



Model created in COMSOL Multiphysics 6.4

# Ohmic Losses and Temperature Distribution in a Passive PEM Fuel Cell

## *Introduction*

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In small PEM (proton exchange membrane) fuel cell systems (in the sub-100 W range), no active devices for cooling or air transport are normally used. This design is chosen to minimize parasitic power losses from pumps and fans and to reduce the system complexity, size, and cost. The reactants at the cathode are therefore transported by passive convection/diffusion. Also, the heat dissipation occurs by passive transport mechanisms to the surrounding environment.

When designing the air side of a passive fuel cell the goal is to ensure an even current density and heat profile over the cell for various surrounding temperatures and current loads.

The holes in the cathode cover plate should typically be large in order to provide good reactant transport to the electrode, but the hole-to-solid material ratio may not be too large since the structural rigidity and electron conductivity of the plate also have to be maintained. Large air holes also cause high local ohmic losses in the gas diffusion layer.

## *Model Definition*

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This example models the current density and heat profile over a passive PEM fuel cell. Mass transport limitations are not accounted for in this model.

The cell is mounted on a printed circuit board (PCB) using a thin film of copper as current collector. Hydrogen inlet holes are made in the copper film. The cathode cover plate is made of steel with larger air inlet holes.

The modeled cell is assumed to be the last unit in a large array of serially connected cells, where the connection to the previous cell is made along the long side of the anode current collector. The cathode current collector short side is used as the positive current terminal of the whole stacked array.

The electrochemical currents are modeled with the Hydrogen Fuel Cell interface and the heat transport is modeled with the Heat Transfer interface, along with the Electrochemical Heating multiphysics coupling node for coupling the heat sources and temperature.

Since the gas diffusion electrodes (GDEs) are very thin in relation to the whole cell, and since mass transport is not accounted for, the GDEs are modeled as planar surfaces (using the Thin H<sub>2</sub> Gas Diffusion Electrode and Thin O<sub>2</sub> Gas Diffusion Electrode nodes, respectively) between the respective gas diffusion layers (GDLs) and the polymer membrane. Two electrode reactions are used, hydrogen reduction at the anode and

oxygen reduction at the cathode. The reference equilibrium potentials and thermoneutral potentials are automatically calculated when the default built-in options are used.

Heat is produced by the electrochemical reactions and joule heating due to the electrical currents. The PCB has low heat conductivity and hence all heat produced dissipates from the cathode cover plate by convective cooling and surface-to-ambient radiation. The heat transfer coefficient used to model the convective cooling depends heavily on the surrounding environment, here a value of  $50 \text{ W}/(\text{m}^2 \cdot \text{K})$  is used. This value is higher than what is normally used for free convection cooling with gases, but may be motivated from the fact that extra convection is induced by the mass transfer processes in the cathode electrode.

All produced water is assumed to leave the system in gas phase, therefore the value used for the equilibrium potential for the oxygen reduction reaction and the entropy value are based on gaseous water. In this way the cooling effect due to vaporizing water is accounted for in the heat sources of the electrochemical reactions.

## Results and Discussion

Figure 1 shows the electronic potential of the cell for a simulated cell voltage of 0.4 V.

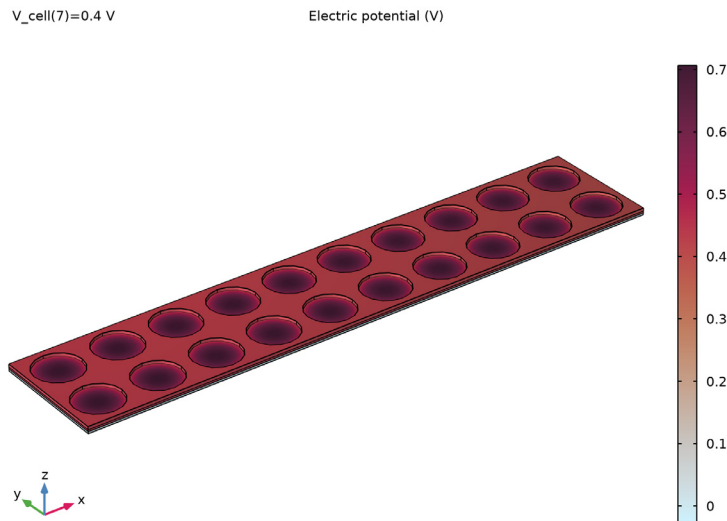


Figure 1: Electronic potential on the surface of the cell.

The potential drop from the center of the air holes to the cover plate is substantial, whereas the potential drop along the cell in the  $x$  direction, resulting from using the short side of the cell as current terminal, is small.

Figure 2 shows the ionic potential of the polymer membrane surface. The cathode air holes have a large impact on the potential profile, the effect of the smaller anode hydrogen inlet holes is less pronounced.

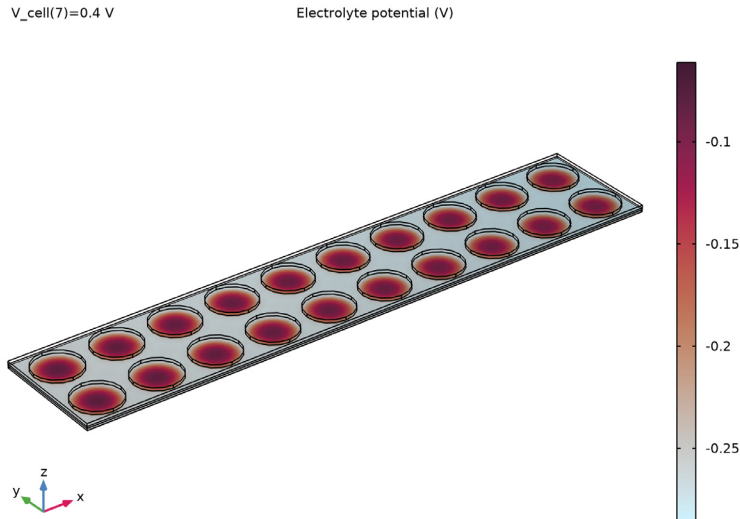


Figure 2: Ionic potential of the polymer membrane surface.

Figure 3 shows the temperature of the whole cell. The cell is warmer toward the cathode current terminal.

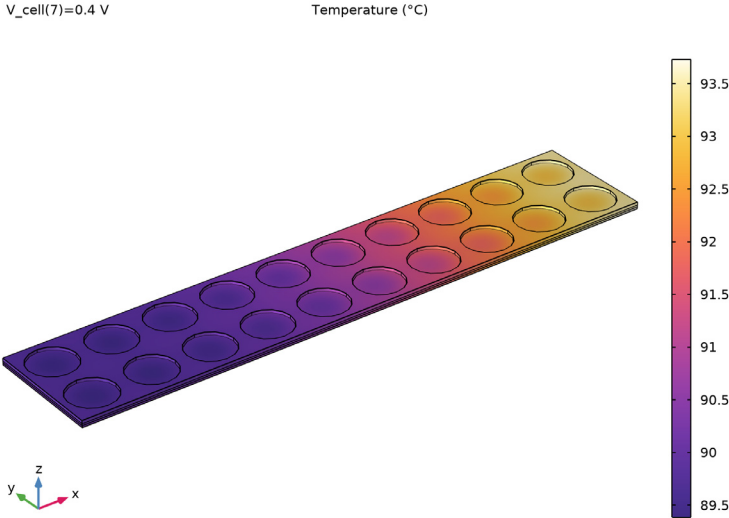
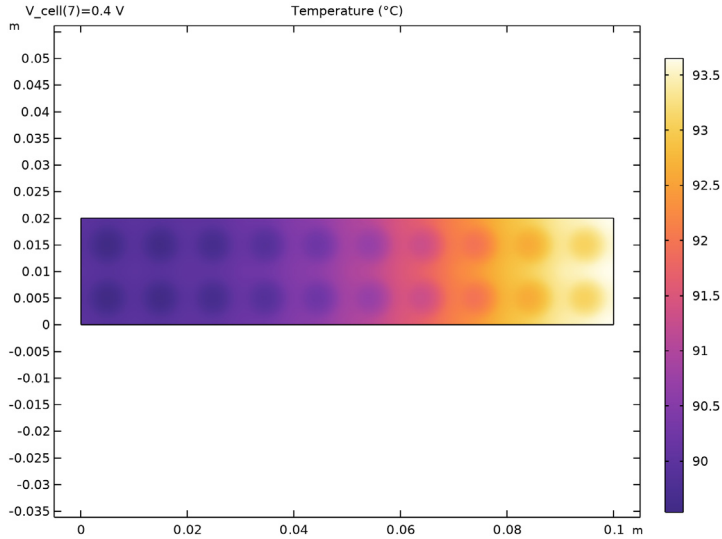


Figure 3: Cell surface temperature.

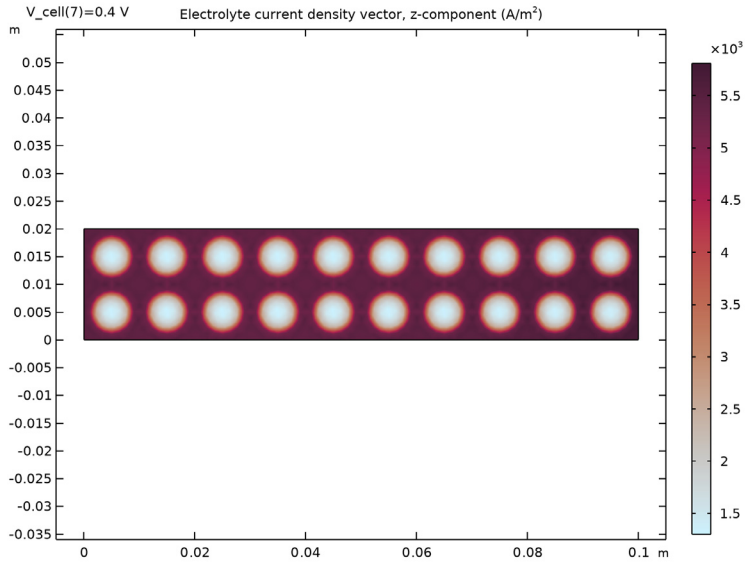


*Figure 4: Temperature in the center of the membrane.*

Figure 4 shows the temperature profile in the center of the membrane. The membrane temperature is very similar to the temperature of the cathode cover plate in Figure 3.

Figure 5 shows the ionic current vector in the  $z$  direction in the center of the membrane. The current density in the parts of the membrane facing the center of the cathode air inlet holes are much lower than other parts of the membrane. It is also seen that the current density is slightly higher toward the current terminal. This is due to higher potential losses on the steel cover plate on the cathode than on the copper film on the anode. The higher

current density toward the cathode current terminal generates more heat, which explains the higher temperature toward the cathode current terminal in [Figure 4](#) and [Figure 5](#).



*Figure 5: Ionic current density in the center of the membrane (z direction).*

[Figure 6](#) shows the polarization plot and [Figure 7](#) the cathode average temperature dependence on the average cell current density.

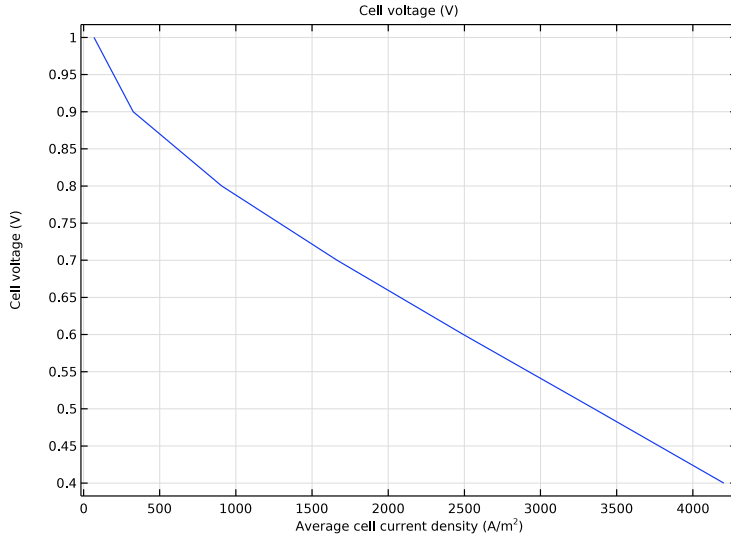


Figure 6: Polarization plot.

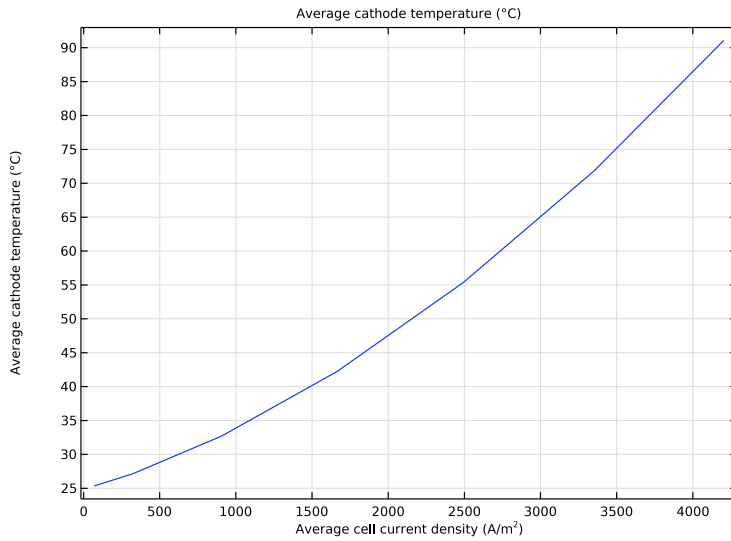


Figure 7: Cathode average temperature dependence on average cell current density.

## *Notes About the COMSOL Implementation*

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The geometry is set up using an assembly of two different parts with an identity pair coupling between the anode current collector and anode GDL domains. The reason for this is to be able to use swept meshes in the normal direction to the cell surface. The identity pair and the corresponding Continuity boundary condition nodes in the physics interfaces are added automatically by default.

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**Application Library path:** Fuel\_Cell\_and\_Electrolyzer\_Module/Fuel\_Cells/passive\_pem


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## *Modeling Instructions*




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

### **NEW**

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


### **MODEL WIZARD**

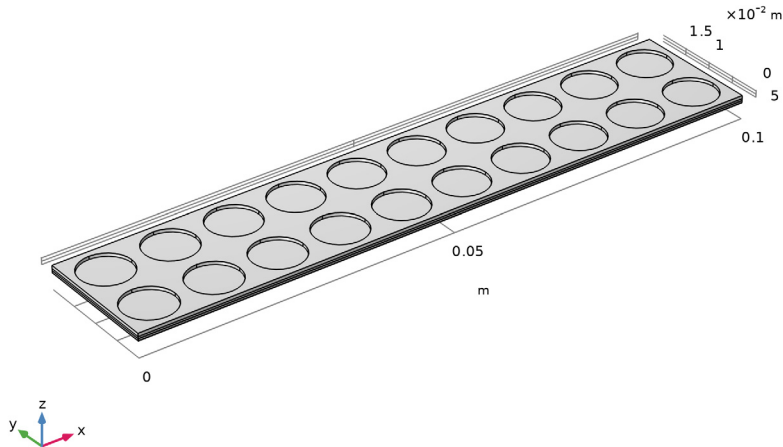
- 1 In the **Model Wizard** window, click  **3D**.
- 2 In the **Select Physics** tree, select **Electrochemistry** > **Hydrogen Fuel Cells** > **Proton Exchange Membrane (fc)**.
- 3 Click **Add**.
- 4 In the **Select Physics** tree, select **Heat Transfer** > **Heat Transfer in Solids (ht)**.
- 5 Click **Add**.
- 6 Click  **Study**.
- 7 In the **Select Study** tree, select **General Studies** > **Stationary**.
- 8 Click  **Done**.

### **GEOMETRY I**

The model geometry is available as a parameterized geometry sequence in a separate MPH file. If you want to build it from scratch, follow the instructions in the section [Appendix — Geometry Modeling Instructions](#). Otherwise load it from file with the following steps.

- 1 In the **Geometry** toolbar, click **Insert Sequence** and choose **Insert Sequence**.


- 2 Browse to the model's Application Libraries folder and double-click the file `passive_pem_geom_sequence.mph`.
- 3 In the **Geometry** toolbar, click  **Build All**.
- 4 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.




## DEFINITIONS

Now create selections of the geometry. You will use them later when setting up the physics.


### *Anode Current Collector*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Anode Current Collector in the **Label** text field.
- 3 Select Domain 1 only.


### *Cathode Current Collector*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Cathode Current Collector in the **Label** text field.
- 3 Select Domain 5 only.


### *GDLs*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type GDLs in the **Label** text field.
- 3 Select Domains 2 and 4 only.


### *Membrane*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Membrane in the **Label** text field.
- 3 Select Domain 3 only.


### *Cathode - Air Boundary*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Cathode - Air Boundary in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundaries 46, 49, 56, 59, 66, 69, 76, 79, 86, 89, 96, 99, 106, 109, 116, 119, 126, 129, 136, and 139 only.


### *Anode Current Terminal*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Anode Current Terminal in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 1 only.


### *Cathode Current Terminal*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Cathode Current Terminal in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 147 only.


### *Anode GDE*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Anode GDE in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 32 only.


### *Cathode GDE*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Cathode GDE in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 35 only.


### *Anode GDL*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Anode GDL in the **Label** text field.
- 3 Select Domain 2 only.

### *Cathode GDL*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Cathode GDL in the **Label** text field.
- 3 Select Domain 4 only.


### *Current Collectors*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Current Collectors in the **Label** text field.
- 3 Select Domains 1 and 5 only.

## **GLOBAL DEFINITIONS**

Load some additional model parameters from a text file.

### *Parameters 1*


- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `passive_pem_parameters.txt`.

## **HYDROGEN FUEL CELL (FC)**


Now set up the physics for the current distribution model (without mass transport effects). The gas stream at the anode side is assumed to be 100% hydrogen, whereas the default species of H<sub>2</sub>O and N<sub>2</sub> are included in the cathode gas stream. Start by assigning the current collector and GDL domains (You will specify the material parameter values under the **Materials** branch later).

- 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 Clear the **H2O** checkbox.
- 4 Locate the **O2 Gas Mixture** section. Find the **Transport mechanisms** subsection. Clear the **Include gas phase diffusion** checkbox.


#### *Current Collector 1*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Current Collector**.
- 2 In the **Settings** window for **Current Collector**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Current Collectors**.
- 4 Locate the **Electrode Charge Transport** section. From the  $\sigma_s$  list, choose **From material**.


#### *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**.
- 4 Locate the **Electrode Charge Transport** section. From the  $\sigma_s$  list, choose **From material**.

#### *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**.
- 4 Locate the **Electrode Charge Transport** section. From the  $\sigma_s$  list, choose **From material**.

#### *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**.

#### *Thin H2 Gas Diffusion Electrode 1*

Now set up the thin GDEs along with the electrochemical reactions. Note that the reference equilibrium potential and the thermoneutral voltage are 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 In the **Settings** window for **Thin H2 Gas Diffusion Electrode**, locate the **Boundary Selection** section.

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

4 Locate the **Electrode Thickness** section. In the  $d_{\text{gde}}$  text field, type d\_gde.

#### *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 **Electrode Kinetics** section.

3 In the  $i_{0,\text{ref}}(T)$  text field, type i0\_refa.

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

#### *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**.

4 Locate the **Electrode Thickness** section. In the  $d_{\text{gde}}$  text field, type d\_gde.

#### *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 **Electrode Kinetics** section.

3 In the  $i_{0,\text{ref}}(T)$  text field, type i0\_refc.

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

#### *O2 Gas Phase 1*

Set up the composition of the O2 gas mixture in the **O2 Gas Phase** node.

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  $\text{RH}_{\text{hum}}$  text field, type RH\_amb.

5 In the  $T_{\text{hum}}$  text field, type T\_amb.

#### *Initial Values 1*




Provide initial values to facilitate numerical convergence.

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Hydrogen Fuel Cell (fc) > Electrolyte Phase 1** click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the  $\phi_1$  text field, type  $-0.1[V]$ .

#### *Electronic Conducting Phase 1*

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

#### *Initial Values 2*


- 1 In the **Physics** toolbar, click  **Attributes** and choose **Initial Values**.
- 2 In the **Settings** window for **Initial Values**, locate the **Domain Selection** section.
- 3 Click  **Clear Selection**.
- 4 Click  **Paste Selection**.
- 5 In the **Paste Selection** dialog, type 4, 5 in the **Selection** text field.
- 6 Click **OK**.
- 7 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 8 In the  $\phi_s$  text field, type  $V_{cell}$ .

#### *Electronic Conducting Phase 1*

Complete the model for the electrochemical currents by grounding the anode current collector, and setting the cathode steel plate to the cell potential.

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 In the **Settings** window for **Electric Ground**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Anode Current Terminal**.

#### *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 In the **Settings** window for **Electric Potential**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Cathode Current Terminal**.
- 4 Locate the **Electric Potential** section. In the  $\phi_{s,bnd}$  text field, type  $V_{cell}$ .

## HEAT TRANSFER IN SOLIDS (HT)

Now set up the model for the heat transport. (You specify all material parameters later). Model the heat lost by convective cooling by using a **Heat Flux** boundary condition.


- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heat Transfer in Solids (ht)**.

### *Heat Flux 1*


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Heat Flux**.
- 2 In the **Settings** window for **Heat Flux**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Cathode - Air Boundary**.
- 4 Select Boundaries 39, 46, 49, 56, 59, 66, 69, 76, 79, 86, 89, 96, 99, 106, 109, 116, 119, 126, 129, 136, and 139 only.  
The boundary selection is easiest to make by first choosing the predefined **Cathode-Air Boundary**, and then adding the top surface of the cathode cover plate.
- 5 Locate the **Heat Flux** section. From the **Flux type** list, choose **Convective heat flux**.
- 6 In the  $h$  text field, type htc.
- 7 In the  $T_{\text{ext}}$  text field, type T\_amb.

### *Surface-to-Ambient Radiation 1*

Include **Surface-to-Ambient Radiation** nodes for the two different surfaces on the cathode side. The emissivity is higher for the carbon GDL than the steel plate.

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Surface-to-Ambient Radiation**.
- 2 In the **Settings** window for **Surface-to-Ambient Radiation**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Cathode - Air Boundary**.
- 4 Locate the **Surface-to-Ambient Radiation** section. From the  $\epsilon$  list, choose **User defined**. In the associated text field, type 0.8.
- 5 In the  $T_{\text{amb}}$  text field, type T\_amb.

### *Surface-to-Ambient Radiation 2*


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Surface-to-Ambient Radiation**.
- 2 Select Boundary 39 only.
- 3 In the **Settings** window for **Surface-to-Ambient Radiation**, locate the **Surface-to-Ambient Radiation** section.
- 4 From the  $\epsilon$  list, choose **User defined**. In the associated text field, type 0.3.

5 In the  $T_{\text{amb}}$  text field, type T\_amb.

### MULTIPHYSICS

Heat will be generated in the domains due to ohmic heating, and on the thin GDEs due to activation losses. Create these heat sources by coupling the **Heat Transfer** interface to the **Hydrogen Fuel Cell** interface, using the **Electrochemical Heating** multiphysics feature. Note that this feature also couples the temperature between the interfaces.



*Electrochemical Heating 1 (ech1)*

In the **Physics** toolbar, click  **Multiphysics Couplings** and choose **Domain > Electrochemical Heating**.

### MATERIALS

This model will use some materials from the built-in library, start by importing these.

#### 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 **Built-in > Copper**.
- 4 Click the **Add to Component** button in the window toolbar.
- 5 In the tree, select **Built-in > Steel AISI 4340**.
- 6 Click the **Add to Component** button in the window toolbar.
- 7 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.

### MATERIALS

*Copper (mat1)*

- 1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 2 From the **Selection** list, choose **Anode Current Collector**.

*Steel AISI 4340 (mat2)*

- 1 In the **Model Builder** window, click **Steel AISI 4340 (mat2)**.
- 2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 3 From the **Selection** list, choose **Cathode Current Collector**.

Set up the required material parameter values for the membrane and GDL manually (The density and heat capacity are actually not needed for this model since this is a stationary heat problem, but they are added here for convenience if one would like to do a time-dependent study).

### GDLs

- 1 In the **Model Builder** window, right-click **Materials** and choose **Blank Material**.
- 2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 3 From the **Selection** list, choose **GDLs**.
- 4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Electric conductivity	sigma_iso ; sigma_ii = sigma_iso, sigma_ij = 0	100	S/m	Basic
Thermal conductivity	k_iso ; k_ii = k_iso, k_ij = 0	25	W/(m·K)	Basic
Density	rho	200	kg/m <sup>3</sup>	Basic
Heat capacity at constant pressure	Cp	700	J/(kg·K)	Basic

- 5 In the **Label** text field, type GDLs.

### Membrane

- 1 Right-click **Materials** and choose **Blank Material**.
- 2 In the **Settings** window for **Material**, type Membrane in the **Label** text field.
- 3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Membrane**.
- 4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Electrolyte conductivity	sigma_iso ; sigma_ii = sigma_iso, sigma_ij = 0	1	S/m	Electrolyte conductivity
Thermal conductivity	k_iso ; k_ii = k_iso, k_ij = 0	0.2	W/(m·K)	Basic
Density	rho	1000	kg/m <sup>3</sup>	Basic
Heat capacity at constant pressure	Cp	4000	J/(kg·K)	Basic

## MESH 1

Build the mesh by meshing the top and bottom surfaces for each part, respectively, and then sweeping in the  $z$  direction.


### *Free Triangular 1*

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Free Triangular**.
- 2 Select Boundary 39 only.

### *Size*

- 1 In the **Model Builder** window, click **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 Click the **Custom** button.
- 4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type  $1.5e-3$ .
- 5 In the **Minimum element size** text field, type  $1e-3$ .

### *Swept 1*

- 1 In the **Mesh** toolbar, click  **Swept**.
- 2 In the **Settings** window for **Swept**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Cathode Current Collector**.



### *Distribution 1*

- 1 Right-click **Swept 1** and choose **Distribution**.
- 2 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 3 In the **Number of elements** text field, type 2.

### *Swept 1*

In the **Model Builder** window, right-click **Swept 1** and choose **Build Selected**.

### *Free Triangular 2*

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Free Triangular**.
- 2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Cathode - Air Boundary**.
- 4 Click  **Build Selected**.

### *Free Triangular 3*

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Free Triangular**.

2 Select Boundary 3 only.

*Size 1*

1 Right-click **Free Triangular 3** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.


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

5 Select the **Maximum element size** checkbox. In the associated text field, type  $0.9e-3$ .

6 Select the **Minimum element size** checkbox. In the associated text field, type  $0.6e-3$ .

7 Click  **Build Selected**.

*Swept 2*

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

*Distribution 1*

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

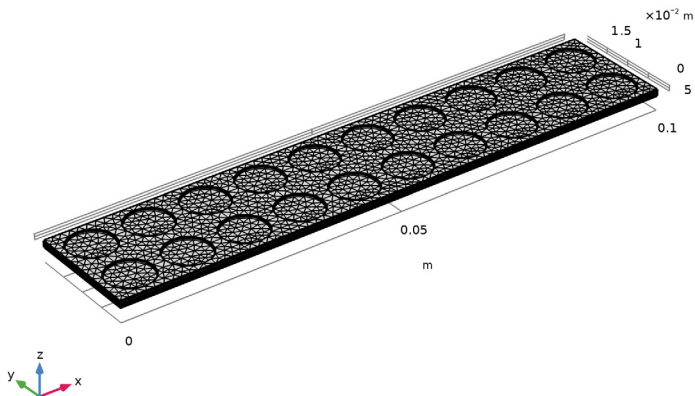
2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 In the **Number of elements** text field, type 2.

*Swept 2*

1 In the **Model Builder** window, right-click **Swept 2** and choose **Build All**.


The finalized mesh should now look as follows:




## DEFINITIONS

Add two probes for calculating the average current density at the anode and temperature at the cathode.

### *Average Cell Current Density Probe*

- 1 In the **Definitions** toolbar, click  **Probes** and choose **Boundary Probe**.
- 2 In the **Settings** window for **Boundary Probe**, type Average Cell Current Density Probe in the **Label** text field.
- 3 In the **Variable name** text field, type  $I_{cell}$ .
- 4 Locate the **Source Selection** section. From the **Selection** list, choose **Anode GDE**.
- 5 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Hydrogen Fuel Cell > Electrode kinetics > fc.iloc\_th2gder1 - Local current density - A/m<sup>2</sup>**.
- 6 Locate the **Expression** section. In the **Expression** text field, type  $fc.iloc\_th2gder1 * Av * d\_gde$ .


### *Average Cell Temperature Probe*

- 1 In the **Definitions** toolbar, click  **Probes** and choose **Boundary Probe**.
- 2 In the **Settings** window for **Boundary Probe**, type Average Cell Temperature Probe in the **Label** text field.
- 3 In the **Variable name** text field, type  $T_{avg}$ .
- 4 Locate the **Source Selection** section. From the **Selection** list, choose **Cathode GDE**.
- 5 Locate the **Expression** section. In the **Expression** text field, type  $T$ .

## STUDY 1



### *Step 1: Stationary*

Use an auxiliary sweep with continuation to solve for a range of different cell voltages.

- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.
- 3 Select the **Auxiliary sweep** checkbox.
- 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



### *Solution 1 (sol1)*

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Dependent Variables 1**.
- 3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 4 From the **Method** list, choose **Initial-value based**.
- 5 In the **Model Builder** window, expand the **Study 1 > Solver Configurations > Solution 1 (sol1) > Stationary Solver 1 > Segregated 1** node, then click **Hydrogen Fuel Cell**.
- 6 In the **Settings** window for **Segregated Step**, click to expand the **Method and Termination** section.
- 7 From the **Jacobian update** list, choose **On first iteration**.
- 8 In the **Model Builder** window, click **Study 1**.
- 9 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 10 Clear the **Generate default plots** checkbox.
- 11 In the **Study** toolbar, click  **Compute**.


## **RESULTS**

Set default units for result presentation.

### *Preferred Units 1*


- 1 In the **Results** toolbar, click  **Configurations** and choose **Preferred Units**.
- 2 In the **Settings** window for **Preferred Units**, locate the **Units** section.
- 3 Click  **Add Physical Quantity**.
- 4 In the **Physical Quantity** dialog, select **General > Temperature (K)** in the tree.
- 5 Click **OK**.
- 6 In the **Settings** window for **Preferred Units**, locate the **Units** section.
- 7 In the table, enter the following settings:

Quantity	Unit	Preferred unit
Temperature	K	°C


- 8 Select the **Apply conversions to expressions with the same dimensions** checkbox.
- 9 In the **Model Builder** window, click **Preferred Units 1**.
- 10 Click  **Apply**.

Follow the steps in this section to reproduce the figures in the [Results and Discussion](#) section.


#### *Electric Potential*

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Electric Potential in the **Label** text field.


#### *Surface 1*

- 1 Right-click **Electric Potential** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type `fc.phis`.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **MetasepiaBlue**.
- 5 In the **Electric Potential** toolbar, click  **Plot**.


#### *Electrolyte Potential*

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Electrolyte Potential in the **Label** text field.


#### *Surface 1*

- 1 Right-click **Electrolyte Potential** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **MetasepiaBlue**.
- 4 In the **Electrolyte Potential** toolbar, click  **Plot**.



#### *Surface Temperature*

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Surface Temperature in the **Label** text field.


#### *Surface 1*

- 1 Right-click **Surface Temperature** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type `T`.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **HeatCameraLight**.
- 5 In the **Surface Temperature** toolbar, click  **Plot**.


### *Cut Plane 1*

- 1 In the **Results** toolbar, click  **Cut Plane**.
- 2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.
- 3 From the **Plane** list, choose **XY-planes**.
- 4 In the **Z-coordinate** text field, type `H_film+H_GDL+H_membrane/2`.
- 5 Click  **Plot**.


### *Membrane Temperature*

- 1 In the **Results** toolbar, click  **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type **Membrane Temperature** in the **Label** text field.


### *Surface 1*

- 1 Right-click **Membrane Temperature** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Plane 1**.
- 4 Locate the **Expression** section. In the **Expression** text field, type `T`.
- 5 Locate the **Coloring and Style** section. From the **Color table** list, choose **HeatCameraLight**.
- 6 In the **Membrane Temperature** toolbar, click  **Plot**.


### *Membrane Current Density*

- 1 In the **Results** toolbar, click  **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type **Membrane Current Density** in the **Label** text field.

### *Surface 1*

- 1 Right-click **Membrane Current Density** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Plane 1**.
- 4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Hydrogen Fuel Cell > Electrolyte current density vector - A/m<sup>2</sup> > fc.llz - Electrolyte current density vector, z-component**.
- 5 Locate the **Coloring and Style** section. From the **Color table** list, choose **MetasepiaBlue**.
- 6 In the **Membrane Current Density** toolbar, click  **Plot**.


### *Polarization Plot*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Polarization Plot in the **Label** text field.
- 3 Locate the **Plot Settings** section.
- 4 Select the **x-axis label** checkbox. In the associated text field, type Average cell current density ( $A/m^{2}$ ).


### *Global I*

- 1 Right-click **Polarization Plot** 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
V_cell	V	Cell voltage

- 4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 5 In the **Expression** text field, type I\_cell.
- 6 Click to expand the **Legends** section. Clear the **Show legends** checkbox.
- 7 In the **Polarization Plot** toolbar, click  **Plot**.

### *Temperature vs. Current Density*


- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Temperature vs. Current Density in the **Label** text field.
- 3 Locate the **Plot Settings** section.
- 4 Select the **x-axis label** checkbox. In the associated text field, type Average cell current density ( $A/m^{2}$ ).

### *Global I*

- 1 Right-click **Temperature vs. Current Density** 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
T_avg	°C	Average cathode temperature

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

- 5 In the **Expression** text field, type `I_cell`.
- 6 Locate the **Legends** section. Clear the **Show legends** checkbox.
- 7 In the **Temperature vs. Current Density** toolbar, click  **Plot**.

## *Appendix — Geometry Modeling Instructions*

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### **ADD COMPONENT**

In the **Home** toolbar, click  **Add Component** and choose **3D**.

### **GLOBAL DEFINITIONS**

First define the geometry parameters.

#### *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 In the table, enter the following settings:

<b>Name</b>	<b>Expression</b>	<b>Value</b>	<b>Description</b>
L	10[cm]	0.1 m	Cell length
D	2[cm]	0.02 m	Cell width
H_film	0.035[mm]	3.5E-5 m	Cu film thickness
H_GDL	0.3[mm]	3E-4 m	GDL thickness
H_membrane	0.02[mm]	2E-5 m	Membrane thickness
H_plate	0.5[mm]	5E-4 m	Steel plate thickness
r_film	2[mm]	0.002 m	Hole radius in Cu film
r_plate	4[mm]	0.004 m	Hole radius in steel plate

### **GEOMETRY 1**



The geometry is based on blocks, with arrays of cylinders to create the holes in the top steel plate and bottom copper film. Use a boolean difference operation to create the two parts that form the final assembly.

#### *Block 1 (blk1)*



- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type L.

- 4 In the **Depth** text field, type D.
- 5 In the **Height** text field, type H\_film.




*Cylinder 1 (cyl1)*

- 1 In the **Geometry** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type r\_film.
- 4 In the **Height** text field, type H\_film.
- 5 Locate the **Position** section. In the **x** text field, type 1 [cm].
- 6 In the **y** text field, type 1 [cm].
- 7 Click  **Build Selected**.

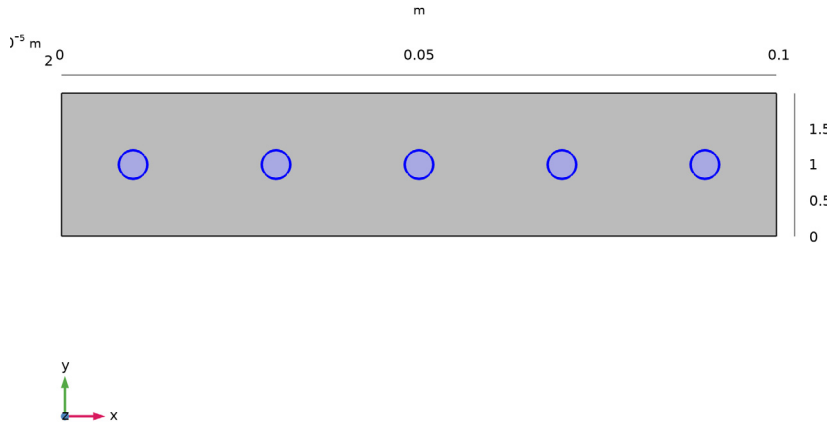
*Array 1 (arr1)*

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Array**.
- 2 Select the object **cyl1** only.
- 3 In the **Settings** window for **Array**, locate the **Size** section.
- 4 In the **x size** text field, type 5.
- 5 Locate the **Displacement** section. In the **x** text field, type 2e-2.
- 6 Click  **Build Selected**.

*Difference 1 (dif1)*

- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Click the  **Go to XY View** button in the **Graphics** toolbar.
- 3 Select the object **blk1** only, to add it to the **Objects to add** list.
- 4 In the **Settings** window for **Difference**, locate the **Difference** section.
- 5 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.



- Click and drag in the **Graphics** window to enclose and high-light all five cylinders, then right-click to confirm the selection.



- Click  **Build Selected**.


- Click the  **Go to Default View** button in the **Graphics** toolbar.

*Block 2 (blk2)*



- In the **Geometry** toolbar, click  **Block**.
- In the **Settings** window for **Block**, locate the **Size and Shape** section.
- In the **Width** text field, type L.
- In the **Depth** text field, type D.
- In the **Height** text field, type H\_GDL.
- Locate the **Position** section. In the **z** text field, type H\_film.
- Click  **Build Selected**.

*Block 3 (blk3)*



- In the **Geometry** toolbar, click  **Block**.
- In the **Settings** window for **Block**, locate the **Size and Shape** section.
- In the **Width** text field, type L.

- 4 In the **Depth** text field, type D.
- 5 In the **Height** text field, type H\_membrane.
- 6 Locate the **Position** section. In the **z** text field, type H\_film+H\_GDL.
- 7 Click  **Build Selected**.



*Block 4 (blk4)*

- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type L.
- 4 In the **Depth** text field, type D.
- 5 In the **Height** text field, type H\_GDL.
- 6 Locate the **Position** section. In the **z** text field, type H\_film+H\_GDL+H\_membrane.
- 7 Click  **Build Selected**.



*Block 5 (blk5)*

- 1 In the **Geometry** toolbar, click  **Block**.
- 2 In the **Settings** window for **Block**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type L.
- 4 In the **Depth** text field, type D.
- 5 In the **Height** text field, type H\_plate.
- 6 Locate the **Position** section. In the **z** text field, type H\_film+H\_GDL+H\_membrane+H\_GDL.
- 7 Click  **Build Selected**.




*Cylinder 2 (cyl2)*

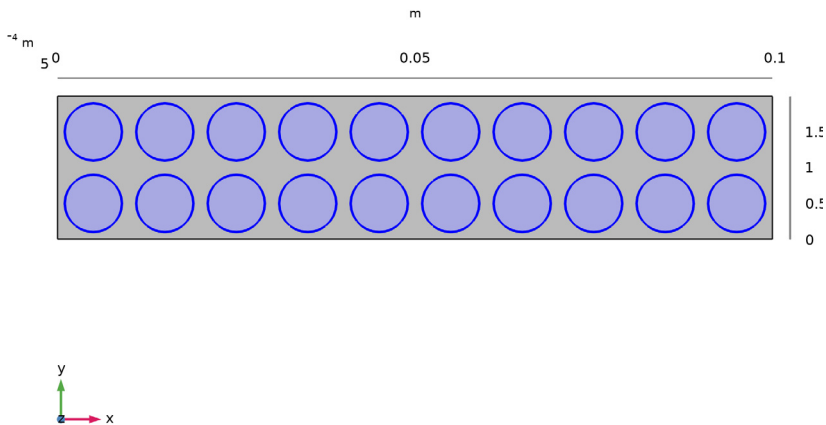
- 1 In the **Geometry** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type r\_plate.
- 4 In the **Height** text field, type H\_plate.
- 5 Locate the **Position** section. In the **x** text field, type 5e-3.
- 6 In the **y** text field, type 5e-3.
- 7 In the **z** text field, type H\_film+H\_GDL+H\_membrane+H\_GDL.
- 8 Click  **Build Selected**.

*Array 2 (arr2)*

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Array**.
- 2 Select the object **cyl1** only.
- 3 In the **Settings** window for **Array**, locate the **Size** section.
- 4 In the **x size** text field, type 10.
- 5 In the **y size** text field, type 2.
- 6 Locate the **Displacement** section. In the **x** text field, type  $1e-2$ .
- 7 In the **y** text field, type  $1e-2$ .
- 8 Click  **Build Selected**.

*Difference 2 (dif2)*

- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Click the  **Go to XY View** button in the **Graphics** toolbar.
- 3 Select the objects **blk2**, **blk3**, **blk4**, and **blk5** only, to add them to the **Objects to add** list.
- 4 In the **Settings** window for **Difference**, locate the **Difference** section.
- 5 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.
- 6 Click and drag in the **Graphics** window to enclose and high-light the 20 cylinders, then right-click to confirm the selection.



7 Click  **Build Selected**.

8 Click the  **Go to Default View** button in the **Graphics** toolbar.

#### *Form Union (fin)*

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

2 In the **Settings** window for **Form Union/Assembly**, locate the **Form Union/Assembly** section.

3 From the **Action** list, choose **Form an assembly**.

4 Click  **Build Selected**.

The model geometry is now complete.