Created in COMSOL Multiphysics 6.2

Water and Carbon Dioxide Co-Electrolysis in a Solid Oxide Electrolyzer Cell

Introduction

In this tutorial, a solid oxide electrolyzer cell model for co-electrolysis of H_2O and CO_2 is presented. The model includes the full coupling between the mass balances and gas flow in the H_2 and O_2 gas diffusion electrodes, the momentum balances in the H_2 and O_2 gas-flow channels, the energy balance across the cell, the balance of the ionic current carried by the oxide ion, and an electronic-current balance. A reversible water–gas shift reaction is included in the H_2 gas-diffusion electrode and the H_2 gas-flow channel.

The model computes the spatial distributions of the various species across the gas-diffusion electrodes and gas-flow channels. The spatial distribution of the total current density along the electrode length is also evaluated using a general projection operator.

Model Definition

On the anode, oxygen ions are oxidized to form oxygen gas,

$$2O^{2-} \leftrightarrow O_2(g) + 4e^- \tag{1}$$

whereas on the cathode, water vapor is reduced to form hydrogen gas and oxygen ions:

$$H_2O(g) + 2e^- \leftrightarrow H_2(g) + O^{2-} \tag{2}$$

A CO_2 electrolysis reaction also occurs on the cathode, where CO_2 gas is reduced to form CO gas and oxygen ions:

$$CO_2(g) + 2e^- \leftrightarrow CO(g) + O^{2-} \tag{3}$$

Figure 1 shows the model geometry. Seven computational domains are used in the model: the two interconnects, H_2 and O_2 gas-flow channels, H_2 and O_2 gas-diffusion electrodes, and the membrane.

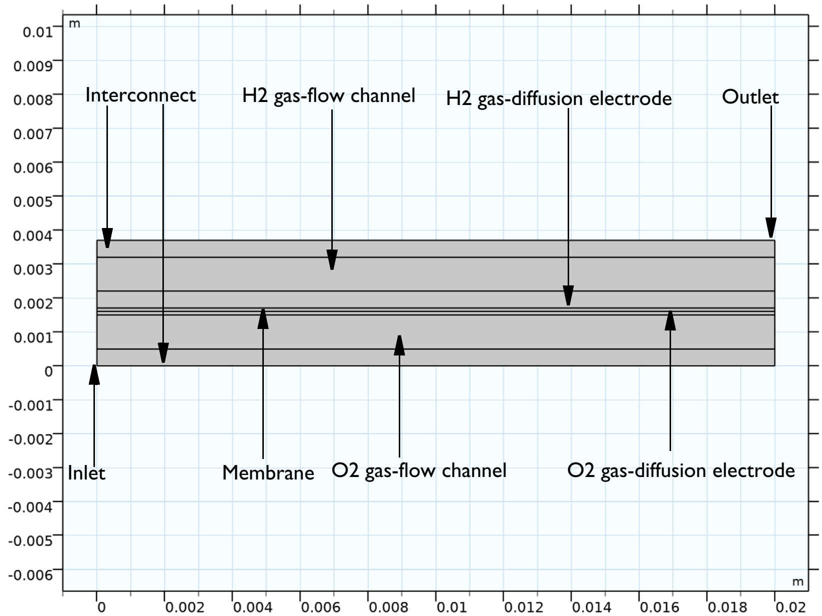


Figure 1: Model geometry. From top: Interconnect, H_2 gas channel, H_2 gas-diffusion electrode, solid oxide electrolyte layer, O_2 gas-diffusion electrode, O_2 gas-flow channel, and interconnect. The inlet and outlet positions are indicated in the figure.

The gas mixture at the cathode consists of H_2, H_2O, CO_2, and CO, whereas that at the anode consists of O_2 and N_2. The composition of the gas mixture will change as a result of the electrochemical reactions and the water–gas shift reaction. The mass transport of the gaseous species is modeled in the gas-flow channels and the gas-diffusion electrodes coupled to the resulting (laminar) flow of the gas mixture.

The current distribution is defined assuming a temperature-dependent electrolyte conductivity of the solid electrolyte. The Water Electrolyzer interface is used to define the electrode reactions and the electrolyte charge transport in the porous gas-diffusion electrodes and the electrolyte layer, as well as the mass transport of the gas mixture. The momentum flow is defined using Darcy's Law in the gas-flow channels and the gas-diffusion electrodes.

On the cathode side, the electrode kinetics depends on the local concentrations of H_2O and H_2 for the H_2O electrolysis reaction and on the local concentrations of CO_2 and CO for the CO_2 electrolysis reaction according to the law of mass action (and the Nernst equation). On the anode side, the electrode kinetics depends on the local concentrations of O_2 for the O_2 evolution reaction according to the law of mass action (and the Nernst equation).

The properties of the gas mixtures at both anode and cathode, as well as the equilibrium potentials of the electrode reactions are automatically defined by the default built-in options of the Water Electrolyzer interface.

Results and Discussion

Figure 2 shows the H_2 concentration distribution in the H_2 gas-flow channel and the H_2 gas-diffusion electrode for an applied potential of 1.5 V. The H_2 concentration is found to increase along the electrode length due to the H_2O electrolysis reaction occurring at the H_2 gas diffusion electrode.

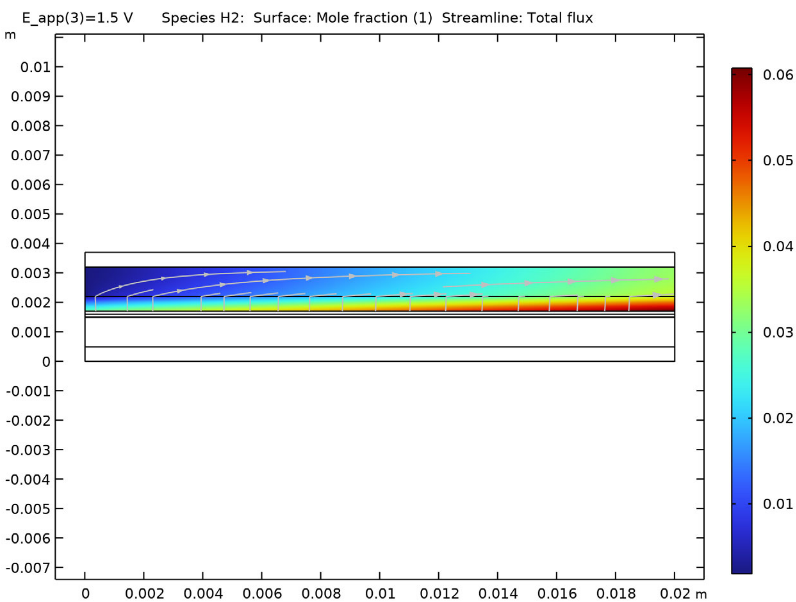


Figure 2: H_2 concentration distribution in the H_2 gas-flow channel and H_2 gas-diffusion electrode for an applied potential of 1.5 V.

Figure 3 shows the CO concentration distribution in the H_2 gas-flow channel and H_2 gas diffusion electrode for applied potential of 1.5 V. CO concentration is found to increase along the electrode length due to the CO_2 electrolysis reaction occurring at the H_2 gas-diffusion electrode. The difference in the CO concentration between the H_2 gas-diffusion electrode and the H_2 gas-flow channel is considerably higher for CO in the downstream when compared to H_2. This can be attributed to slower diffusion of CO than H_2.

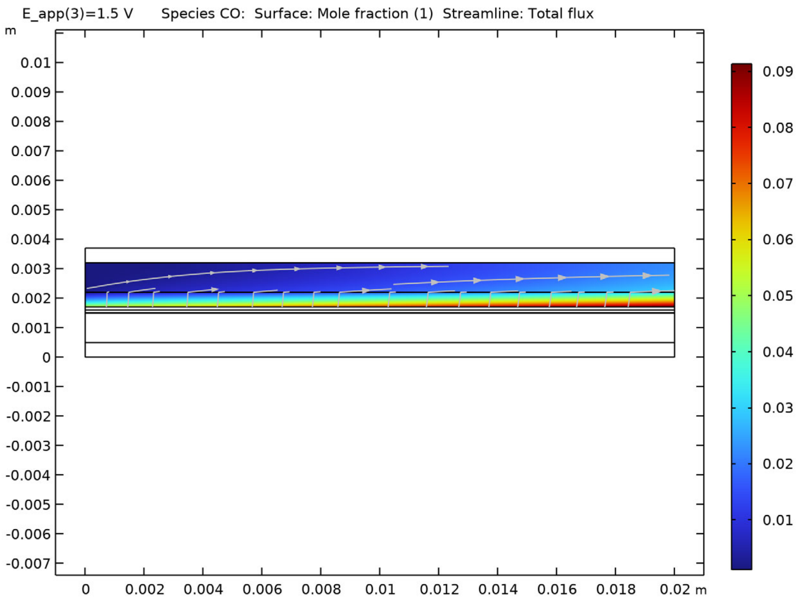


Figure 3: CO concentration distribution in the H_2 gas-flow channel and the H_2 gas-diffusion electrode for an applied potential of 1.5 V.

Figure 4 shows the change in temperature across a solid oxide electrolyzer cell for an applied potential of 1.5 V. Although both the H_2O and CO_2 electrolysis reactions are endothermic, the cell temperature is increased by about 25 K from the inlet to the outlet for an applied potential of 1.5 V. As this applied potential is higher than the cell thermoneutral potential, the heat generated from overpotential losses is more than the heat required for electrolysis reactions.

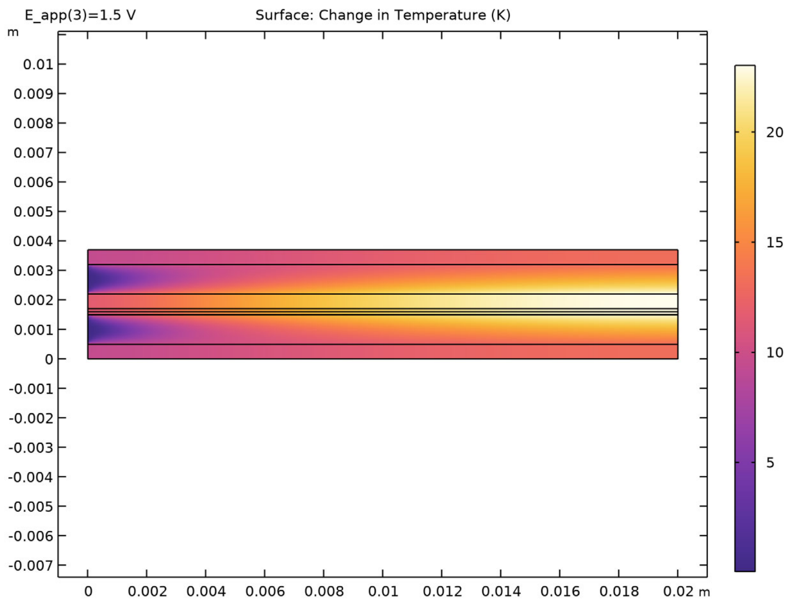


Figure 4: Change in temperature across a solid oxide electrolyzer cell for an applied potential of 1.5 V.

Figure 5 shows the distribution of the water–gas shift reaction rate in the H_2 gas-flow channel and the H_2 gas-diffusion electrode for an applied potential of 1.5 V. The water–gas shift reaction rate is found to be higher closer to the H_2 gas-diffusion electrode-membrane interface for an applied potential of 1.5 V, which is attributed to the high CO concentration in the region.

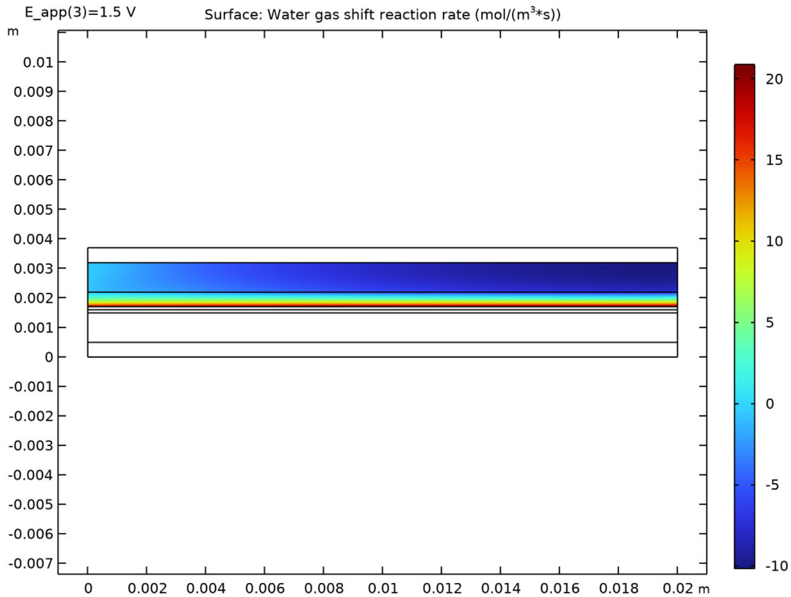


Figure 5: Water–gas shift reaction rate in the H_2 gas-flow channel and the H_2 gas-diffusion electrode for an applied potential of 1.5 V.

Finally, Figure 6 shows that the total cathodic (negative) current density, which is integrated along the *y* direction for each grid point along the *x* direction using a general projection operator, decreases for H_2O electrolysis and increases for CO_2 electrolysis along the electrode length.

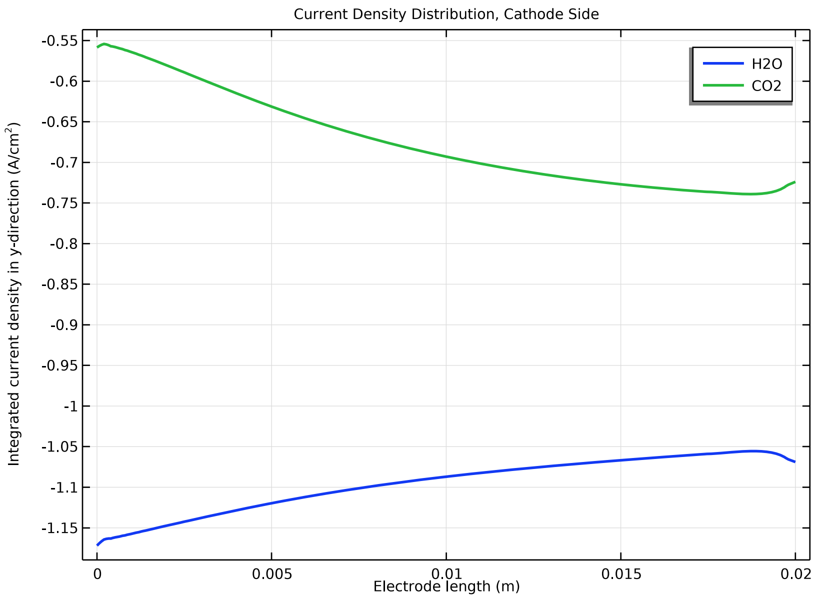


Figure 6: The total cathodic current density for H_2O and CO_2 electrolysis along the electrode length for an applied potential of 1.5 V.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Electrolyzers/soec_co2`

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>Water Electrolyzers>Solid Oxide (we)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Heat Transfer>Heat Transfer in Solids and Fluids (ht)**.

5 Click **Add**.

6 Click **Study**.

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

8 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 `soec_co2_parameters.txt`.

GEOMETRY 1

Draw the model geometry using a rectangle and six layers.

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

Rectangle 1 (r1)

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**, locate the **Size and Shape** section.

4 In the **Width** text field, type `L`.

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

6 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
`Layer 1`	`di`
`Layer 2`	`dg`
`Layer 3`	`da`
`Layer 4`	`dm`

Layer name	Thickness (m)
Layer 5	dc
Layer 6	dg

7 Click **Build All Objects**.

DEFINITIONS

Variables 1

Next, add variables.

1 In the **Home** toolbar, click **Variables** and choose **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 `soec_co2_variables.txt`.

General Projection 1 (genproj1)

Next, add a **General Projection** coupling.

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

2 Select Domain 5 only.

WATER ELECTROLYZER (WE)

Start setting up the electrochemistry part of the model.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Water Electrolyzer (we)**.

2 In the **Settings** window for **Water Electrolyzer**, locate the **H2 Gas Mixture** section.

3 Select the **CO2** check box.

4 Select the **CO** check box.

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

6 Locate the **O2 Gas Mixture** section. Select the **N2** check box.

7 Select the **Include gas phase diffusion** check box.

8 Select the **Use Darcy's Law for momentum transport** check box.

Membrane 1

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

2 Select Domain 4 only.

H2 Gas Diffusion Electrode 1

1. In the **Physics** toolbar, click **Domains** and choose **H2 Gas Diffusion Electrode**.
2. Select Domain 5 only.
3. In the **Settings** window for **H2 Gas Diffusion Electrode**, locate the **Effective Electrolyte Charge Transport** section.
4. In the ε_l text field, type `epsl`.
5. Locate the **Gas Transport** section. From the **Effective diffusivity correction** list, choose **Tortuosity**.
6. In the ε_g text field, type `epsg`.
7. In the τ_g text field, type `taug`.
8. In the κ_g text field, type `kappag_GDE`.

H2 Gas Diffusion Electrode Reaction: Water Electrolysis

1. In the **Model Builder** window, under **Component 1 (comp1)>Water Electrolyzer (we)> H2 Gas Diffusion Electrode 1** click **H2 Gas Diffusion Electrode Reaction 1**.
2. In the **Settings** window for **H2 Gas Diffusion Electrode Reaction**, type `H2 Gas Diffusion Electrode Reaction: Water Electrolysis` in the **Label** text field.
3. Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_HER`.
4. In the α_a text field, type `0.5`.
5. Locate the **Active Specific Surface Area** section. In the a_v text field, type `S`.

H2 Gas Diffusion Electrode 1

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

H2 Gas Diffusion Electrode Reaction: CO2 Electrolysis

1. In the **Physics** toolbar, click **Attributes** and choose **H2 Gas Diffusion Electrode Reaction**.
2. In the **Settings** window for **H2 Gas Diffusion Electrode Reaction**, type `H2 Gas Diffusion Electrode Reaction: CO2 Electrolysis` in the **Label** text field.
3. Locate the **Stoichiometric Coefficients** section. In the ν_{CO2} text field, type `-1`.
4. In the ν_{CO} text field, type `1`.
5. Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_COER`.
6. Locate the **Active Specific Surface Area** section. In the a_v text field, type `S`.

O2 Gas Diffusion Electrode 1

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

2 Select Domain 3 only.

3 In the **Settings** window for **O2 Gas Diffusion Electrode**, locate the **Effective Electrolyte Charge Transport** section.

4 In the ε_l text field, type `epsl`.

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

6 In the ε_g text field, type `epsg`.

7 In the τ_g text field, type `taug`.

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

O2 Gas Diffusion Electrode Reaction 1

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

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

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_OER`.

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

H2 Gas Flow Channel 1

Next, add the **H2 Gas Flow Channel**.

1 In the **Physics** toolbar, click **Domains** and choose **H2 Gas Flow Channel**.

2 Select Domain 6 only.

3 In the **Settings** window for **H2 Gas Flow Channel**, locate the **Gas Transport** section.

4 From the list, choose **Straight channels**.

5 In the H text field, type `dg`.

6 In the W text field, type `dg`.

O2 Gas Flow Channel 1

Next, add the **O2 Gas Flow Channel**.

1 In the **Physics** toolbar, click **Domains** and choose **O2 Gas Flow Channel**.

2 Select Domain 2 only.

3 In the **Settings** window for **O2 Gas Flow Channel**, locate the **Gas Transport** section.

4 From the list, choose **Straight channels**.

5 In the H text field, type `dg`.

6 In the W text field, type `dg`.

Current Collector 1

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

2 Select Domains 1 and 7 only.

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

4 From the σ_s list, choose **From material**.

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, click **Electronic Conducting Phase 1**.

Initial Values, O2 Domains 1

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

2 Select Domain 3 only.

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

4 In the ϕ_s text field, type `E_app`.

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 12 only.

Electronic Conducting Phase 1

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

Electric Potential 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electric Potential**.

2 Select Boundary 6 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the $\phi_{s,bnd}$ text field, type `E_app`.

H2 Gas Phase 1

Next, specify initial values, add the water gas shift reaction, and set the hydrogen inlet and outlet boundary conditions.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

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

3 In the $x_{0,\mathrm{H2O}}$ text field, type x0_H2O.

4 In the $x_{0,\mathrm{CO2}}$ text field, type x0_CO2.

5 In the $x_{0,\mathrm{CO}}$ text field, type x0_CO.

H2 Gas Phase 1

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

Water Gas Shift Reaction 1

1 In the **Physics** toolbar, click **Attributes** and choose **Water Gas Shift Reaction**.

2 In the **Settings** window for **Water Gas Shift Reaction**, locate the **Water Gas Shift Reaction Rate** section.

3 In the k_{WGSR} text field, type k_wgsr.

4 In the p_{ref} text field, type 1[Pa].

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 11 only.

3 In the **Settings** window for **H2 Inlet**, locate the **Mixture Specification** section.

4 From the list, choose **Mass flow rates**.

5 In the $J_{0,\mathrm{H2O}}$ text field, type Mflux_in*w0_H2O.

6 In the $J_{0,\mathrm{CO2}}$ text field, type Mflux_in*w0_CO2.

7 In the $J_{0,\mathrm{CO}}$ text field, type Mflux_in*w0_CO.

8 In the $\omega_{0,\mathrm{bnd,H2O}}$ text field, type w0_H2O.

9 In the $\omega_{0,\mathrm{bnd,CO2}}$ text field, type w0_CO2.

10 In the $\omega_{0,\mathrm{bnd,CO}}$ text field, type w0_CO.

11 Locate the **Flow Boundary Condition** section. From the list, choose **Total mass flow rate**.

12 In the J_0 text field, type Mflux_in.

H2 Gas Phase 1

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

H2 Outlet 1

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

2 Select Boundary 21 only.

O2 Gas Phase 1

Next, set the initial values and the oxygen inlet and outlet boundary conditions.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

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

3 In the $x_{0,\mathrm{N2}}$ text field, type `x0_N2`.

O2 Gas Phase 1

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

O2 Inlet 1

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

2 Select Boundary 3 only.

3 In the **Settings** window for **O2 Inlet**, locate the **Mixture Specification** section.

4 From the list, choose **Mass flow rates**.

5 In the $J_{0,\mathrm{N2}}$ text field, type `Mflux_in*w0_N2`.

6 In the $\omega_{0,\mathrm{bnd,N2}}$ text field, type `w0_N2`.

7 Locate the **Flow Boundary Condition** section. From the list, choose **Total mass flow rate**.

8 In the J_0 text field, type `Mflux_in`.

O2 Gas Phase 1

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

O2 Outlet 1

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

2 Select Boundary 17 only.

HEAT TRANSFER IN SOLIDS AND FLUIDS (HT)

Next, set the heat transfer physics.

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

2 In the **Settings** window for **Heat Transfer in Solids and Fluids**, locate the **Physical Model** section.

3 In the T_{ref} text field, type `T_in`.

Solid: Interconnects

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

2 In the **Settings** window for **Solid**, type `Solid: Interconnects` in the **Label** text field.

Fluid: Flow Channels

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

2 In the **Settings** window for **Fluid**, type `Fluid: Flow Channels` in the **Label** text field.

3 Select Domains 2 and 6 only.

4 Locate the **Model Input** section. From the p_A list, choose **User defined**. In the associated text field, type `we.pA`.

5 Locate the **Heat Convection** section. Specify the **u** vector as

we.u	x
we.v	y

6 Locate the **Heat Conduction, Fluid** section. From the k list, choose **Thermal conductivity, gas phase (we)**.

7 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.

8 From the ρ list, choose **Density of gas phase (we)**.

9 From the C_p list, choose **Heat capacity at constant pressure, gas phase (we)**.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

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

3 In the T text field, type `T_in`.

Porous Medium: Cathode GDE

Next, add thermal conductivities for the gas diffusion electrode domains.

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

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

3 Select Domain 5 only.

Fluid 1

1 In the **Model Builder** window, click **Fluid 1**.
2 In the **Settings** window for **Fluid**, locate the **Model Input** section.
3 From the p_A list, choose **User defined**. In the associated text field, type `we.pA`.
4 Locate the **Heat Convection** section. Specify the **u** vector as

`we.u`	x
`we.v`	y

5 Locate the **Heat Conduction, Fluid** section. From the k_f list, choose **Thermal conductivity, gas phase (we)**.
6 Locate the **Thermodynamics, Fluid** section. From the ρ_f list, choose **Density of gas phase (we)**.
7 From the $C_{p,\mathrm{f}}$ list, choose **Heat capacity at constant pressure, gas phase (we)**.

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.
2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.
3 From the ε_p list, choose **User defined**. In the associated text field, type `epsg`.
4 Locate the **Heat Conduction, Porous Matrix** section. From the k_b list, choose **User defined**. In the associated text field, type `kc`.
5 Locate the **Thermodynamics, Porous Matrix** section. From the ρ_b list, choose **User defined**. From the $C_{\mathrm{p,b}}$ list, choose **User defined**.

Porous Medium: Anode GDE

1 In the **Physics** toolbar, click **Domains** and choose **Porous Medium**.
2 In the **Settings** window for **Porous Medium**, type `Porous Medium: Anode GDE` in the **Label** text field.
3 Select Domain 3 only.

Fluid 1

1 In the **Model Builder** window, click **Fluid 1**.
2 In the **Settings** window for **Fluid**, locate the **Model Input** section.
3 From the p_A list, choose **User defined**. In the associated text field, type `we.pA`.

4 Locate the **Heat Convection** section. Specify the **u** vector as

`we.u`	x
`we.v`	y

5 Locate the **Heat Conduction, Fluid** section. From the k_f list, choose **Thermal conductivity, gas phase (we)**.

6 Locate the **Thermodynamics, Fluid** section. From the ρ_f list, choose **Density of gas phase (we)**.

7 From the $C_{p,\mathrm{f}}$ list, choose **Heat capacity at constant pressure, gas phase (we)**.

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.

3 From the ε_p list, choose **User defined**. In the associated text field, type `epsg`.

4 Locate the **Heat Conduction, Porous Matrix** section. From the k_b list, choose **User defined**. In the associated text field, type `ka`.

5 Locate the **Thermodynamics, Porous Matrix** section. From the ρ_b list, choose **User defined**. From the $C_{\mathrm{p,b}}$ list, choose **User defined**.

Solid: Membrane

Next, add thermal conductivity for the membrane domains.

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

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

3 Select Domain 4 only.

4 Locate the **Heat Conduction, Solid** section. From the k list, choose **User defined**. In the associated text field, type `km`.

5 Locate the **Thermodynamics, Solid** section. From the ρ list, choose **User defined**. From the C_p list, choose **User defined**.

Inflow 1

Next, add the inflow, outflow, and periodic condition boundary conditions.

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

2 Select Boundaries 3 and 11 only.

3 In the **Settings** window for **Inflow**, locate the **Upstream Properties** section.

4 In the T_ustr text field, type `T_in`.

Outflow 1

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

2 Select Boundaries 17 and 21 only.

Periodic Condition 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.

2 Select Boundaries 2 and 15 only.

MULTIPHYSICS

Next, add an electrochemical heating multiphysics coupling.

Electrochemical Heating 1 (ech1)

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

MATERIALS

Now, add materials from the Material Library.

ADD MATERIAL

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

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

3 In the tree, select **Fuel Cell and Electrolyzer>Solid Oxides>Yttria-Stabilized Zirconia, 8YSZ, (ZrO2)0.92-(Y2O3)0.08**.

4 Click **Add to Component** in the window toolbar.

MATERIALS

Yttria-Stabilized Zirconia, 8YSZ, (ZrO2)0.92-(Y2O3)0.08 (mat1)

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

2 Click **Clear Selection**.

3 Select Domains 3–5 only.

ADD MATERIAL

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

2 In the tree, select **Built-in>Steel AISI 4340**.

3 Click **Add to Component** in the window toolbar.

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

MATERIALS

Steel AISI 4340 (mat2)

Select Domains 1 and 7 only.

MESH 1

Next, set up a user-controlled mesh.

Distribution 1

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Distribution**.
2. Select Boundaries 2, 4, 6, 8, 10, 12, 14, and 15 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 **Model Builder** window, right-click **Mesh 1** and choose **Distribution**.
2. Select Boundaries 1, 13, 16, and 22 only.
3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. In the **Number of elements** text field, type 2.

Distribution 3

1. Right-click **Mesh 1** and choose **Distribution**.
2. Select Boundaries 3, 11, 17, and 21 only.
3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. In the **Number of elements** text field, type 10.

Distribution 4

1. Right-click **Mesh 1** and choose **Distribution**.
2. Select Boundaries 7 and 19 only.
3. In the **Settings** window for **Distribution**, locate the **Distribution** section.
4. In the **Number of elements** text field, type 2.

Distribution 5

1. Right-click **Mesh 1** and choose **Distribution**.
2. Select Boundaries 9 and 20 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 20.

6 In the **Element ratio** text field, type 10.

7 From the **Growth rate** list, choose **Exponential**.

Distribution 6

1 Right-click **Mesh 1** and choose **Distribution**.

2 Select Boundaries 5 and 18 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 10.

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

7 From the **Growth rate** list, choose **Exponential**.

8 Select the **Reverse direction** check box.

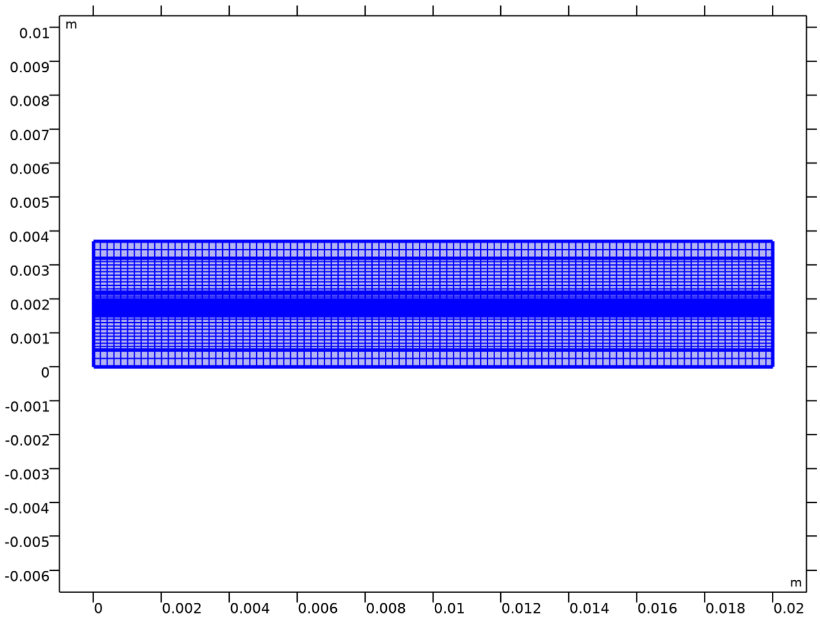
Mapped 1

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

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

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

The mesh should look like this:



STUDY 1

Finally, set the study settings using an auxiliary sweep for the applied potential to complete the model setup.

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, under **Study 1** click **Step 1: Current Distribution Initialization**.

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

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

Step 2: Stationary

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

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E_app (SOEC operating potential)	`0.5 1 1.5`	V

6 In the **Home** toolbar, click **Compute**.

RESULTS

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

Mole Fraction, H2 (we)

1 In the **Model Builder** window, under **Results** click **Mole Fraction, H2 (we)**.

2 In the **Mole Fraction, H2 (we)** toolbar, click **Plot**.

The plot should look like Figure 2.

Mole Fraction, CO (we)

1 In the **Model Builder** window, click **Mole Fraction, CO (we)**.

2 In the **Mole Fraction, CO (we)** toolbar, click **Plot**.

The plot should look like Figure 3.

Surface 1

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

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

3 In the **Expression** text field, type `T-T_in`.

Temperature (ht)

1 In the **Model Builder** window, click **Temperature (ht)**.

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

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

4 In the **Title** text area, type `Surface: Change in Temperature (K)`.

5 In the **Temperature (ht)** toolbar, click **Plot**.

The plot should look like Figure 4.

Water Gas Shift Reaction Rate

Next, plot the water gas shift reaction rate over the hydrogen gas diffusion electrode and flow channel domains.

1. In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.
2. In the **Settings** window for **2D Plot Group**, type `Water Gas Shift Reaction Rate` in the **Label** text field.

Surface 1

1. In the **Water Gas Shift Reaction Rate** toolbar, click **Surface**.
2. In the **Settings** window for **Surface**, locate the **Expression** section.
3. In the **Expression** text field, type `we.r_wgsr`.
4. In the **Water Gas Shift Reaction Rate** toolbar, click **Plot**.

   The plot should look like Figure 5.

Current Density Distribution

Finally, add a plot for the total integrated current density across the electrode length.

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Current Density Distribution` in the **Label** text field.
3. Locate the **Data** section. From the **Parameter selection (E_app)** list, choose **Last**.
4. Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
5. In the **Title** text area, type `Current Density Distribution, Cathode Side`.
6. Locate the **Plot Settings** section.
7. Select the **x-axis label** check box. In the associated text field, type `Electrode length (m)`.
8. Select the **y-axis label** check box. In the associated text field, type `Integrated current density in y-direction (A/cm<sup>2</sup>)`.

Line Graph 1

1. In the **Current Density Distribution** toolbar, click **Line Graph**.
2. Select Boundary 10 only.
3. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
4. In the **Expression** text field, type `genproj1(we.iv_h2gder1)`.
5. In the **Unit** field, type `A/cm^2`.
6. Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.
7. Click to expand the **Legends** section. Select the **Show legends** check box.
8. From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
H2O

Current Density Distribution

In the **Model Builder** window, click **Current Density Distribution**.

Line Graph 2

1 In the **Current Density Distribution** toolbar, click **Line Graph**.

2 Select Boundary 10 only.

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

4 In the **Expression** text field, type `genproj1(we.iv_h2gder2)`.

5 In the **Unit** field, type `A/cm^2`.

6 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

7 Locate the **Legends** section. Select the **Show legends** check box.

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

9 In the table, enter the following settings:

Legends
CO2

Current Density Distribution

1 In the **Model Builder** window, click **Current Density Distribution**.

2 In the **Current Density Distribution** toolbar, click **Plot**.

The plot should look like Figure 6.