, then click **Line Graph 1**.

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

3 Click to select the **Activate Selection** toggle button.

4 Select Boundary 6 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `fc.iloc_to2gder1`.

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

Legends
Oxygen Reduction/Evolution

Line Graph 2

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

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

3 Click to select the **Activate Selection** toggle button.

4 Select Boundary 6 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `fc.iloc_to2gder2`.

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

Legends
`Carbon Corrosion`

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

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

3 Click to select the **Activate Selection** toggle button.

4 Select Boundary 6 only.

Oxygen-Side Current Density

1 In the **Model Builder** window, click **Oxygen-Side Current Density**.

2 In the **Oxygen-Side Current Density** toolbar, click **Plot**.

The plot should look like Figure 9.

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

Surface 1

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

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

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

Arrow Surface 1

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

Surface 1

1 In the **Model Builder** window, expand the **Electrolyte Potential (fc)** node, then click **Surface 1**.

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

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

Arrow Surface 1

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

Surface 1

1 In the **Model Builder** window, expand the **Mole Fraction, H2O (fc)** node, then click **Surface 1**.

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

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

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.

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

3 In the **Density level** text field, type 8.

4 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **Cyan**.

Surface 1

1 In the **Model Builder** window, expand the **Pressure (fc)** node, then click **Surface 1**.

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

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

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

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.

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

3 In the **Density level** text field, type 8.

4 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **White**.

Mole Fraction, N2 (fc)

In the **Model Builder** window, under **Results** right-click **Mole Fraction, N2 (fc)** and choose **Delete**.