Model created in COMSOL Multiphysics 6.4

Ohmic and Activation Losses in a Polymer Electrolyte Membrane Water Electrolyzer Cell

Introduction

In a polymer electrolyte membrane water electrolyzer cell, hydrogen and oxygen gas is produced by electrolysis. The hydrogen and oxygen compartments are separated by a polymer membrane, which also acts as electrolyte.

This introductory tutorial computes the ohmic and activation losses in a membrane–electrode assembly (MEA) in a polymer–electrolyte membrane water electrolyzer. The model geometry is in 1D and comprises two porous transport layers (PTLs) and one membrane domain.

The exterior boundaries of the hydrogen and oxygen PTLs are assumed to be at equilibrium with fully humidified gas streams, and gas diffusion is assumed to be fast. Hence no mass transport or momentum transfer is included in the model.

Model Definition

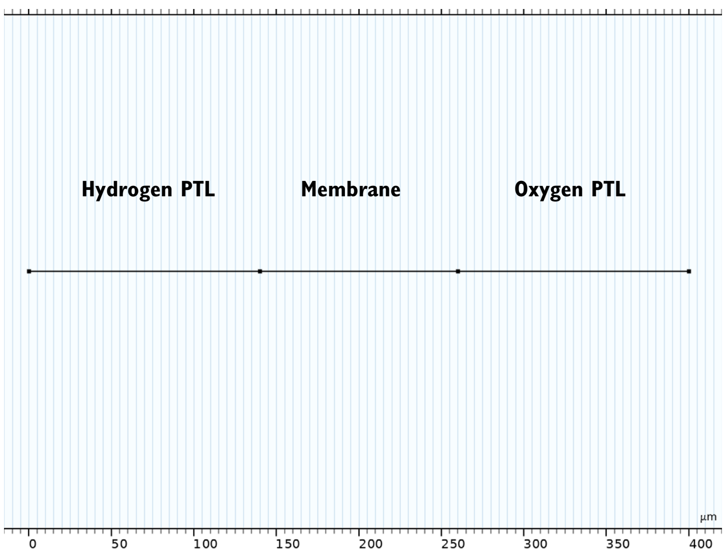


Figure 1: Model geometry.

Figure 1 shows the model geometry. The geometry consists of two PTLs (140 µm thick each) and one membrane (120 µm thick) domain.

The conductivity of the Nafion® electrolyte is added from the Fuel Cell and Electrolyzer Material Library.

The model is setup using the **Water Electrolyzer** interface. The electrodes are assumed to be very thin and are hence modeled as internal boundary conditions at the membrane–PTL boundaries, using Butler–Volmer kinetics. Ohmic losses are included in the electrode and electrolyte phases are included in the PTLs and Membrane, respectively. Any effects due to gas phase mass transport limitations are neglected (this is also known as a secondary current distribution model). The model is isothermal.

The equilibrium potentials of the electrode reactions are defined using the built-in thermodynamic functions, defining the oxygen and hydrogen gas streams to be at 100% relative humidity at the operating cell temperature (80°C) and pressure (1 atm)

The model is solved using an **Auxiliary Sweep**, sweeping the stationary cell voltage from 1.4 V to 2.2 V.

Results and Discussion

Figure 2 shows the electric potential in the electrode phase of the PTLs at varied cell voltages. As the cell voltages increases, increasing potential gradients are observed in the cell. At the highest cell voltage, the potential drop in each PTL is about 60 mV.

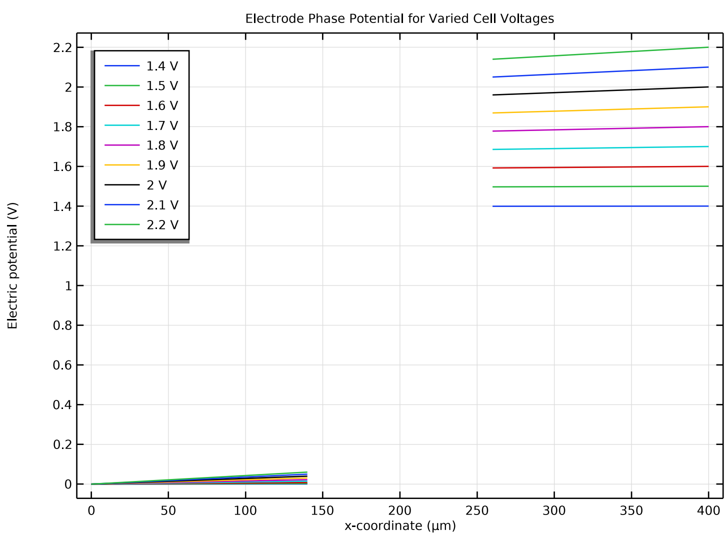


Figure 2: Electrode phase potential at varied cell voltages.

Figure 3 shows the corresponding electrolyte phase potentials. Also here, increased potential gradients are observed with the increasing cell voltage, with a maximum voltage drop of about 325 mV at the highest cell voltage.

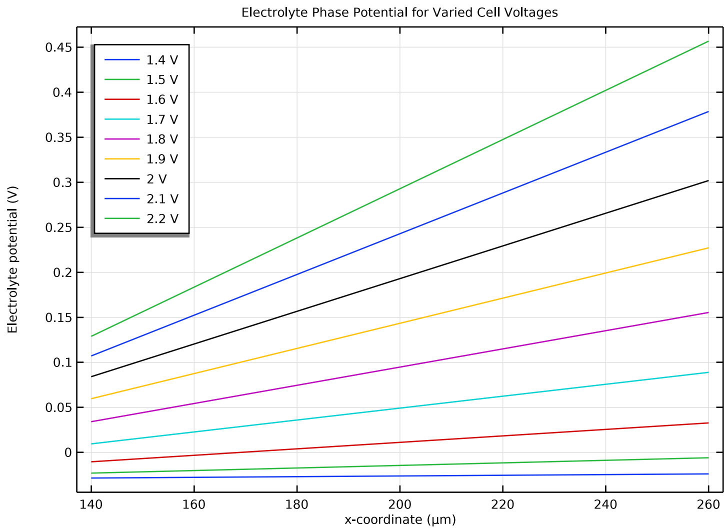


Figure 3: Electrolyte phase potential at varied cell voltages.

Figure 4 shows a polarization plot of the cell. As the cell voltage is increased, the current increases exponentially at first, with a transition to a linear behavior with respect to the cell voltage at higher voltages. This behavior can be ascribed to the exponential Butler–Volmer kinetics dominating cell polarization at low current densities, in combination with the cell membrane resistance significantly impacting the cell polarization at higher cell current densities.

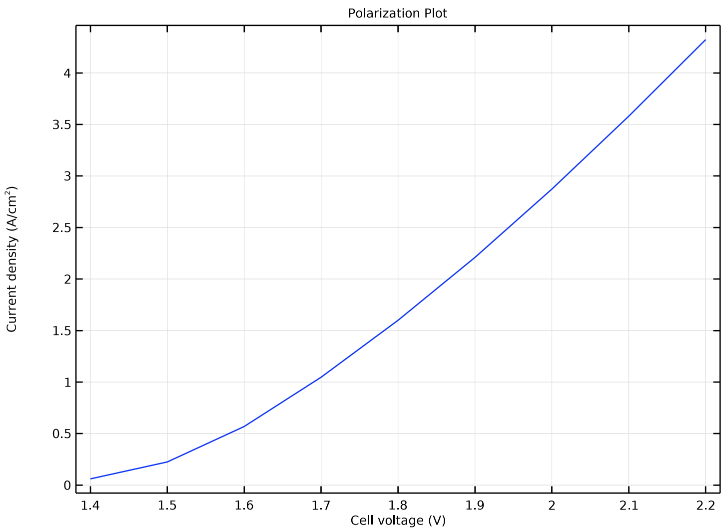


Figure 4: Polarization plot.

Finally, Figure 5 depicts the activation overpotentials of the individual electrode reactions. The oxygen evolution reaction, being a more sluggish reaction, exhibits an about five times larger potential loss at the highest cell voltage than the hydrogen evolution reaction.

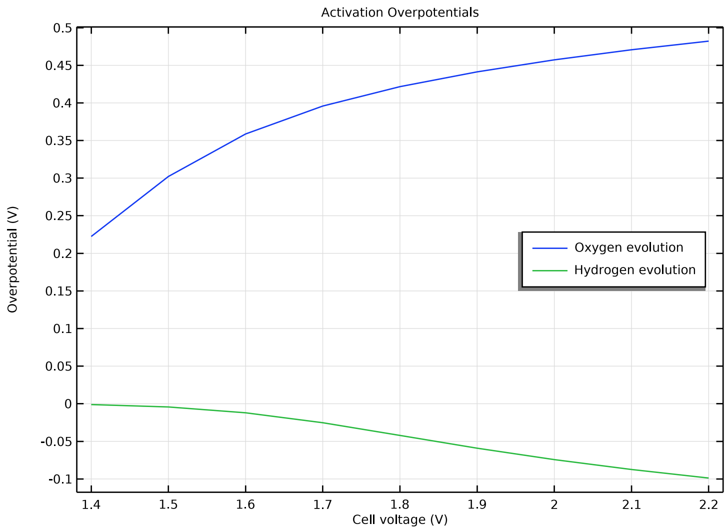


Figure 5: Activation overpotentials.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Electrolyzers/pemwe_1d`

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 **1D**.

2 In the **Select Physics** tree, select **Electrochemistry** > **Water Electrolyzers** > **Proton Exchange Membrane (we)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Add the model parameters from a text file as follows:

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 `pemwe_1d_parameters.txt`.

GEOMETRY 1

The model geometry consists of three domains: the hydrogen-side porous transport layer (PTL), the membrane, and the oxygen-side PTL.

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

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

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

Interval 1 (i1)

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

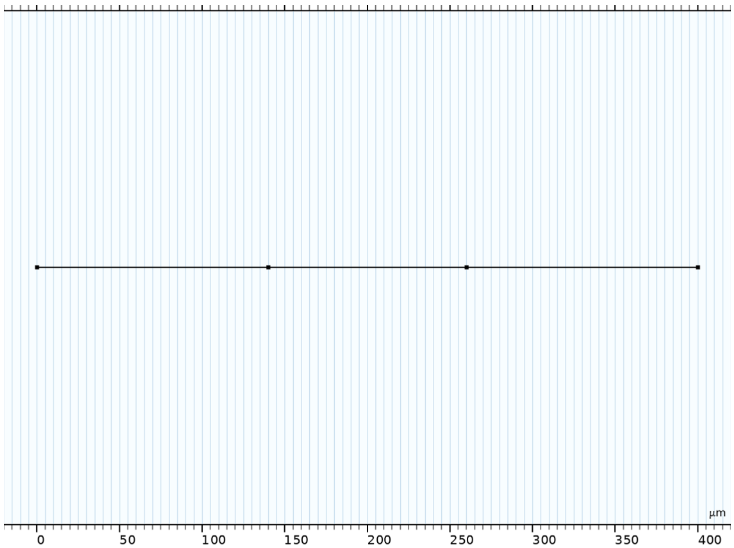
2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 From the **Specify** list, choose **Interval lengths**.

4 In the table, enter the following settings:

Lengths (µm)
L_ptl
L_mem
L_ptl

5 Click **Build All Objects**.



MATERIALS

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

ADD MATERIAL

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

MATERIALS

Nafion®, EW 1100, Liquid Equilibrated, Protonated (mat1)
Select Domain 2 only.

WATER ELECTROLYZER (WE)

Now start defining the actual physics of the model. Begin by turning off diffusion in the gas phase mixtures as follows:

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 Find the **Transport mechanisms** subsection. Clear the **Include gas phase diffusion** checkbox.

4 Locate the **O2 Gas Mixture** section. Clear the **Include gas phase diffusion** checkbox.

H2 Gas Diffusion Layer 1

Add nodes for the different components of the electrolyzer and assign them to the different domains. This will define what phases are active where.

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

2 Select Domain 1 only.

3 In the **Settings** window for **H2 Gas Diffusion Layer**, locate the **Electrode Charge Transport** section.

4 In the σ_s text field, type `sigmas_ptl`.

O2 Gas Diffusion Layer 1

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

2 Select Domain 3 only.

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

4 In the σ_s text field, type `sigmas_ptl`.

Membrane 1

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

2 Select Domain 2 only.

Thin H2 Gas Diffusion Electrode 1

Now add the electrodes, and the modify some of the corresponding default electrode reaction settings as follows:

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

2 Select Boundary 2 only.

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

4 In the d_{gde} text field, type `d_H2_electrode`.

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_ref_H2`.

4 Locate the **Active Specific Surface Area** section. In the a_{v} text field, type `Av_H2_electrode`.

Note that the reference equilibrium potential of the electrode reaction in the **Equilibrium Potential** section is set to **Built in** by default. Keep this setting as is. This will compute the equilibrium potential automatically based on the settings of the gas phase nodes, which will be specified later.

Thin O2 Gas Diffusion Electrode 1

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

2 Select Boundary 3 only.

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

4 In the d_{gde} text field, type `d_O2_electrode`.

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_ref_O2`.

4 Locate the **Active Specific Surface Area** section. In the a_{v} text field, type `Av_O2_electrode`.

Electronic Conducting Phase 1

As external boundary conditions to the model you will make use of a **Ground** and an **Electric Potential** node.

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

Electric Ground 1

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

2 Select Boundary 1 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 4 only.

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

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

H2 Gas Phase 1

Now specify the gas mixtures in each gas compartment. As mentioned earlier, this will impact how the **Built-in** equilibrium potentials of the electrode reactions are defined.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Water Electrolyzer (we)** click **H2 Gas Phase 1**.

2 In the **Settings** window for **H2 Gas Phase**, locate the **Composition** section.

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

4 In the T_{hum} text field, type `T`.

5 In the $p_{A,hum}$ text field, type `p_cell`.

O2 Gas Phase 1

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

4 In the T_{hum} text field, type `T`.

5 In the $p_{A,hum}$ text field, type `p_cell`.

GLOBAL DEFINITIONS

Default Model Inputs

The **Default Model Inputs** node allows you to set a common pressure and temperature for all physics nodes of the model.

1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General** > **Pressure (Pa) - minput.pA**.

4 Find the **Expression for remaining selection** subsection. In the **Pressure** text field, type `p_cell`.

5 In the tree, select **General** > **Temperature (K) - minput.T**.

6 In the **Temperature** text field, type T.

STUDY 1

Step 2: Stationary

The model is now ready for solving. Solve for a range of cell voltages by using an **Auxiliary Sweep** as follows:

1 In the **Model Builder** window, under **Study 1** click **Step 2: 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
E_cell (Cell voltage (sweep parameter))		V

6 Click **Range**.

7 In the **Range** dialog, type 1.4 in the **Start** text field.

8 In the **Step** text field, type 0.1.

9 In the **Stop** text field, type 2.2.

10 Click **Replace**.

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

RESULTS

Electrode Phase Potential for Varied Cell Voltages

Inspect and modify some of the default plots as follows:

1 In the **Settings** window for **1D Plot Group**, type Electrode Phase Potential for Varied Cell Voltages in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

3 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

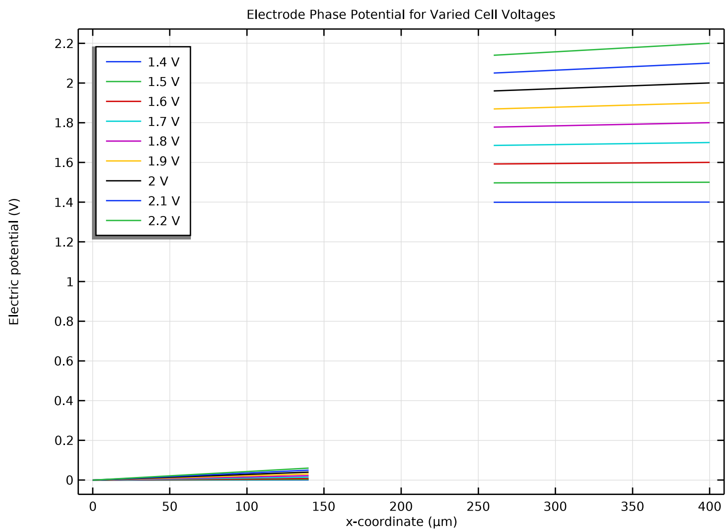
Line Graph 1

1 In the **Model Builder** window, expand the **Electrode Phase Potential for Varied Cell Voltages** node, then click **Line Graph 1**.

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

3 Select the **Show legends** checkbox.

4 In the **Electrode Phase Potential for Varied Cell Voltages** toolbar, click **Plot**.



Electrolyte Phase Potential for Varied Cell Voltages

1 In the **Model Builder** window, under **Results** click **Electrolyte Potential (we)**.

2 In the **Settings** window for **1D Plot Group**, type `Electrolyte Phase Potential for Varied Cell Voltages` in the **Label** text field.

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

4 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

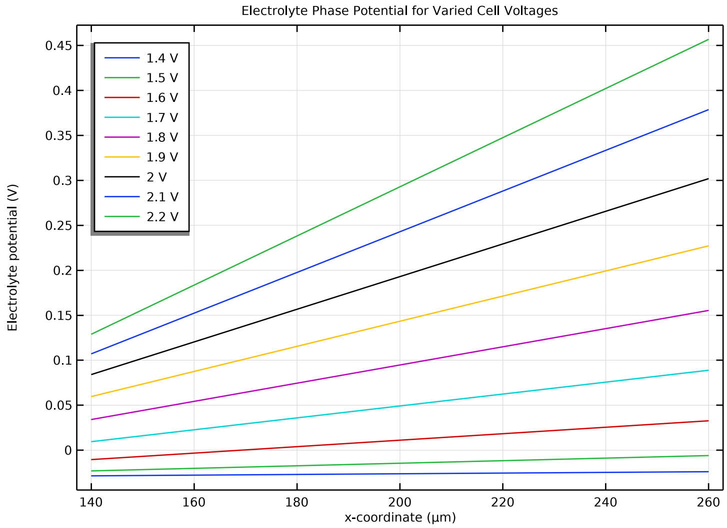
Line Graph 1

1 In the **Model Builder** window, expand the **Electrolyte Phase Potential for Varied Cell Voltages** node, then click **Line Graph 1**.

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

3 Select the **Show legends** checkbox.

4 In the **Electrolyte Phase Potential for Varied Cell Voltages** toolbar, click **Plot**.



Polarization Plot

Now add a user-defined polarization plot by following these steps:

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

2 In the **Settings** window for **1D Plot Group**, type `Polarization Plot` in the **Label** text field.

Point Graph 1

1 Right-click **Polarization Plot** and choose **Point Graph**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Water Electrolyzer** > **we.nls - Normal electrode current density - A/m²**.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `-we.nIs`.

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

Polarization Plot

1 In the **Model Builder** window, click **Polarization Plot**.

2 In the **Settings** window for **1D Plot Group**, locate the **Title** section.

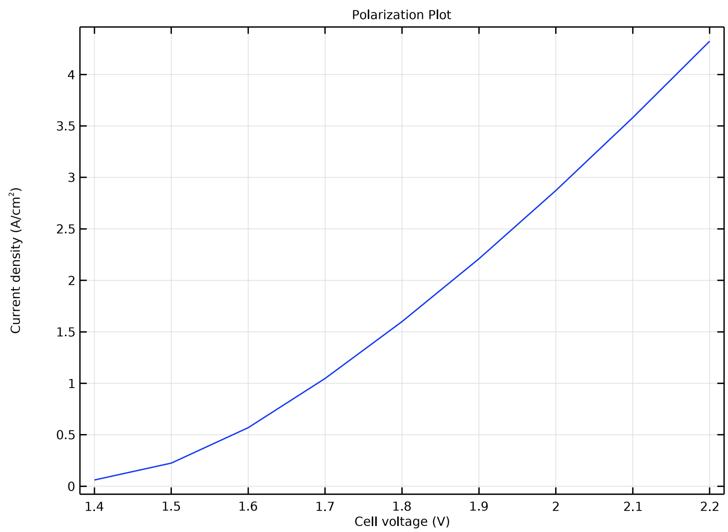
3 From the **Title type** list, choose **Label**.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type Cell voltage (V).

6 Select the **y-axis label** checkbox. In the associated text field, type Current density (A/cm²).

7 In the **Polarization Plot** toolbar, click **Plot**.



Activation Overpotentials

Add a final plot for evaluating the activation overpotentials in each electrode:

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

2 In the **Settings** window for **1D Plot Group**, type Activation Overpotentials in the **Label** text field.

Point Graph 1

1 Right-click **Activation Overpotentials** and choose **Point Graph**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Water Electrolyzer** > **Electrode kinetics** > **we.eta_to2gder1 - Overpotential - V**.

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

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

6 In the table, enter the following settings:

Legends
`Oxygen evolution`

Point Graph 2

1 In the **Model Builder** window, right-click **Activation Overpotentials** and choose **Point Graph**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Water Electrolyzer** > **Electrode kinetics** > **we.eta_th2gder1 - Overpotential - V**.

4 Locate the **Legends** section. Select the **Show legends** checkbox.

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

6 In the table, enter the following settings:

Legends
`Hydrogen evolution`

Activation Overpotentials

1 In the **Model Builder** window, click **Activation Overpotentials**.

2 In the **Settings** window for **1D Plot Group**, locate the **Title** section.

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

4 Locate the **Plot Settings** section.

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

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

7 In the **Activation Overpotentials** toolbar, click **Plot**.