Model created in COMSOL Multiphysics 6.4

Ammonia-Fed Solid Oxide Fuel Cell

Introduction

In this model of an ammonia-fed solid oxide fuel cell (SOFC), the required hydrogen is supplied through endothermic thermal decomposition of ammonia. 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 thermal decomposition reaction of ammonia is included in the H_2 gas diffusion electrode domain.

The model computes the spatial distributions of the various species across the gas-diffusion electrodes and gas-flow channels. It demonstrates that the SOFC is cooled down at the lower applied current density and heated up at the higher applied current density.

The model also demonstrates the use of auxiliary species in the H_2 gas mixture. The model is based on Ref. 1.

Model Definition

On the cathode, oxygen gas is reduced to form oxygen ions,

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

whereas on the anode, hydrogen gas is oxidized to form water vapor:

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

A thermal decomposition reaction of ammonia is included in the H_2 gas-diffusion electrode domain:

$$NH_3(g) \rightarrow 1.5H_2(g) + 0.5N_2(g) \tag{3}$$

Since the ammonia decomposition is an endothermic reaction, this reaction will absorb heat and cool down the SOFC. The cooling rate from decomposition will hence depend on the fuel flow rate into the cell.

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.

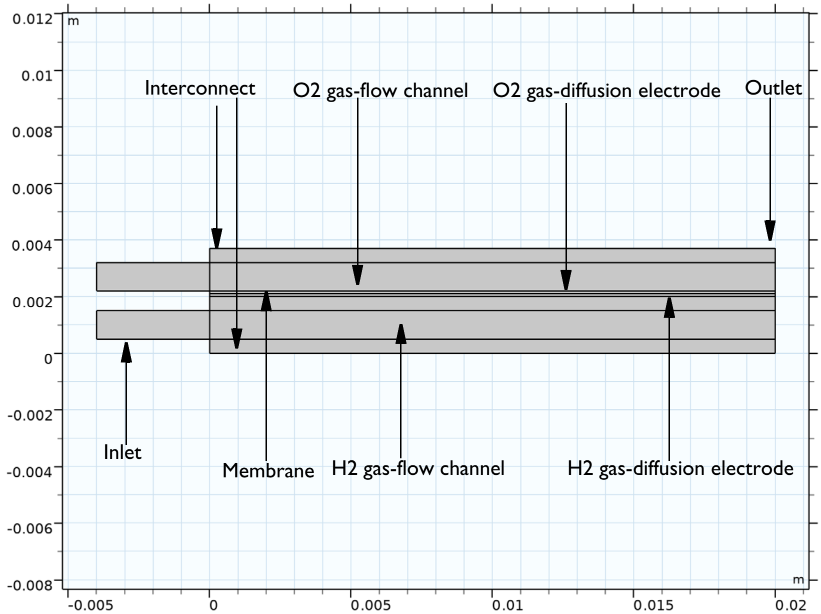


Figure 1: Model geometry. From top: Interconnect, O_2 gas channel, O_2 gas-diffusion electrode, solid oxide electrolyte layer, H_2 gas-diffusion electrode, H_2 gas-flow channel, and interconnect. The inlet and outlet positions are indicated in the figure.

The **Hydrogen Fuel Cell** 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 current distribution is defined assuming a temperature-dependent electrolyte conductivity of the solid electrolyte.

The gas mixture at the anode consists of H_2, H_2O, N_2, and NH_3, whereas that at the cathode the mixture consists of O_2 and N_2. NH_3 is added as an **Auxiliary Species** in the H_2 gas mixture and its properties are set using the **Thermodynamics** node. The molar fraction initial values for the H_2 gas mixture are derived assuming a close to 100% decomposition of NH_3, since this reaction is so fast.

The composition of the gas mixture changes as a result of the electrochemical reactions and the thermal decomposition reaction of ammonia. On the anode side, the electrode kinetics depends on the local concentrations of H_2O and H_2 and on the cathode side, the electrode kinetics depends on the local concentrations of O_2, according to the law of mass action (and the Nernst equation).

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 momentum flow is defined using the **Free and Porous Media Flow, Brinkman** interface for the H_2 and O_2 gas mixtures separately in the gas-flow channels and the gas-diffusion electrodes.

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 Hydrogen Fuel Cell interface.

For average cell currents above 0.1 A/cm^2, the molar flow rates of ammonia and oxygen are set to be proportional to the total current, with a 25% excess of ammonia and a 300% excess of oxygen (that is, using ammonia and oxygen flow stoichiometries of 1.25 and 4, respectively). Below 0.1 A/cm^2 the flow rates are held constant, corresponding to the flow rates values for a 1.25/4 stoichiometry at 0.1 A/cm^2.

The model is solved using an Auxiliary sweep, ramping up the average cell current density from 0.01 to 1 A/cm^2.

Results and Discussion

Figure 2 shows the change in the cell voltage and outlet temperature for different applied current densities. It can be seen in Figure 2 that the cell voltage decreases and the cell outlet temperature increases with an increase in the applied current density. The cell is cooled down for an applied current density of up to 0.1 A/cm^2, which is attributed to constant thermal decomposition of NH_3. Since the fuel stoichiometry for the flow rate is higher than 1.25/4 at currents below 0.1 A/cm^2, the decomposition reaction will cool the cell relatively more for low currents. In addition, the lower overpotentials at lower currents will generate relatively less heat for lower currents. The increase in the cell temperature beyond applied current density of 0.1 A/cm^2 is attributed to the increased cell heating due to the increased voltage losses.

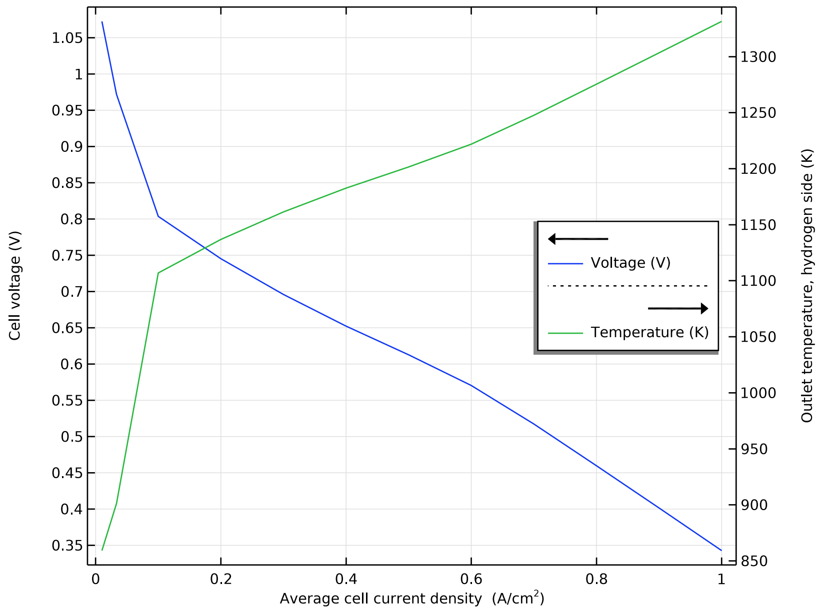


Figure 2: Change in cell voltage and outlet temperature at different applied current densities.

Figure 3 shows the change in temperature across the SOFC cell for applied current densities of 0.01 A/cm^2 (left) and 1 A/cm^2 (right). The negative change in temperature indicates that the cell is cooled down at an applied current density of 0.01 A/cm^2, whereas the positive change in temperature indicates that the cell is heated up at an applied current density of 1 A/cm^2.

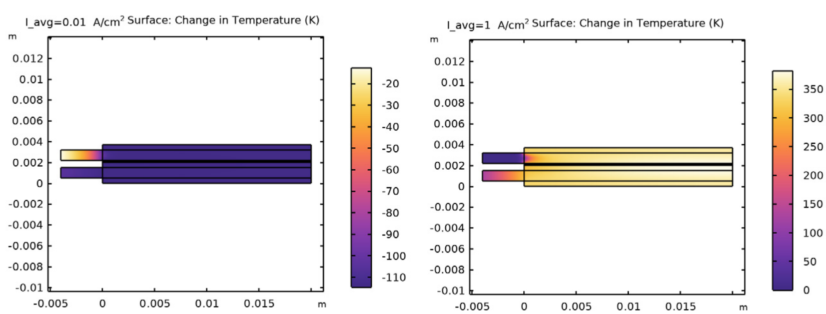


Figure 3: Change in temperature at applied current density 0.01 A/cm^2 (left) and 1 A/cm^2 (right).

Figure 4 shows the change in thermal decomposition reaction rate of ammonia across the SOFC cell for applied current densities of 0.01 A/cm^2 (left) and 1 A/cm^2 (right). The ammonia thermal decomposition rate increases with an increase in the applied current density, which is attributed to the increased cell temperature.

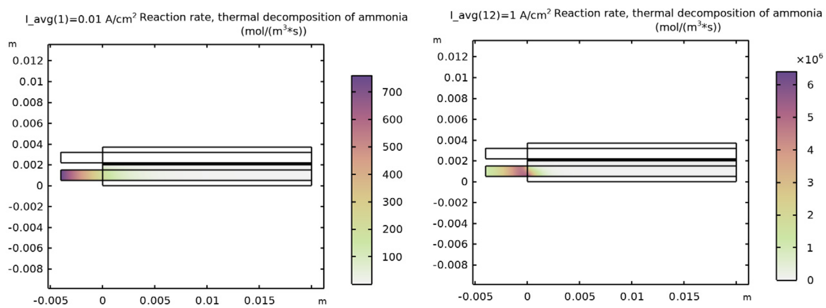


Figure 4: Change in thermal decomposition reaction rate of ammonia at applied current density 0.01 A/cm^2 (left) and 1 A/cm^2 (right).

Figure 5 shows the change in ammonia concentration across the SOFC cell for applied current densities of 0.01 A/cm^2 (left) and 1 A/cm^2 (right). The ammonia concentration is more uniform at 0.01 A/cm^2 as compared to 1 A/cm^2, which is attributed to the higher ammonia thermal decomposition rate at the higher applied current density.

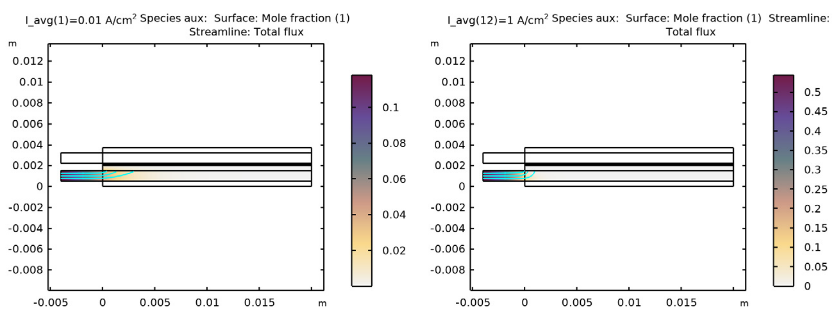


Figure 5: Change in ammonia concentration at applied current density 0.01 A/cm^2 (left) and 1 A/cm^2 (right).

Reference

1. M. Ni, "Thermo-electrochemical modeling of ammonia-fueled solid oxide fuel cells considering ammonia thermal decomposition in the anode," *Int. J. Hydrog. Energy*, vol. 36, p. 3153, 2011.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/sofc_nh3`

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** > **Solid Oxide (fc)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Fluid Flow** > **Porous Media and Subsurface Flow** > **Free and Porous Media Flow, Brinkman (fp)**.

5 Click **Add**.

6 In the **Velocity field (m/s)** text field, type `ua`.

7 In the **Velocity field components** table, enter the following settings:

ua
va
wa

8 In the **Pressure (Pa)** text field, type `pa`.

9 Click **Add**.

10 In the **Velocity field (m/s)** text field, type `uc`.

11 In the **Velocity field components** table, enter the following settings:

uc
vc
wc

12 In the **Pressure (Pa)** text field, type `pc`.

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

14 Click **Add**.

15 Click **Study**.

16 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Hydrogen Fuel Cell** > **Stationary with Initialization**.

17 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 `sofc_nh3_parameters.txt`.

GEOMETRY 1

Draw the model geometry using a rectangle and six layers and two inlets for extended inlets.

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 5	dc
Layer 6	dg

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

Rectangle 2 (r2)

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

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

3 In the **Width** text field, type `din`.

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

5 Locate the **Position** section. In the **x** text field, type `-din`.

6 In the **y** text field, type `di`.

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

Rectangle 3 (r3)

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

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

3 In the **Width** text field, type `din`.

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

5 Locate the **Position** section. In the **x** text field, type `-din`.

6 In the **y** text field, type `di+dg+da+dm+dc`.

7 Click **Build All Objects**.

8 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 `sofc_nh3_variables.txt`.

GLOBAL DEFINITIONS

Add thermodynamic properties for ammonia.

1 In the **Physics** toolbar, click **Thermodynamics** and choose **Thermodynamic System**.

SELECT SYSTEM

1 Go to the **Select System** window.
2 Click the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.
2 In the **Species** list box, select **ammonia (7664-41-7, H3N)**.
3 Click + **Add Selected**.
4 Click the **Next** button in the window toolbar.

SELECT THERMODYNAMIC MODEL

1 Go to the **Select Thermodynamic Model** window.
2 Click the **Finish** button in the window toolbar.

GLOBAL DEFINITIONS

Gas System 1 (pp1)

Right-click **Global Definitions** > **Thermodynamics** > **Gas System 1 (pp1)** and choose **Species Property**.

SELECT PROPERTIES

1 Go to the **Select Properties** window.
2 In the list, choose **Enthalpy of formation (J/mol)**, **Entropy of formation (J/(K*mol))**, **Fuller diffusion volume (cm^3)**, **Heat capacity (Cp) (J/(K*mol))**, **Molar mass (g/mol)**, **Normal boiling-point temperature (K)**, **Thermal conductivity (W/(m*K))**, and **Viscosity (Pa*s)**.
3 Click + **Add Selected**.
4 Click the **Next** button in the window toolbar.

SELECT PHASE

1 Go to the **Select Phase** window.
2 Click the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.
2 In the list box, select **ammonia**.
3 Click + **Add Selected**.

4 Click the **Next** button in the window toolbar.

SPECIES PROPERTY OVERVIEW

1 Go to the **Species Property Overview** window.

2 Click the **Finish** button in the window toolbar.

HYDROGEN FUEL CELL (FC)

Start setting up the electrochemistry part of the model.

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 **Domain Selection** section.

3 In the list box, select **9**.

4 Click **Remove from Selection**.

5 Select Domains 1–8 only.

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

7 Click **Remove from Selection**.

8 Select Domains 1, 2, and 4–8 only.

9 Locate the **H2 Gas Mixture** section. Select the **N2** checkbox.

10 Select the **Auxiliary species** checkbox.

11 Click to expand the **Electrode Reaction Settings** section. Find the **Built-in thermodynamic expressions** subsection. In the T_{RHE} text field, type `T_in`.

12 Locate the **Out-of-Plane Thickness** section. In the d_z text field, type `D`.

Membrane 1

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

2 Select Domain 6 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 Select the **Include pore-wall interaction** checkbox.

9 In the d_{pore} text field, type d_pore.

H2 Gas Diffusion Electrode Reaction 1

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

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

3 In the $i_{0,ref}(T)$ text field, type i0_ref_H2.

4 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 7 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 Select the **Include pore-wall interaction** checkbox.

9 In the d_{pore} text field, type d_pore.

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 $i_{0,ref}(T)$ text field, type i0_ref_O2.

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 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 Domains 1 and 4 only.

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 Domains 2 and 8 only.

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 7 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 12 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 18 only.
3 In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.
4 In the $I_{s,total}$ text field, type `-I_tot`.

H2 Gas Phase 1

Set dynamic viscosity to built in and set thermodynamics properties for auxiliary species.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Hydrogen Fuel Cell (fc)** click **H2 Gas Phase 1**.
2 In the **Settings** window for **H2 Gas Phase**, locate the **Auxiliary Species** section.
3 In the M_{aux} text field, type `M_aux`.
4 In the $H_{aux}(T)$ text field, type `H_aux`.
5 In the $S_{aux}(T)$ text field, type `S_aux`.

6 In the $C_{p,aux}(T)$ text field, type `Cp_aux`.

7 In the ν_{aux} text field, type `nu_aux`.

8 In the μ_{aux} text field, type `mu_aux`.

9 In the k_{aux} text field, type `k_aux`.

10 In the $T_{b,aux}$ text field, type `Tb_aux`.

Next, specify initial values, add the ammonia decomposition 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 $x_{0,H2O}$ text field, type `x0_H2O_an`.

4 In the $x_{0,N2}$ text field, type `x0_N2_an`.

5 In the $x_{0,aux}$ text field, type `x0_NH3_an`.

H2 Gas Phase 1

1 Click the **Show More Options** button in the **Model Builder** toolbar.

2 In the **Show More Options** dialog, select **Physics** > **Advanced Physics Options** in the tree.

3 In the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

4 Click **OK**.

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

Reaction Sources 1

1 In the **Physics** toolbar, click **Attributes** and choose **Reaction Sources**.

2 Select Domain 5 only.

3 In the **Settings** window for **Reaction Sources**, locate the **Reaction Sources** section.

4 From the **Source type** list, choose **Molar**.

5 In the r_{H2} text field, type `1.5*r_NH3`.

6 In the r_{N2} text field, type `0.5*r_NH3`.

7 In the r_{aux} text field, type `-r_NH3`.

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 1 only.

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

4 Clear the **Stoichiometric feed** checkbox.

5 Locate the **Mass Flow Rates** section. In the $J_{0,\text{aux}}$ text field, type `m_NH3_an`.

6 Locate the **Boundary Initial Values** section. From the list, choose **User defined**.

7 In the $\omega_{0,\text{bnd,H2O}}$ text field, type `w0_H2O_an`.

8 In the $\omega_{0,\text{bnd,N2}}$ text field, type `w0_N2_an`.

9 In the $\omega_{0,\text{bnd,aux}}$ text field, type `w0_NH3_an`.

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 Boundaries 23 and 24 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, expand the **O2 Gas Phase 1** node, then click **Initial Values 1**.

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

3 In the $x_{0,\text{N2}}$ text field, type `x0_N2_cath`.

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 4 only.

3 In the **Settings** window for **O2 Inlet**, locate the **Stoichiometric Feed** section.

4 In the I text field, type `I_flow`.

5 In the S_{O2} text field, type `stoich_O2`.

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 Boundaries 26 and 27 only.

FREE AND POROUS MEDIA FLOW, BRINKMAN - H2 SIDE

Next set flow physics at H2 and O2 sides separately.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free and Porous Media Flow, Brinkman (fp)**.

2 In the **Settings** window for **Free and Porous Media Flow, Brinkman**, type `Free and Porous Media Flow, Brinkman - H2 side` in the **Label** text field.

3 Locate the **Domain Selection** section. Click **Clear Selection**.

4 Select Domains 1, 4, and 5 only.

5 Locate the **Physical Model** section. From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Porous Medium 1

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

2 Select Domain 5 only.

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 From the κ list, choose **User defined**. In the associated text field, type `kappag_GDE`.

Inlet 1

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

2 Select Boundary 1 only.

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

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

5 Locate the **Mass Flow** section. In the m text field, type `m_NH3_an`.

Outlet 1

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

2 Select Boundary 23 only.

FREE AND POROUS MEDIA FLOW, BRINKMAN - O2 SIDE

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Free and Porous Media Flow, Brinkman 2 (fp2)**.

2 In the **Settings** window for **Free and Porous Media Flow, Brinkman**, type `Free and Porous Media Flow, Brinkman - O2 Side` in the **Label** text field.

3 Locate the **Domain Selection** section. Click **Clear Selection**.

4 Select Domains 2, 7, and 8 only.

5 Locate the **Physical Model** section. From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Porous Medium 1

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

2 Select Domain 7 only.

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 From the κ list, choose **User defined**. In the associated text field, type `kappag_GDE`.

Inlet 1

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

2 Select Boundary 4 only.

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

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

5 Locate the **Mass Flow** section. In the m text field, type `fc.o2gasph1.o2in1.J0`.

Outlet 1

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

2 Select Boundary 27 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 1, 2, 4, and 8 only.
4. Locate the **Heat Conduction, Fluid** section. From the k list, choose **Thermal conductivity, gas phase (fc)**.
5. Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.
6. From the ρ list, choose **Density of gas phase (fc)**.
7. From the C_p list, choose **Heat capacity at constant pressure, gas phase (fc)**.

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: Anode GDE

Next, add thermal conductivity, density and heat capacity 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: Anode 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 **Heat Conduction, Fluid** section.
3. From the k_{f} list, choose **Thermal conductivity, gas phase (fc)**.
4. Locate the **Thermodynamics, Fluid** section. From the ρ_{f} list, choose **Density of gas phase (fc)**.
5. From the $C_{p,\mathrm{f}}$ list, choose **Heat capacity at constant pressure, gas phase (fc)**.

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 $C_{p,b}$ list, choose **User defined**.

Porous Medium: Cathode GDE

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 7 only.

Fluid 1

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

2 In the **Settings** window for **Fluid**, locate the **Heat Conduction, Fluid** section.

3 From the k_f list, choose **Thermal conductivity, gas phase (fc)**.

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

5 From the $C_{p,f}$ list, choose **Heat capacity at constant pressure, gas phase (fc)**.

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 $C_{p,b}$ 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 6 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 1 and 4 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 23, 24, 26, and 27 only.

Periodic Condition 1

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

2 Select Boundaries 8 and 21 only.

MULTIPHYSICS

Next, add a few multiphysics coupling nodes for electrochemical heating, nonisothermal flow and reacting flow.

Electrochemical Heating 1 (ech1)

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

Nonisothermal Flow 1 (nitf1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain** > **Nonisothermal Flow**.

Nonisothermal Flow 2 (nitf2)

1 In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain** > **Nonisothermal Flow**.

2 In the **Settings** window for **Nonisothermal Flow**, locate the **Coupled Interfaces** section.

3 From the **Fluid flow** list, choose **Free and Porous Media Flow, Brinkman - O2 Side (fp2)**.

Reacting Flow, H2 Gas Phase 1 (rfh1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain** > **Reacting Flow, H2 Gas Phase**.

Reacting Flow, O2 Gas Phase 1 (rfo1)

1 In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain** > **Reacting Flow, O2 Gas Phase**.

2 In the **Settings** window for **Reacting Flow, O2 Gas Phase**, locate the **Coupled Interfaces** section.

3 From the **Fluid flow** list, choose **Free and Porous Media Flow, Brinkman - O2 Side (fp2)**.

DEFINITIONS

Next, add a couple of probes to be used later in postprocessing.

Global Variable Probe 1 (var1)

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 Click to expand the **Table and Window Settings** section. From the **Output table** list, choose **New table**.

5 Click **Add Plot Window**.

Point Probe 1 (point1)

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

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

3 Click **Clear Selection**.

4 Select Point 14 only.

5 Locate the **Expression** section. In the **Expression** text field, type `T`.

6 Click to expand the **Table and Window Settings** section. From the **Output table** list, choose **New table**.

7 From the **Plot window** list, choose **Probe Plot 1**.

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 the **Add to Component** button 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 5–7 only.

ADD MATERIAL

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

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

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

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

MATERIALS

Steel AISI 4340 (mat2)

Select Domains 3 and 9 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 8, 10, 12, 14, 16, 18, 20, and 21 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 `100`.

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

7 Select the **Reverse direction** checkbox.

Distribution 2

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

2 Select Boundaries 7, 19, 22, and 28 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 1, 4, 9, 17, 23, and 27 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 2.
7 Select the **Symmetric distribution** checkbox.

Distribution 4

1 Right-click **Mesh 1** and choose **Distribution**.
2 Select Boundaries 13 and 25 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 15 and 26 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 40.
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 11 and 24 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 40.
6 In the **Element ratio** text field, type 10.

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

8 Select the **Symmetric distribution** checkbox.

Distribution 7

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

2 Select Boundaries 2, 3, 5, and 6 only.

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

4 In the **Number of elements** text field, type 20.

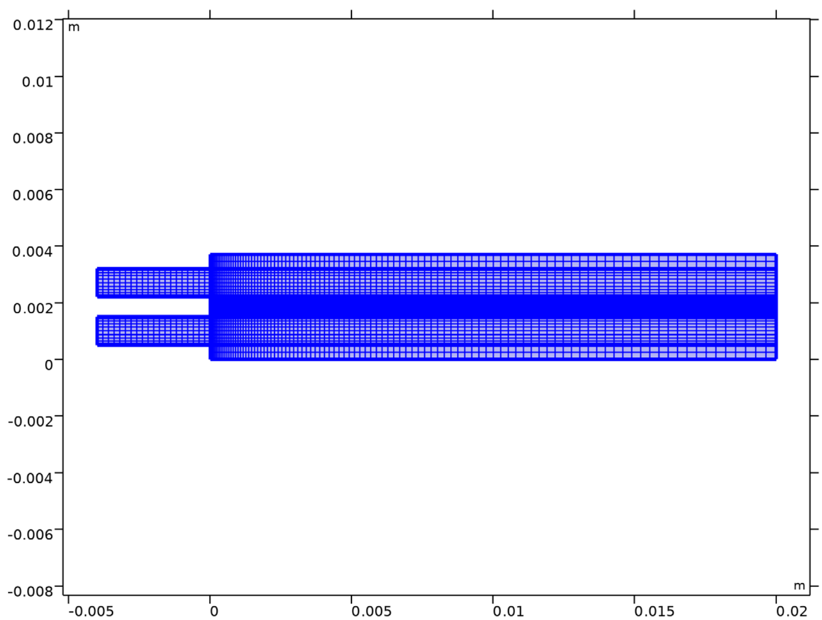
Mapped 1

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 current distribution initialization, flow initialization, and stationary study settings using an auxiliary sweep for the average cell current density to complete the model setup.

Step 3: Stationary 2

In the **Study** toolbar, click **Stationary**.

Step 1: Current Distribution Initialization

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

Stationary - Flow Initialization

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

2 In the **Settings** window for **Stationary**, type `Stationary - Flow Initialization` in the **Label** text field.

3 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Hydrogen Fuel Cell (fc)** and **Heat Transfer in Solids and Fluids (ht)**.

4 In the **Solve for** column of the table, under **Component 1 (comp1)** > **Multiphysics**, clear the checkboxes for **Electrochemical Heating 1 (ech1)**, **Nonisothermal Flow 1 (nitf1)**, and **Nonisothermal Flow 2 (nitf2)**.

Stationary - All Physics

1 In the **Model Builder** window, under **Study 1** click **Step 3: Stationary 2**.

2 In the **Settings** window for **Stationary**, type `Stationary - All Physics` in the **Label** text field.

3 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
I_avg (Average cell current density)	`I_avg_init I_avg_final/30 range(I_avg_final/10, I_avg_final/10, I_avg_final)`	`A/cm^2`

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Stationary Solver 3** node.

4 Right-click **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Stationary Solver 3** and choose **Fully Coupled**.

5 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.

6 In the **Maximum number of iterations** text field, type `100`.

7 From the **Termination criterion** list, choose **Solution**.

8 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.

Voltage and Temperature

1 In the **Model Builder** window, expand the **Results** > **Probe Plot Group 1** node, then click **Probe Plot Group 1**.

2 In the **Settings** window for **1D Plot Group**, type `Voltage and Temperature` 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/cm<sup>2</sup>)`.

5 Select the **Two y-axes** checkbox.

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

7 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Outlet temperature, hydrogen side (K)`.

8 In the table, enter the following settings:

Plot	Plot on secondary y-axis
Probe Table Graph 1	
Probe Table Graph 2	√

9 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Probe Table Graph 1

1 In the **Model Builder** window, click **Probe Table Graph 1**.

2 In the **Settings** window for **Table Graph**, click to expand the **Legends** section.

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

4 In the table, enter the following settings:

Legends
Voltage (V)

Probe Table Graph 2

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

2 In the **Settings** window for **Table Graph**, locate the **Legends** section.

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

4 In the table, enter the following settings:

Legends
Temperature (K)

Voltage and Temperature

1 In the **Model Builder** window, click **Voltage and Temperature**.

2 In the **Voltage and Temperature** toolbar, click **Plot**.

The plot should look like Figure 2.

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 **Parameter indicator** text field, type I_avg=eval(I_avg,A/cm^2) A/cm².

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

7 Locate the **Data** section. From the **Parameter value (I_avg (A/cm^2))** list, choose **0.01**.

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

The plots should look like Figure 3.

Ammonia Decomposition Reaction Rate

Next, plot ammonia thermal decomposition reaction rate over the hydrogen gas diffusion electrode and flow channel domains.

1 In the **Results** toolbar, click **2D Plot Group**.
2 In the **Settings** window for **2D Plot Group**, type `Ammonia Decomposition Reaction Rate` in the **Label** text field.

Surface 1

1 In the **Ammonia Decomposition Reaction Rate** toolbar, click **Surface**.
2 In the **Settings** window for **Surface**, locate the **Expression** section.
3 In the **Expression** text field, type `r_NH3`.
4 Locate the **Coloring and Style** section. From the **Color table** list, choose **HelfrichiZero**.

Ammonia Decomposition Reaction Rate

1 In the **Model Builder** window, click **Ammonia Decomposition Reaction Rate**.
2 In the **Ammonia Decomposition Reaction Rate** toolbar, click **Plot**.
3 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
4 From the **Parameter value (I_avg (A/cm^2))** list, choose **0.01**.
5 In the **Ammonia Decomposition Reaction Rate** toolbar, click **Plot**.

The plots should look like Figure 4.

Surface 1

1 In the **Model Builder** window, expand the **Results** > **Mole Fraction, aux (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 **ConopiformisZero**.

Streamline 1

1 In the **Model Builder** window, expand the **Results** > **Mole Fraction, aux (fc)** node, then click **Streamline 1**.
2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3 From the **Positioning** list, choose **Magnitude controlled**.
4 In the **Maximum density level** text field, type `10`.
5 Locate the **Coloring and Style** section. Find the **Point style** subsection.
6 Select the **Scale factor** checkbox. In the associated text field, type `0.06`.

7 From the **Color** list, choose **Cyan**.

The plots should look like Figure 5.

8 In the **Mole Fraction, aux (fc)** toolbar, click **Plot**.

Mole Fraction, aux (fc)

1 In the **Model Builder** window, click **Mole Fraction, aux (fc)**.

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

3 From the **Parameter value (I_avg (A/cm^2))** list, choose **0.01**.

Streamline 1

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

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

3 From the **Positioning** list, choose **Magnitude controlled**.

4 In the **Maximum density level** text field, type `8.8`.

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. In the **Scale factor** text field, type `0.6`.

6 In the **Mole Fraction, aux (fc)** toolbar, click **Plot**.

Follow the instructions below to improve the appearance of the remaining 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

1 In the **Model Builder** window, click **Arrow Surface 1**.

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

3 From the **Color** list, choose **Yellow**.

Surface 1

1 In the **Model Builder** window, expand the **Results** > **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 **ConopiformisZero**.

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.
2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3 From the **Positioning** list, choose **Magnitude controlled**.
4 In the **Maximum density level** text field, type 12.
5 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 **Results** > **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 **ConopiformisZero**.

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.
2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3 From the **Positioning** list, choose **Magnitude controlled**.
4 In the **Maximum density level** text field, type 10.
5 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 **Results** > **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 **ConopiformisZero**.

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.
2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3 From the **Positioning** list, choose **Magnitude controlled**.
4 In the **Maximum density level** text field, type 10.
5 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 **Results** > **Mole Fraction, N2 (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 **ConopiformisZero**.

Streamline 1

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

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

3 From the **Positioning** list, choose **Magnitude controlled**.

4 In the **Maximum density level** text field, type `10`.

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