Alkaline Electrolyzer

Introduction

Alkaline water electrolysis is a well-established industrial process for producing hydrogen gas. In the cell, hydrogen gas is formed at the cathode whereas oxygen gas is formed at the anode.

The electrolyte is an aqueous liquid, and when the evolved gases form bubbles, the effective ionic conductivity is lowered. The generated gases may have a detrimental effect on cell performance also due to a lowered accessible surface area for the electrode reactions.

This example investigates the impact of the gas formation on the performance of an alkaline electrolysis cell.

Model Definition

Figure 1 shows the model geometry. Electrolyte enters the cell from below, hydrogen and oxygen evolve on the two vertical electrode surfaces, with the gas/electrolyte mixtures exiting the cell at the top. An ion-conducting separator (diaphragm) separates the two electrolyte compartments

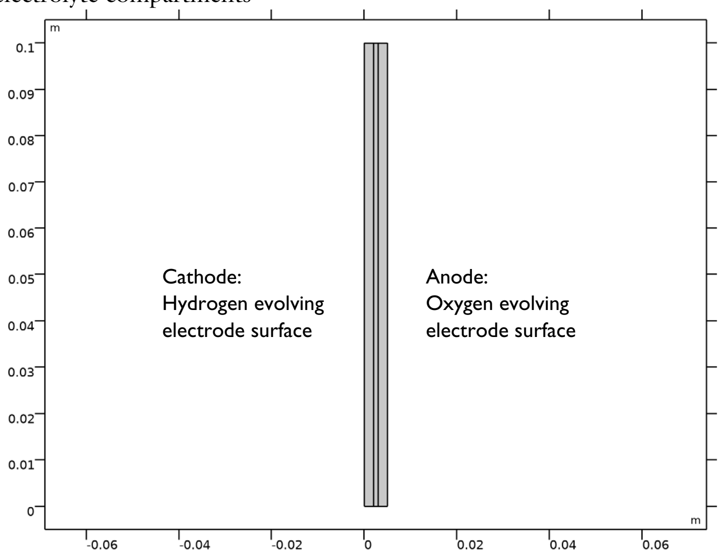


Figure 1: Model geometry.

The Water Electrolyzer interface is used in the model, which defines a current distribution model using Butler–Volmer kinetics on both electrodes.

On the negative cathode, hydrogen evolution occurs according to:

$$2H_2O(l) + 2e^- \rightarrow H_2(g) + 2OH^- \tag{1}$$

whereas on the positive anode, oxygen evolution occurs according to

$$2OH^- \rightarrow \frac{1}{2}O_2(g) + H_2O(l) + 2e^- \tag{2}$$

A supporting electrolyte assumption is assumed for the electrolyte charge transport, assuming the liquid electrolyte conductivity not to change as a result of the electrode reactions. However, when gas evolution is introduced in the model, a correction of the effective electrolyte conductivity is made so that it depends on the gas volume fraction and the bulk electrolyte conductivity according to the Bruggeman correlation

$$\sigma_{l,\,\mathrm{eff}} = (1-\phi_d)^{1.5}\sigma_l \tag{3}$$

where ϕ_d is the gas volume fraction. Also, when including gas evolution, the effective exchange current density for the electrode reactions depends on the local gas volume fraction according to

$$i_{0,\,\mathrm{eff}} = (1-\phi_d)i_0 \tag{4}$$

When including gas evolution, the Euler–Euler model is used in the electrolyte compartments, solving for the velocity vector in both the liquid and gas phases and the gas volume fraction. Gas and liquid mass flux boundary conditions are used on the electrodes surfaces, coupled to the current distribution model. At the separator boundaries, a liquid phase mass flux corresponding to ionic flux of OH^- from the current distribution model is applied.

The gas properties and mass flow rates assume that the gases are fully humidified, considering the dew point at the operating temperature

In the Euler–Euler model, bubble dispersion (Ref. 1) is included in the momentum equations using a volume force according to

$$F_{\mathrm{BD}} = -\phi_d\rho_1\frac{K_{\mathrm{g}}}{d_{\mathrm{b}}}|u_{\mathrm{slip}}|\nabla\phi_d \tag{5}$$

were ρ_l is the liquid phase density, K_g is a gas phase dispersion factor, d_b the bubble diameter, and u_{slip} the slip velocity.

Results and Discussion

Figure 2 shows the polarization curves for the two cases of including and not including gas evolution in the model. Including gas evolution in the current distribution model indicates a small, but significant, polarization effect due to the generated bubbles.

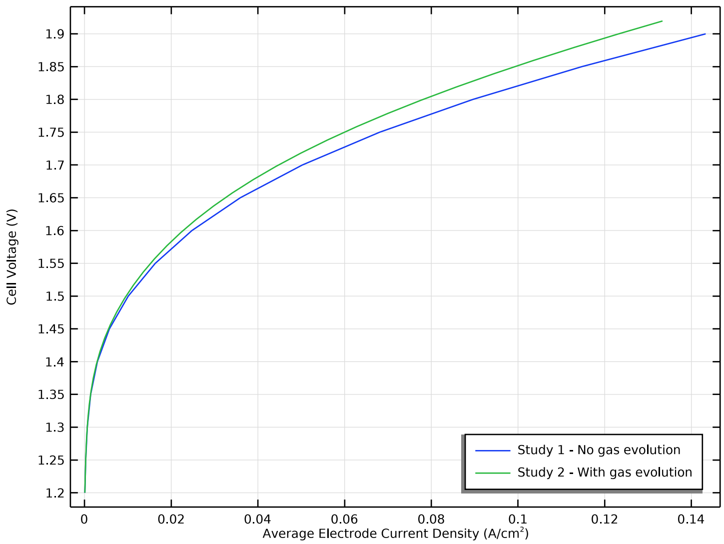


Figure 2: Polarization curve comparison when including vs not including gas evolution.

Figure 3 shows the gas volume fractions. Gas volume fractions increase towards the outlet. Due to the differences in reaction stoichiometries, more hydrogen than oxygen is generated.

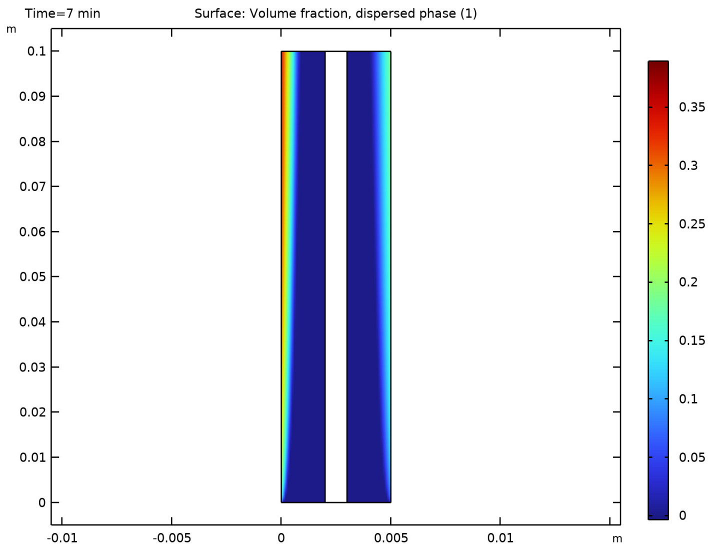


Figure 3: Gas volume fraction at a cell voltage of 1.9 V. The hydrogen gas volume fraction (left) is higher than for oxygen (right).

Figure 4 shows a line plot along the *y* direction in the middle of the separator of the electrolyte current density. At high cell polarization, the generated gas results in an approximately 15% difference in the *y* direction for the cross-separator electrolyte current density. This also implies a nonuniform utilization of the electrodes, which may lead to wear and shortened life for the cell.

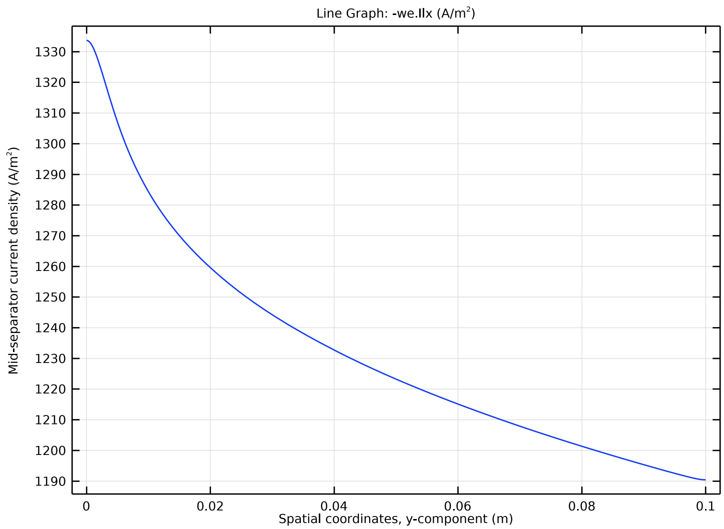


Figure 4: Current distribution along a cut line placed in the middle of the separator at a cell voltage of 1.9 V.

Notes About the COMSOL Implementation

Study 1 does not solve for Euler–Euler, that is: it does not include two-phase effects.

At high cell voltages (gas evolution rates) vortices are formed, making it hard to converge to a stationary solution. Hence a time-dependent solver is used in Study 2, ramping up the voltage in time.

Reference

1. Le Bideau and others, "Eulerian Two-Fluid Model of Alkaline Water Electrolysis for Hydrogen Production," *Energies*, vol. 13, p. 3394, 2020.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Electrolyzers/alkaline_electrolyzer`

Modeling Instructions

This tutorial is divided into two steps. In the first step, a polarization curve for the water electrolyzer is simulated without the effect of the gas evolution. In the second step the gas evolution is considered, using the Euler-Euler interface. The polarization curves are then compared.

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>Hydroxide Exchange (we)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Fluid Flow>Multiphase Flow>Euler-Euler Model>Euler-Euler Model, Laminar Flow (ee)**.

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

Load the model parameters from a text file.

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 `alkaline_electrolyzer_parameters.txt`.

GEOMETRY 1

Create the geometry as a union of three rectangles. By labeling the rectangles and enabling the **Result objects selection** check box, properly named selections are created that will be used later when setting up the physics.

Hydrogen Gas Compartment

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

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

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_H2`.

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

5 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

6 Click **Build Selected**.

Separator

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

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

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

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

5 Locate the **Position** section. In the **x** text field, type `W_H2`.

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

7 Click **Build Selected**.

Oxygen Gas Compartment

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

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

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_O2`.

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

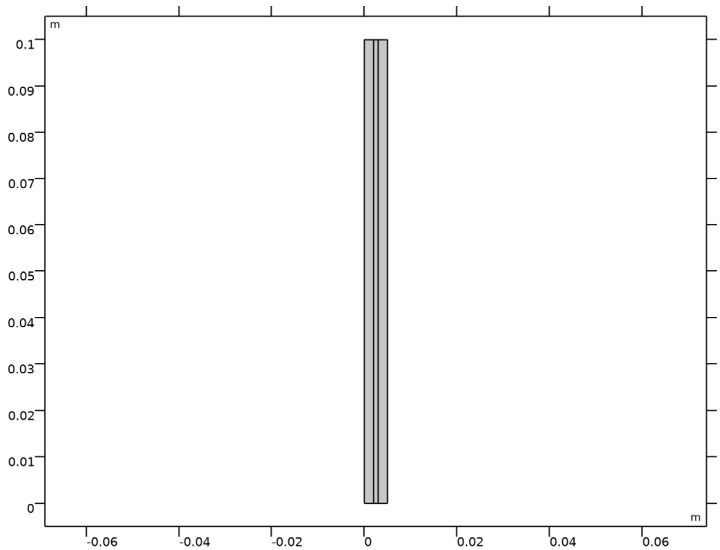
5 Locate the **Position** section. In the **x** text field, type `W_H2+W_sep`.

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

Form Union (fin)

1 In the **Model Builder** window, right-click **Form Union (fin)** and choose **Build Selected**.

The final geometry should now look as follows:



Proceed to create some additional selections, that will also be used when setting up the physics later.

Hydrogen Electrode

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Hydrogen Electrode` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 1 only.

Oxygen Electrode

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Oxygen Electrode` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundary 10 only.

Inlets

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Inlets` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundaries 2 and 8 only.

Outlets

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Outlets` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundaries 3 and 9 only.

Separator Boundaries

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Separator Boundaries` in the **Label** text field.

3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.

4 On the object **fin**, select Boundaries 4 and 7 only.

Electrodes

1 In the **Geometry** toolbar, click **Selections** and choose **Union Selection**.

2 In the **Settings** window for **Union Selection**, type `Electrodes` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click **Add**.

5 In the **Add** dialog box, in the **Selections to add** list, choose **Hydrogen Electrode** and **Oxygen Electrode**.

6 Click **OK**.

Gas Compartments

1 In the **Geometry** toolbar, click **Selections** and choose **Union Selection**.

2 In the **Settings** window for **Union Selection**, type `Gas Compartments` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Hydrogen Gas Compartment** and **Oxygen Gas Compartment**.

5 Click **OK**.

DEFINITIONS

View 1

In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.

Axis

Change the scaling of the geometry in the graphics window. This is only for viewing purposes and has no other impact on the model.

1 In the **Model Builder** window, expand the **View 1** node, then click **Axis**.

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

3 From the **View scale** list, choose **Manual**.

4 In the **y scale** text field, type `0.2`.

5 Click **Update**.

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

ADD MATERIAL

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

Add the electrolyte properties from the material library.

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

3 In the tree, select **Fuel Cell and Electrolyzer>Aqueous Alkali>Potassium Hydroxide, KOH**.

4 Right-click and choose **Add to Component 1 (comp1)**.

The gas phase properties will defined using built-in variables in the **Water Electrolyzer** interface and are not defined using **Materials**.

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

WATER ELECTROLYZER (WE)

This model will not consider concentration gradients of the reactant gases. The gas mixtures are assumed to be humidified to a 100% relative humidity.

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

2 Find the **Transport mechanisms** subsection. Clear the **Include gas phase diffusion** check box.

When specifying the electrode reaction, we will assume the electrolysis reactions proceed with liquid water as reactant (not water vapor). This will have an impact on the built-in calculation of the equilibrium potentials.

3 Find the **Reactions** subsection. Select the **Include H2O(l) in reaction stoichiometry** check box.

4 Locate the **O2 Gas Mixture** section. Find the **Transport mechanisms** subsection. Clear the **Include gas phase diffusion** check box.

5 Find the **Reactions** subsection. Select the **Include H2O(l) in reaction stoichiometry** check box.

H2 Gas Phase 1

1 In the **Model Builder** window, expand the **Water Electrolyzer (we)** node, then 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 $p_{\mathrm{A,hum}}$ text field, type `p_gas`.

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 $p_{\mathrm{A,hum}}$ text field, type `p_gas`.

Separator 1

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

The effective electrolyte conductivity in the separator will be based on the bulk value for KOH in **Materials**, corrected for by the electrolyte volume fraction of the separator.

2 Select Domain 2 only.

3 In the **Settings** window for **Separator**, locate the **Effective Electrolyte Charge Transport** section.

4 In the ε_{l} text field, type `eps_sep`.

H2 Gas-Electrolyte Compartment 1

1 In the **Physics** toolbar, click **Domains** and choose **H2 Gas-Electrolyte Compartment**.

2 Select Domain 1 only.

3 In the **Settings** window for **H2 Gas-Electrolyte Compartment**, locate the **Domain Selection** section.

4 From the **Selection** list, choose **Hydrogen Gas Compartment**.

O2 Gas-Electrolyte Compartment 1

1 In the **Physics** toolbar, click **Domains** and choose **O2 Gas-Electrolyte Compartment**.

2 In the **Settings** window for **O2 Gas-Electrolyte Compartment**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Oxygen Gas Compartment**.

H2 Electrode Surface 1

1 In the **Physics** toolbar, click **Boundaries** and choose **H2 Electrode Surface**.

2 In the **Settings** window for **H2 Electrode Surface**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Hydrogen Electrode**.

H2 Electrode Reaction 1

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

2 In the **Settings** window for **H2 Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{H2O} text field, type `0`.

4 In the $\nu_{H2O(l)}$ text field, type `-1`.

5 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_H2`.

O2 Electrode Surface 1

1 In the **Physics** toolbar, click **Boundaries** and choose **O2 Electrode Surface**.

2 In the **Settings** window for **O2 Electrode Surface**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Oxygen Electrode**.

4 Locate the **Electrode Phase Potential Condition** section. In the $\phi_{s,\mathrm{ext}}$ text field, type `E_cell`.

O2 Electrode Reaction 1

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

2 In the **Settings** window for **O2 Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{H2O} text field, type `0`.

4 In the $\nu_{H2O(l)}$ text field, type `-1`.

5 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_ref_O2`.

GLOBAL DEFINITIONS

Default Model Inputs

Specify the default model inputs in the model. These are used by all physics nodes.

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>Concentration (mol/m^3) - minput.c**.

The properties (density and viscosity) of the electrolyte are concentration dependent.

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

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

6 In the **Pressure** text field, type `p_gas`.

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

8 In the **Temperature** text field, type `T`.

DEFINITIONS

The model settings for the electrolyzer, excluding the effect of gas evolution, are now complete. Before solving, add a probe for the average cell current density. The probe will provide a scalar output for each step taken by the solver, and will be plotted while solving.

Boundary Probe 1 (bnd1)

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

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

3 From the **Selection** list, choose **Oxygen Electrode**.

4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Water Electrolyzer>Electrode kinetics> we.iloc_o2er1 - Local current density - A/m²**.

5 Locate the **Expression** section. In the **Table and plot unit** field, type `A/cm^2`.

6 Select the **Description** check box. In the associated text field, type `Average cell current density`.

STUDY 1 - NO GAS EVOLUTION

1 In the **Model Builder** window, click **Study 1**.
2 In the **Settings** window for **Study**, type `Study 1 - No Gas Evolution` in the **Label** text field.

Step 2: Stationary

1 In the **Model Builder** window, expand the **Study 1 - No Gas Evolution** node, then click **Step 2: Stationary**.
2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
3 In the table, clear the **Solve for** check box for **Euler-Euler Model, Laminar Flow (ee)**.
4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.
5 Click + **Add**.
6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E_cell (Cell voltage)	`range(1.2,0.05,1.9)`	V

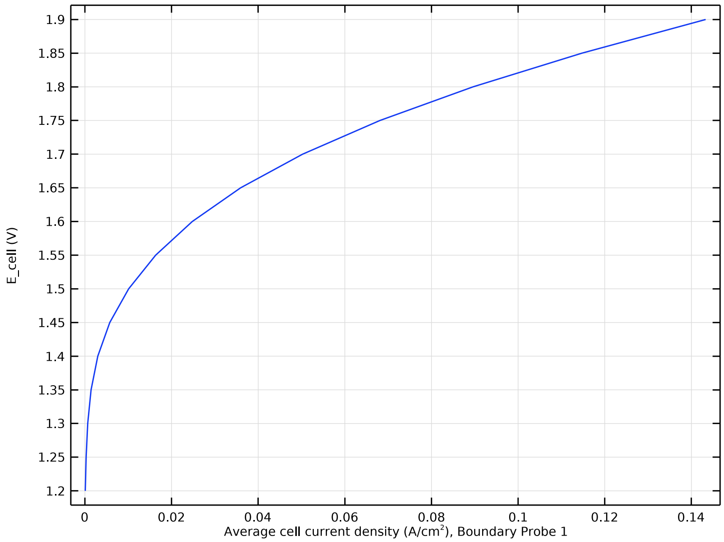
7 In the **Home** toolbar, click = **Compute**.

RESULTS

Probe Plot Group 2

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 2**.
2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.
3 Select the **Flip the x- and y-axes** check box.
4 Locate the **Legend** section. Clear the **Show legends** check box.

5 In the **Probe Plot Group 2** toolbar, click **Plot**.



DEFINITIONS

Now proceed to set up the gas evolution. First add some variable definitions from text files. Note that the different variable nodes should be selected on different domains and boundaries of the geometry.

Variables 1 - Hydrogen Gas Compartment

1 In the **Model Builder** window, expand the **Component 1 (comp1)** node.

2 Right-click **Component 1 (comp1)>Definitions** and choose **Variables**.

3 In the **Settings** window for **Variables**, type `Variables 1 - Hydrogen Gas Compartment` in the **Label** text field.

4 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

5 From the **Selection** list, choose **Hydrogen Gas Compartment**.

6 Locate the **Variables** section. Click **Load from File**.

7 Browse to the model's Application Libraries folder and double-click the file `alkaline_electrolyzer_h2_comp_variables.txt`.

Variables 2 - Oxygen Gas Compartment

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables 2 - Oxygen Gas Compartment` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Oxygen Gas Compartment**.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `alkaline_electrolyzer_o2_comp_variables.txt`.

Variables 3 - Hydrogen Electrode

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables 3 - Hydrogen Electrode` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Hydrogen Electrode**.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `alkaline_electrolyzer_h2_elec_variables.txt`.

Variables 4 - Oxygen Electrode

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables 4 - Oxygen Electrode` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Oxygen Electrode**.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `alkaline_electrolyzer_o2_elec_variables.txt`.

WATER ELECTROLYZER (WE)

H2 Gas-Electrolyte Compartment 1

Similarly to the separator, the electrolyte-gas compartments should now use corrected electrolyte conductivity values, based on the electrolyte volume fraction. As gas evolves in the cell, the electrolyte volume fraction decreases.

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

2 In the **Settings** window for **H2 Gas-Electrolyte Compartment**, locate the **Effective Electrolyte Charge Transport** section.

3 In the ε_l text field, type `eps_liquid`.

O2 Gas-Electrolyte Compartment 1

1 In the **Model Builder** window, click **O2 Gas-Electrolyte Compartment 1**.

2 In the **Settings** window for **O2 Gas-Electrolyte Compartment**, locate the **Effective Electrolyte Charge Transport** section.

3 In the ε_l text field, type `eps_liquid`.

H2 Electrode Reaction 1

Also the kinetics now gets affected by the gas volume fraction.

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

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

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_H2*eps_liquid`.

O2 Electrode Reaction 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Water Electrolyzer (we)> O2 Electrode Surface 1** click **O2 Electrode Reaction 1**.

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

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_O2*eps_liquid`.

EULER-EULER MODEL, LAMINAR FLOW (EE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Euler-Euler Model, Laminar Flow (ee)**.

2 In the **Settings** window for **Euler-Euler Model, Laminar Flow**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Gas Compartments**.

4 Locate the **Physical Model** section. From the **Dispersed phase** list, choose **Liquid droplets/ bubbles**.

Phase Properties 1

1 In the **Model Builder** window, expand the **Euler-Euler Model, Laminar Flow (ee)** node, then click **Phase Properties 1**.

2 In the **Settings** window for **Phase Properties**, locate the **Model Input** section.

3 From the *c* list, choose **Common model input**.

The liquid phase properties are taken from KOH in **Materials**. The gas phase properties are taken from the built-in properties of the **Water Electrolyzer** interface.

4 Locate the **Dispersed Phase Properties** section. From the ρ_d list, choose **Density of gas phase (we)**.

5 From the μ_d list, choose **Dynamic viscosity of gas phase (we)**.

6 In the d_d text field, type `d_bubble`.

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 Specify the **uc** vector as

0	x
v_in	y

4 Specify the **ud** vector as

0	x
v_in	y

5 In the *p* text field, type `g_const*1000[kg/m^3]*(H_elec-y)`.

Gravity 1

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

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

3 From the **Selection** list, choose **All domains**.

Volume Force - Bubble Dispersion

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

2 In the **Settings** window for **Volume Force**, type `Volume Force - Bubble Dispersion` in the **Label** text field.

3 Locate the **Volume Force** section. Specify the $\mathbf{F}_c$ vector as

FC_BDx	x
FC_BDy	y

4 Specify the $\mathbf{F}_{\mathrm{d}}$ vector as

FD_BDx	x
FD_BDy	y

5 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

Inlet 1

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

2 In the **Settings** window for **Inlet**, locate the **Continuous Phase Boundary Condition** section.

3 Specify the $\mathbf{u}_{\mathrm{c},0}$ vector as

0	x
v_in	y

4 Locate the **Dispersed Phase Boundary Condition** section. Specify the $\mathbf{u}_{\mathrm{d},0}$ vector as

0	x
v_in	y

5 From the **Dispersed phase boundary condition** list, choose **No flux**.

6 Locate the **Boundary Selection** section. From the **Selection** list, choose **Inlets**.

Outlet 1

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

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

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

Wall 2 - Electrodes

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

2 In the **Settings** window for **Wall**, type `Wall 2 - Electrodes` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Electrodes**.

4 Locate the **Continuous Phase Boundary Condition** section. Select the **Leakage** check box.

5 In the m_c text field, type `m_liquid`.

6 Locate the **Dispersed Phase Boundary Condition** section. From the **Dispersed phase boundary condition** list, choose **Leakage**.

7 In the m_d text field, type `m_gas`.

Wall 3 - Separator

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

2 In the **Settings** window for **Wall**, type `Wall 3 - Separator` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Separator Boundaries**.

4 Locate the **Continuous Phase Boundary Condition** section. Select the **Leakage** check box.

5 In the m_c text field, type `m_OH`.

The gas evolution polarization curve will be calculated using a time-dependent simulation, where the cell voltage is made time dependent using a ramp function.

DEFINITIONS

Ramp 1 (rm1)

In the **Home** toolbar, click f(x) **Functions** and choose **Local>Ramp**.

WATER ELECTROLYZER (WE)

O2 Electrode Surface 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Water Electrolyzer (we)** node, then click **O2 Electrode Surface 1**.

2 In the **Settings** window for **O2 Electrode Surface**, locate the **Electrode Phase Potential Condition** section.

3 In the $\phi_{s,ext}$ text field, type `E_cell+rm1(t[1/min])*0.1[V]`.

Use a separate probe for the time-dependent simulation, with output to a separate table.

DEFINITIONS

Boundary Probe 2 (bnd2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** right-click **Boundary Probe 1 (bnd1)** and choose **Duplicate**.

2 In the **Settings** window for **Boundary Probe**, click to expand the **Table and Window Settings** section.

3 Click + **Add Table**.

The gas evolution needs to be accurately resolved in the mesh close to the electrode boundaries. Set up the meshing sequence manually as follows:

MESH 1

Distribution 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Distribution**.
2 Select Boundaries 1, 4, 7, and 10 only.
3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
4 In the **Number of elements** text field, type 500.

Distribution 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Distribution**.
2 Select Boundaries 2, 3, 8, and 9 only.
3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
4 In the **Number of elements** text field, type 20.

Distribution 3

1 Right-click **Mesh 1** and choose **Distribution**.
2 Select Boundaries 5 and 6 only.

Given the rectangular shape of the geometry, a mapped mesh is suitable for this model.

Mapped 1

1 In the **Mesh** toolbar, click **Mapped**.
2 In the **Settings** window for **Mapped**, click **Build Selected**.

Add boundary layers in the mesh at the electrode surfaces as follows:

Boundary Layers 1

1 In the **Mesh** toolbar, click **Boundary Layers**.
2 In the **Settings** window for **Boundary Layers**, click to expand the **Transition** section.
3 Clear the **Smooth transition to interior mesh** check box.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.
2 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **Electrodes**.
4 Locate the **Layers** section. In the **Number of layers** text field, type 2.
5 From the **Thickness specification** list, choose **First layer**.

6 In the **Thickness** text field, type `3e-5`.

7 Click **Build All**.

ROOT

For the gas evolution simulation we will use a study sequence with several steps. The first two steps will calculate suitable initial values for the third time-dependent step.

ADD STUDY

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

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

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

4 Right-click and choose **Add Study**.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2 - INCLUDING GAS EVOLUTION

In the **Settings** window for **Study**, type `Study 2 - Including Gas Evolution` in the **Label** text field.

Time Dependent

1 In the **Study** toolbar, click **Study Steps** and choose **Time Dependent>Time Dependent**.

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

3 From the **Time unit** list, choose **min**.

4 In the **Output times** text field, type `range(0,1,7)`.

Modify the probe settings of the studies in order to not overwrite the probe output when not desired.

Step 2: Stationary

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

2 In the **Settings** window for **Stationary**, click to expand the **Results While Solving** section.

3 From the **Probes** list, choose **None**.

Step 3: Time Dependent

1 In the **Model Builder** window, click **Step 3: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, click to expand the **Results While Solving** section.

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

4 In the **Probes** list, select **Boundary Probe 1 (bnd1)**.

5 Under **Probes**, click **Delete**.

STUDY 1 - NO GAS EVOLUTION

Step 2: Stationary

1 In the **Model Builder** window, under **Study 1 - No Gas Evolution** click **Step 2: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Results While Solving** section.

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

4 In the **Probes** list, select **Boundary Probe 2 (bnd2)**.

5 Under **Probes**, click **Delete**.

STUDY 2 - INCLUDING GAS EVOLUTION

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

RESULTS

Polarization Plots

1 In the **Model Builder** window, under **Results** right-click **Probe Plot Group 2** and choose **Move Up**.

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

3 Locate the **Plot Settings** section.

4 Select the **x-axis label** check box. In the associated text field, type `Average Electrode Current Density (A/cm<sup>2</sup>)`.

5 Select the **y-axis label** check box. In the associated text field, type `Cell Voltage (V)`.

6 Locate the **Legend** section. Select the **Show legends** check box.

7 From the **Position** list, choose **Lower right**.

Probe Table Graph 1

1 In the **Model Builder** window, expand the **Polarization Plots** node, then 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
`Study 1 - No gas evolution`

Probe Table Graph 2

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

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

3 Find the **x-axis column** subsection. From the **Preprocessing** list, choose **Linear**.

4 In the **Scaling** text field, type `0.1`.

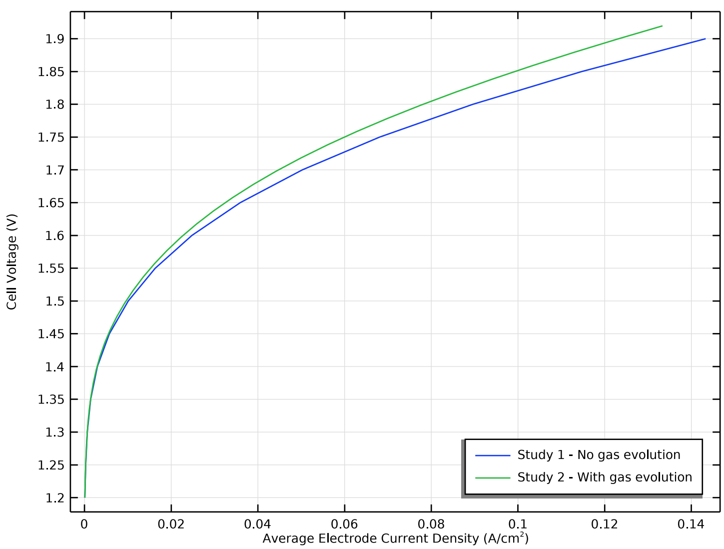
5 In the **Shift** text field, type `E_cell`.

6 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
`Study 2 - With gas evolution`

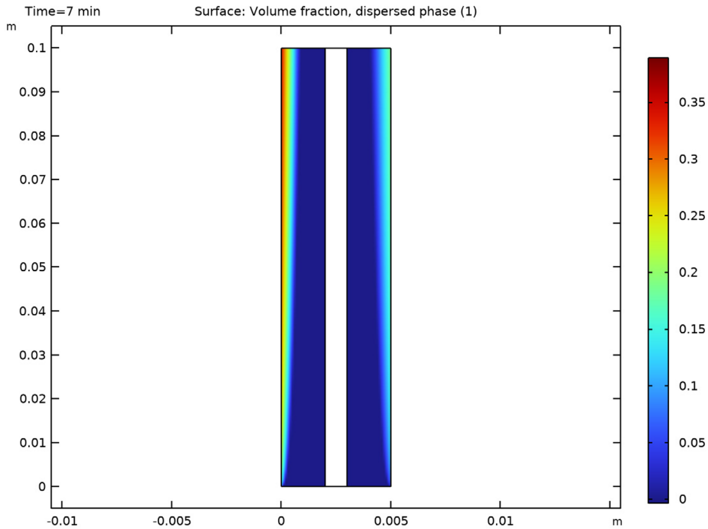
8 In the **Polarization Plots** toolbar, click **Plot**.



Dispersed Phase (ee)

1 In the **Model Builder** window, under **Results** click **Dispersed Phase (ee)**.

2 In the **Dispersed Phase (ee)** toolbar, click **Plot**.



Create a cut line dataset in order to plot the electrolyte current density along a line in the middle of the separator.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

2 In the **Settings** window for **Cut Line 2D**, locate the **Data** section.

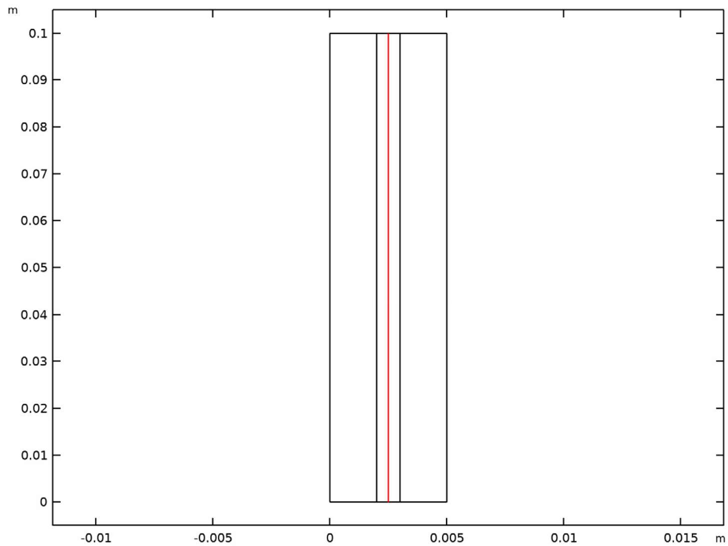
3 From the **Dataset** list, choose **Study 2 - Including Gas Evolution/Solution 3 (sol3)**.

4 Locate the **Line Data** section. In row **Point 1**, set **x** to `W_cell/2`.

5 In row **Point 2**, set **x** to `W_cell/2`.

6 In row **Point 2**, set **y** to `H_elec`.

7 Click **Plot**.



Mid-separator Current Density

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Time selection** list, choose **Last**.

5 Locate the **Plot Settings** section.

6 Select the **y-axis label** check box. In the associated text field, type Mid-separator current density (A/m²).

Line Graph 1

1 Right-click **Mid-separator Current Density** and choose **Line Graph**.

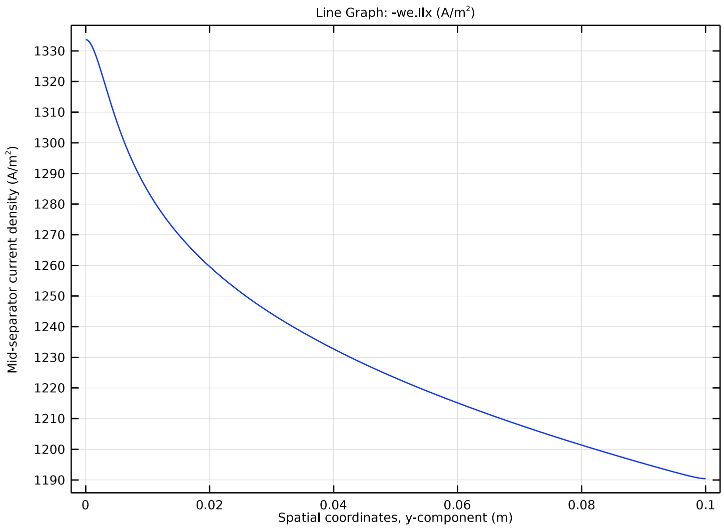
2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type -we.Ilx.

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

5 In the **Expression** text field, type y.

6 In the **Mid-separator Current Density** toolbar, click **Plot**.



Electrolyte Potential (we)

In the **Model Builder** window, under **Results** right-click **Electrolyte Potential (we)** and choose **Group**.

Group 1 - Study 1

In the **Settings** window for **Group**, type `Group 1 - Study 1` in the **Label** text field.

Continuous Phase (ee), Dispersed Phase (ee), Electrolyte Potential (we) 1, Mid-separator Current Density

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Electrolyte Potential (we) 1**, **Continuous Phase (ee)**, **Dispersed Phase (ee)**, and **Mid-separator Current Density**.

2 Right-click and choose **Group**.

Group 2 - Study 2

In the **Settings** window for **Group**, type `Group 2 - Study 2` in the **Label** text field.