Model created in COMSOL Multiphysics 6.4

Liquid Alkaline Electrolyzer with Concentrated Electrolyte Transport

Introduction

This tutorial demonstrates how to modify a concentration-independent (also known as a secondary current distribution) liquid alkaline water electrolyzer with concentrated electrolyte theory to explicitly resolve local electrolyte and solvent concentrations (thereby creating a tertiary current distribution). A liquid alkaline electrolyzer is defined in a 2D model with a separator, two gas–electrolyte compartments, and negative hydrogen and positive oxygen electrodes at the boundaries. A stationary solver is used with the cell voltage swept over a range of potentials to generate a polarization curve.

The model is first solved for a secondary current distribution only. Concentrated electrolyte theory is then taken into account and the cell performance is compared between the secondary and tertiary current distribution cases.

Model Definition

The model geometry can be seen in Figure 1.

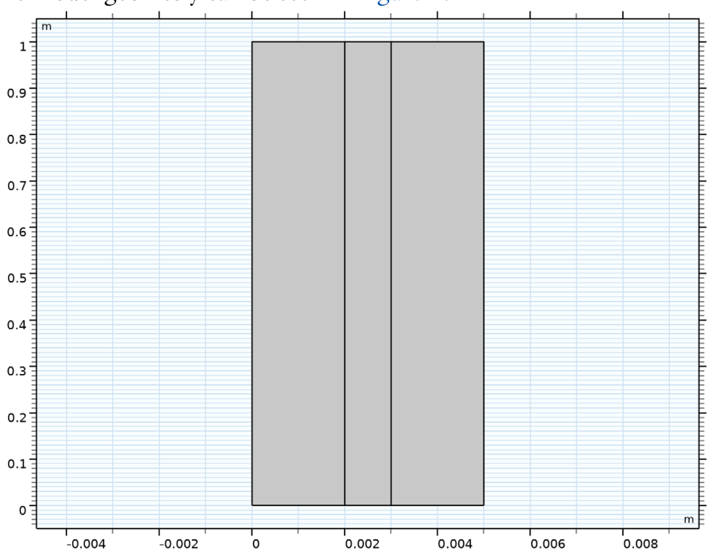


Figure 1: Alkaline electrolyzer geometry. The x-axis is scaled by a factor of 100.

The geometry is identical to that found in the Alkaline Electrolyzer tutorial model. The geometry in Figure 1 and all subsequent figures is scaled on the x-axis by a factor of 100. In brief, two electrolyte compartments are placed on either side of an ion-conducting porous separator, with the entire system permeated by 6M KOH. Liquid flows in from the bottom of the electrolyzer and exits the top. The electrodes are located on left and right exterior walls of the electrolyte compartments.

In the standard case, the **Water Electrolyzer** interface is used in a secondary current distribution formulation to capture the behavior of the system. Butler–Volmer kinetics is used at both electrodes to describe the reaction rates, with the following reactions:

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

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

Reaction 1 is hydrogen evolution (reduction) and occurs at the cathode (left electrode). Reaction 2 is oxygen evolution (oxidation) and occurs at the anode (right electrode). The electrodes are considered to be flat plates (not porous electrodes).

When using a secondary current distribution, electrolyte charge transport is computed using Ohm's law, assuming a constant conductivity and neglecting gradients in species concentration. In the second and main case examined here, this assumption is replaced with a more strict calculation of the ion and solvent concentrations everywhere in the electrolyte using the Maxwell–Stefan–Onsager theory of concentrated electrolyte transport. This behavior is captured by the **Concentrated Electrolyte Transport** interface.

To describe species transport using the CET interface, it is necessary to know the binary diffusion coefficients for each species pair (potassium–water, hydroxide–water, and potassium–hydroxide). These are typically determined by experimental measurements.

For a binary electrolyte in a single solvent, the three parameters conductivity, transport number of the positive ion, and salt diffusivity may be used to determine the three required binary diffusion coefficients. The three diffusion coefficients are calculated as follows:

$$D_{\mathrm{K,\,H_2O}} = \frac{D_{\mathrm{KOH}}}{2(1-t_{\mathrm{K}})} \tag{3}$$

$$D_{\mathrm{OH,\,H_2O}} = \frac{D_{\mathrm{KOH}}}{2t_{\mathrm{K}}} \tag{4}$$

$$D_{\mathrm{K,\,OH}} = \frac{\kappa R T c_{\mathrm{K}} D_{\mathrm{KOH}}}{c_{\mathrm{K}} c_{\mathrm{T}} F^2 D_{\mathrm{KOH}} - 2\kappa R T c_{\mathrm{H_2O}}(1-t_{\mathrm{K}})t_{\mathrm{K}}} \tag{5}$$

where F is Faraday's constant (C/mol), T is the temperature (K), c_i is the concentration of species i (mol/m^3), c_{T} is the total concentration (mol/m^3), $D_{i,j}$ is the binary diffusion coefficient (m^2/s), D_{KOH} is the KOH diffusivity in water (m^2/s), t_K is the transport number of potassium, and κ is the conductivity (S/m). The conductivity is determined as a function of concentration and temperature from an analytical expression based on experimental data. A plot of the conductivity can be seen in Figure 2.

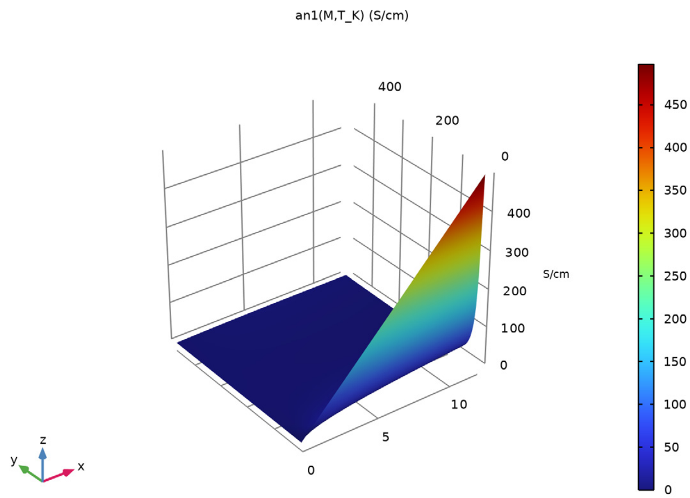


Figure 2: Conductivity of potassium hydroxide as a function of concentration (x-axis, M) and temperature (y-axis, °C).

In the **Free and Porous Media Flow** interface, laminar flow in the electrolyte compartments is combined with porous media flow in the separator. This fluid flow is coupled to the CET interface by using the density as computed by CET as the fluid density and setting the velocity field in CET to that of the Free and Porous Media Flow computed field. Flow at the electrodes due to electrochemical reaction is defined by the current at the electrode and Faraday's Law.

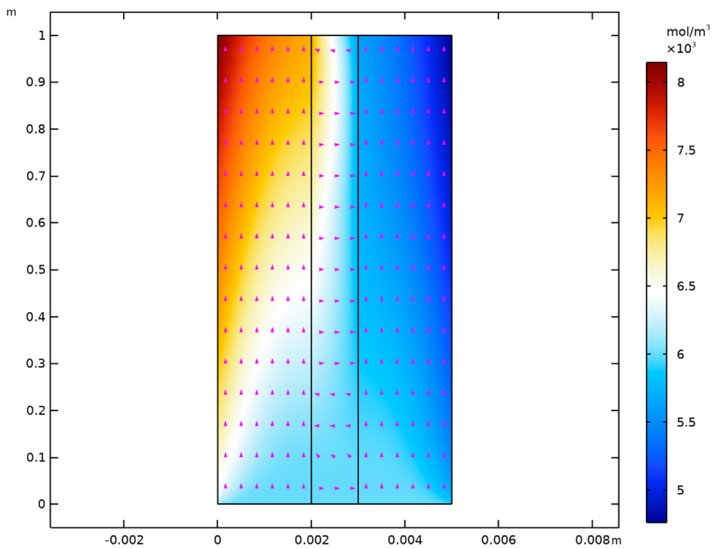


Figure 3: Concentration profile (surface) and total flux direction (arrow surface) of potassium ion.

The concentration of potassium ion in the electrolyzer in the CET case can be seen in Figure 3. The concentration is higher near the outlet of the electrolyzer as well as near the cathode, where hydroxide ions are produced. Electroneutrality requires that the potassium concentration increases with the hydroxide concentration.

Figure 4 shows how the conductivity in the electrolyzer changes with applied voltage (and therefore concentration). As the voltage increases, conductivity increases in areas of higher concentration and decreases in areas of lower concentration.

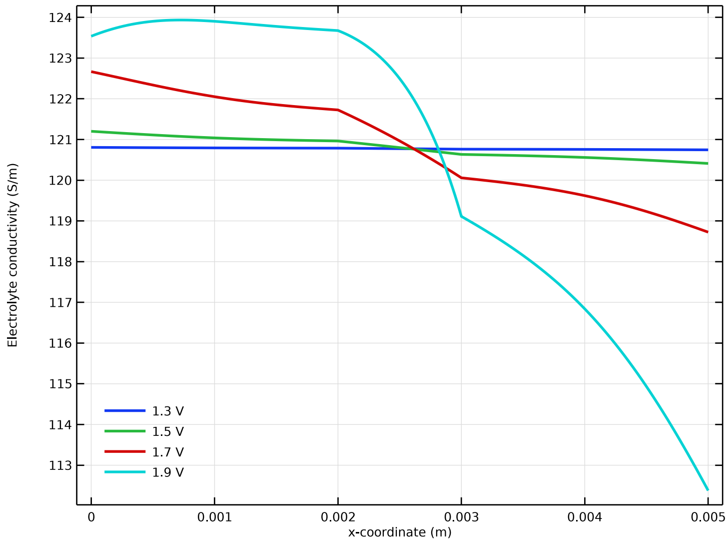


Figure 4: Electrolyte conductivity as a function of x at y = 0.85 m.

Figure 5 demonstrates the difference between the polarization curves calculated in the WE case and the CET case. The difference in conductivity caused by the concentration gradients in the CET case results in slightly more resistance and lower current density at the same voltage compared to when the system is solved without considering concentration gradients.

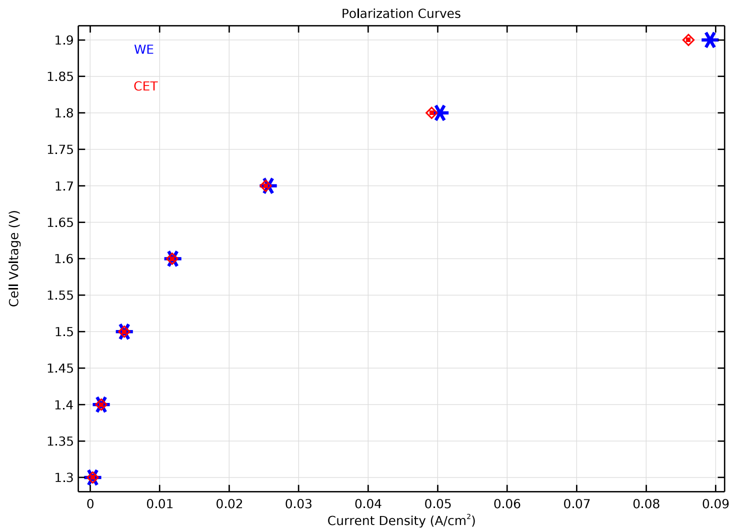


Figure 5: Comparison of polarization curves between the WE (blue star) and CET (red diamond) cases.

Reference

1. J. Newman and K.E. Thomas-Alyea, *Electrochemical Systems*, 3rd Ed. John Wiley & Sons, Hoboken, NJ, 2004.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Electrolyzers/aec_concentrated_electrolyte`

Modeling Instructions

This tutorial is in two parts. First, a polarization curve for a standard liquid alkaline water electrolyzer is generated using the **Water Electrolyzer** interface only. Then, the **Concentrated Electrolyte Transport** and **Free and Porous Media Flow, Brinkman** interfaces are activated, the concentration and velocity profiles are examined, and the new polarization curve is compared with the initial polarization curve.

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** > **Alkaline (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

Load model parameters from a text file.

Parameters 1

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

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

3 Click **Load from File**.

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

GEOMETRY 1

The basic geometry is the same as that used in Alkaline Electrolyzer, so it is imported here. The height parameter is then modified for this model. Since the aspect ratio of the geometry is large define a View that scales the x-axis 100 times.

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

2 Browse to the model's Application Libraries folder and double-click the file `alkaline_electrolyzer.mph`.

GLOBAL DEFINITIONS

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

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

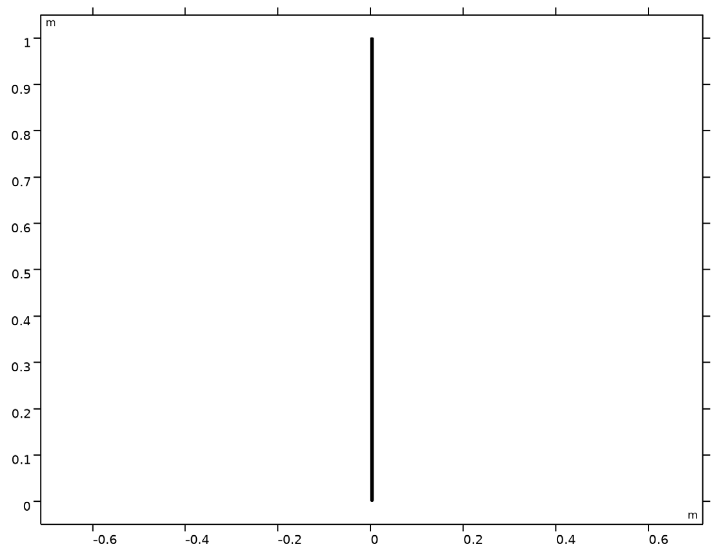
3 In the table, enter the following settings:

Name	Expression	Value	Description
H_elec	1[m]	1 m	Electrode height

GEOMETRY 1

1 In the **Geometry** toolbar, click **Build All**.

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



Since the aspect ratio of the geometry is large define a View that scales the x-axis 100 times.

DEFINITIONS

View 2

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

2 Right-click **Definitions** and choose **View**.

Axis

1 In the **Model Builder** window, expand the **View 2** node, then click **Axis**.

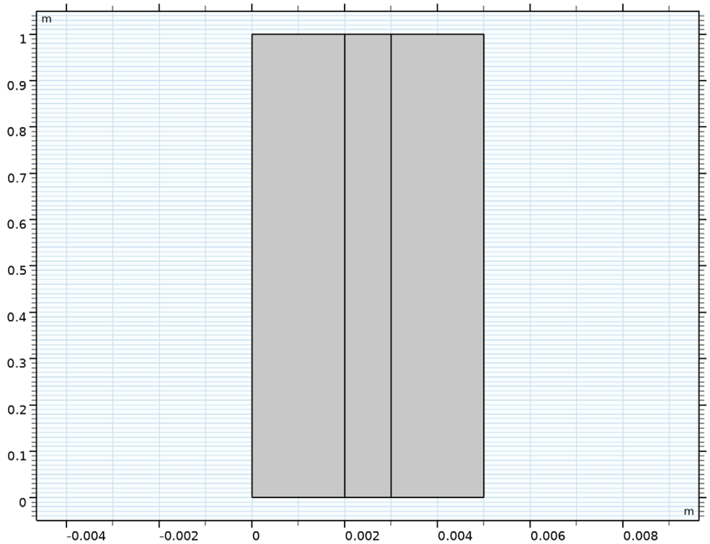
2 In the **Settings** window for **Axis**, locate the **Axis** section.

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

4 In the **x scale** text field, type 100.

5 Click **Update**.

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



Variables - Electrodes

Load local variables from a text file. Note that the Electrodes variables are only active on the electrode boundaries.

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Definitions**, in the **Graphics** window toolbar, click next to **Go to Default View**, then choose **Go to View 2**.

3 In the **Model Builder** window, click **Variables 1**.

4 In the **Settings** window for **Variables**, locate the **Variables** section.

5 Click **Load from File**.

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

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

8 From the **Selection** list, choose **Electrodes**.

9 In the **Label** text field, type `Variables - Electrodes`.

Electrode Average

Define an averaging function on the oxygen electrode to use for determining the cell current density for the polarization curves in both studies.

1. In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Average**.
2. In the **Settings** window for **Average**, type `Electrode Average` in the **Label** text field.
3. Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.
4. From the **Selection** list, choose **Oxygen Electrode**.

MATERIALS

Add the electrolyte material for KOH here. The electrolyte conductivity varies with the dimensionless concentration and temperature, as shown in the plot.

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** > **Aqueous Alkali** > **Potassium Hydroxide, KOH**.
4. Click the right end of the **Add to Global Materials** split button in the window toolbar.
5. From the menu, choose **Add to Component**.
6. In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

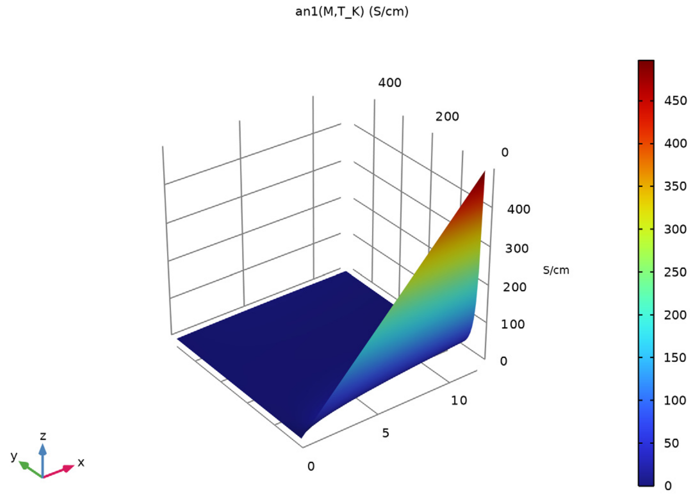
Potassium Hydroxide, KOH (mat1)

In the **Model Builder** window, expand the **Component 1 (comp1)** > **Materials** > **Potassium Hydroxide, KOH (mat1)** node.

Analytic 1 (an1)

1. In the **Model Builder** window, expand the **Component 1 (comp1)** > **Materials** > **Potassium Hydroxide, KOH (mat1)** > **Electrolyte conductivity (ionc)** node, then click **Analytic 1 (an1)**.

2 In the **Settings** window for **Analytic**, click **Plot**.



GLOBAL DEFINITIONS

Default Model Inputs

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** > **Temperature (K) - minput.T**.

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

5 In the tree, select **General** > **Concentration (mol/m^3) - minput.c**.

6 In the **Concentration** text field, type `c`.

WATER ELECTROLYZER (WE)

Now, the **Water Electrolyzer** interface can be set up for the first case, without using CET and Fluid Flow. Note that gas-phase diffusion in the electrolyte is not considered here.

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 Phase 1

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.

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.

H2 Gas-Electrolyte Compartment 1

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

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

3 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**.

Separator 1

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

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

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

4 Locate the **Effective Electrolyte Charge Transport** section. In the ε_{l} text field, type eps_sep.

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 **Electrode Kinetics** section.
3 In the $i_{0,ref}(T)$ text field, type `i0_ref_H2*i0_f_H2`.
4 Locate the **Stoichiometric Coefficients** section. In the ν_{H2O} text field, type `0`.
5 In the $\nu_{H2O(l)}$ text field, type `-1`.

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 $\phi_{s,ext}$ 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 **Electrode Kinetics** section.
3 In the $i_{0,ref}(T)$ text field, type `i0_ref_O2*i0_f_O2`.
4 Locate the **Stoichiometric Coefficients** section. In the $\nu_{H2O(l)}$ text field, type `-1`.
5 In the ν_{H2O} text field, type `0`.

MESH 1

To ensure that the flows near the domain boundaries are accurately resolved, refine the mesh near the electrode and separator surfaces using the **Boundary Layer** mesh functionality. This improves convergence in the second part of the study. Set up the meshing sequence manually as follows:

Mapped 1

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

Size

1 In the **Model Builder** window, click **Size**.
2 In the **Settings** window for **Size**, locate the **Element Size** section.
3 From the **Predefined** list, choose **Finer**.
4 Click to expand the **Element Size Parameters** section.

Distribution 1

1 In the **Mesh** toolbar, click **Distribution**.
2 In the **Settings** window for **Distribution**, locate the **Distribution** section.
3 In the **Number of elements** text field, type 8.
4 Select Boundaries 2, 3, 5, 6, 8, and 9 only.

Boundary Layers 1

1 In the **Mesh** toolbar, click **Boundary Layers**.
2 In the **Settings** window for **Boundary Layers**, locate the **Domain Selection** section.
3 From the **Geometric entity level** list, choose **Domain**.
4 From the **Selection** list, choose **Gas Compartments**.
5 Click to expand the **Transition** section. Clear the **Smooth transition to interior mesh** checkbox.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.
2 Select Boundaries 1, 4, 7, and 10 only.
3 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.
4 In the **Number of layers** text field, type 3.

STUDY 1 - WE ONLY

1 In the **Model Builder** window, click **Study 1**.
2 In the **Settings** window for **Study**, type `Study 1 - WE Only` in the **Label** text field.

Step 2: Stationary

1 In the **Model Builder** window, under **Study 1 - WE Only** 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)	1.3 1.4 1.5 1.6 1.7 1.8 1.9	V

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

RESULTS

Polarization Curves

Plot the polarization curve for the WE model to confirm that the system solved appropriately.

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

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

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

4 In the **Title** text area, type `Polarization Curve`.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `Current Density (A/cm<sup>2</sup>)`.

7 Locate the **Title** section. In the **Title** text area, type `Polarization Curves`.

8 In the **Label** text field, type `Polarization Curves`.

Line Graph 1

1 In the **Polarization Curves** toolbar, click **Line Graph**.

2 Select Boundary 10 only.

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

4 In the **Expression** text field, type `E_cell`.

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

6 In the **Expression** text field, type `aveop1(we.itot)`.

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

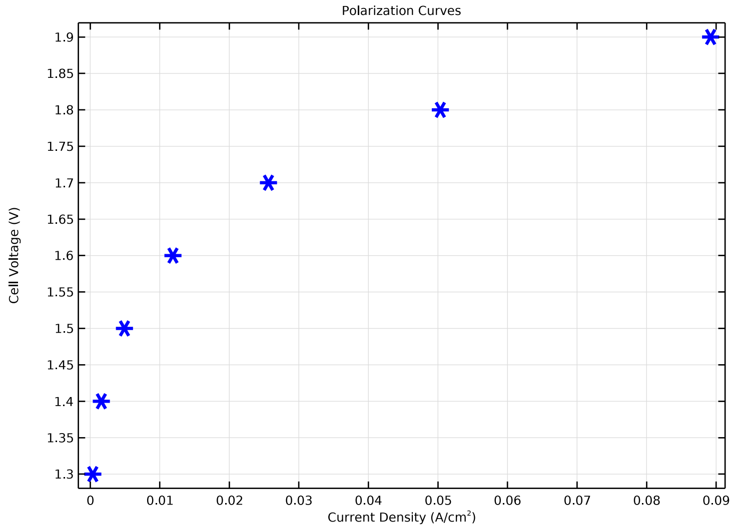
8 Click to expand the **Coloring and Style** section. Locate the **Data** section. From the **Dataset** list, choose **Study 1 - WE Only/Solution 1 (sol1)**.

9 Locate the **Coloring and Style** section. From the **Color** list, choose **Blue**.

10 From the **Width** list, choose **2**.

11 Find the **Line markers** subsection. From the **Marker** list, choose **Asterisk**.

12 In the **Polarization Curves** toolbar, click **Plot**.



ADD PHYSICS

Now add the appropriate physics to solve the system with **CET**.

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

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

3 In the tree, select **Electrochemistry** > **Concentrated Electrolyte Transport (cet)**.

4 Click the **Add to Component 1** button in the window toolbar.

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

6 Click the **Add to Component 1** button in the window toolbar.

7 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

DEFINITIONS

Additional variables and the inlet velocity profile must be added for the **CET** model.

Variables - KOH Properties, CET

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 Click **Load from File**.

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

5 In the **Label** text field, type `Variables - KOH Properties, CET`.

Inlet Velocity Profile

1 In the **Home** toolbar, click f(X) **Functions** and choose **Local** > **Piecewise**.

2 In the **Settings** window for **Piecewise**, type `Inlet Velocity Profile` in the **Label** text field.

3 Locate the **Definition** section. Find the **Intervals** subsection. Click **Load from File**.

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

5 Locate the **Units** section. In the **Arguments** text field, type `m`.

6 In the **Function** text field, type `m/s`.

WATER ELECTROLYZER (WE)

To properly couple the **CET** interface to the **Water Electrolyzer** interface, **Solve for electrolyte phase potential** must be cleared and `cet.phil` used as the electrolyte potential variable in the **Water Electrolyzer** interface.

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

2 In the **Settings** window for **Water Electrolyzer**, click to expand the **Electrolyte and Membrane Transport** section.

3 Find the **Electrolyte transport** subsection. Clear the **Solve for electrolyte phase potential** checkbox.

Electrolyte Phase 1

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

2 In the **Settings** window for **Electrolyte Phase**, locate the **Electrolyte Phase Potential** section.

3 In the ϕ_l text field, type `cet.phil`.

CONCENTRATED ELECTROLYTE TRANSPORT (CET)

The **Concentrated Electrolyte Transport** interface can now be used with KOH as the dissolved species and water as the solvent.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Concentrated Electrolyte Transport (cet)**.

2 In the **Settings** window for **Concentrated Electrolyte Transport**, locate the **Species** section.

3 Find the **Cations** subsection. In the table, enter the following settings:

Name	Molar mass (kg/mol)	Charge
K	M_K	+1

4 Find the **Anions** subsection. In the table, enter the following settings:

Name	Molar mass (kg/mol)	Charge
OH	M_OH	-1

5 Find the **Neutral species** subsection. In the table, enter the following settings:

Name	Molar mass (kg/mol)
H2O	M_H2O

Reference Electrode 1

Hydrogen evolution is used as the reference reaction here.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Concentrated Electrolyte Transport (cet)** click **Reference Electrode 1**.

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

3 In the s_{K} text field, type 0.

4 In the s_{OH} text field, type 1.

5 In the s_{H2O} text field, type -1.

Electrolyte 1

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

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

3 From the T list, choose **User defined**. In the associated text field, type T.

4 Locate the **Convection** section. From the $\mathbf{u}$ list, choose **Velocity field (fp)**. In the corresponding text fields, type V_KOH for potassium hydroxide and V_w for water, respectively.

Diffusion Coefficients 1

The binary diffusion coefficients are defined in the variables imported in an earlier step. The values are calculated from the conductivity, diffusion coefficient, and transport number; see the Model Definition section.

1 In the **Model Builder** window, click **Diffusion Coefficients 1**.
2 In the **Settings** window for **Diffusion Coefficients**, locate the **Maxwell–Stefan Diffusivities** section.
3 In the $D_{\mathrm{K,OH}}$ text field, type D_K_OH.
4 In the $D_{\mathrm{K,H2O}}$ text field, type D_K_H2O.
5 In the $D_{\mathrm{OH,H2O}}$ text field, type D_OH_H2O.

Initial Values 1

. In the corresponding text field, type c.

Separator 1

1 In the **Physics** toolbar, click **Domains** and choose **Separator**.
2 In the **Settings** window for **Separator**, locate the **Domain Selection** section.
3 From the **Selection** list, choose **Separator**.
4 Locate the **Separator** section. In the ε_l text field, type eps_sep.

Flow Out

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **Outlets**.
4 In the **Label** text field, type Flow Out.

Flow In

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.
2 In the **Settings** window for **Inflow**, locate the **Inflow** section.
3 From the **Boundary condition type** list, choose **Flux (Danckwerts)**.
4 Locate the **Boundary Selection** section. From the **Selection** list, choose **Inlets**.
5 In the **Label** text field, type Flow In.

Reaction Fluxes

1 In the **Physics** toolbar, click **Boundaries** and choose **Flux**.
2 In the **Settings** window for **Flux**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **Electrodes**.
4 Locate the **Inward Species Fluxes** section. In the $N_{\mathrm{OH},0}$ text field, type R_OH.
5 In the $N_{\mathrm{H2O},0}$ text field, type R_H2O.
6 In the **Label** text field, type Reaction Fluxes.

FREE AND POROUS MEDIA FLOW, BRINKMAN (FP)

Use a **Free and Porous Media Flow** to capture laminar flow in the electrolyte compartments and porous flow in the separator. Use P2+P1 discretization to improve the resolution of the computed velocity profile. The flow is weakly compressible because the density as computed by the **Concentrated Electrolyte Transport** interface is not necessarily constant.

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**, locate the **Physical Model** section.
3 From the **Compressibility** list, choose **Weakly compressible flow**.
4 Click to expand the **Discretization** section. From the **Discretization of fluids** list, choose **P2+P1**.
5 Click to collapse the **Discretization** section.

Fluid Properties 1

Both here and in the fluid properties for the porous domain, the density is directly coupled to the CET interface and the dynamic viscosity is specified by the material property defined earlier.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Free and Porous Media Flow, Brinkman (fp)** click **Fluid Properties 1**.
2 In the **Settings** window for **Fluid Properties**, locate the **Model Input** section.
3 From the T list, choose **User defined**. In the associated text field, type `T`.
4 In the c text field, type `cet.c_K_OH`.
5 Locate the **Fluid Properties** section. From the ρ list, choose **User defined**. In the associated text field, type `cet.rho`.

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 **u** vector as

pw1(x)	y

Initial Values 2

1 In the **Physics** toolbar, click **Domains** and choose **Initial Values**.
2 In the **Settings** window for **Initial Values**, locate the **Domain Selection** section.

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

Wall 1

In the **Model Builder** window, collapse the **Component 1 (comp1)** > **Free and Porous Media Flow, Brinkman (fp)** > **Wall 1** node.

Porous Medium 1

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

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

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

Fluid 1

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

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

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

4 In the c text field, type `cet.c_K_OH`.

5 Locate the **Fluid Properties** section. From the ρ list, choose **User defined**. In the associated text field, type `cet.rho`.

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 `eps_sep`.

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

FREE AND POROUS MEDIA FLOW, BRINKMAN (FP)

Porous Medium 1

In the **Model Builder** window, collapse the **Component 1 (comp1)** > **Free and Porous Media Flow, Brinkman (fp)** > **Porous Medium 1** node.

Wall - Electrodes

Define `v_leak` based on the mass flux from Faraday's Law at the electrode surface.

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

2 In the **Settings** window for **Wall**, locate the **Boundary Condition** section.

3 From the **Wall condition** list, choose **Leaking wall**.

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

5 Locate the **Boundary Condition** section. Specify the $\mathbf{u}_1$ vector as

v_leak	x

6 In the **Label** text field, type `Wall - Electrodes`.

Inlet 1

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

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

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

4 Locate the **Velocity** section. Click the **Velocity field** button.

5 Specify the $\mathbf{u}_0$ vector as

pw1(x)	y

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**.

ADD STUDY

1 In the **Study** 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** > **Suggested by Some Physics Interfaces** > **Stationary with Initialization**.

4 Click the **Add Study** button in the window toolbar.

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

STUDY 2 - USING CET

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

Step 2: Stationary

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

2 In the **Settings** window for **Stationary**, locate 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)	1.3 1.4 1.5 1.6 1.7 1.8 1.9	V

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

RESULTS

Now add the CET study to the polarization curve for comparison.

Polarization Curves

In the **Model Builder** window, under **Results** click **Polarization Curves**.

Line Graph 2

1 In the **Polarization Curves** toolbar, click **Line Graph**.

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

3 From the **Dataset** list, choose **Study 2 - Using CET/Solution 3 (sol3)**.

4 Select Boundary 10 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `E_cell`.

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

7 In the **Expression** text field, type `aveop1(we.itot)`.

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

9 Locate the **Coloring and Style** section. From the **Color** list, choose **Red**.

10 Find the **Line markers** subsection. From the **Marker** list, choose **Diamond**.

11 From the **Width** list, choose **2**.

12 In the **Polarization Curves** toolbar, click **Plot**.

Annotation 1

1 Right-click **Polarization Curves** and choose **Annotation**.

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

3 In the **Text** text field, type `WE`.

4 Locate the **Position** section. In the **X** text field, type `0.005`.

5 In the **Y** text field, type `1.9`.

6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

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

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

Annotation 2

1 Right-click **Annotation 1** and choose **Duplicate**.

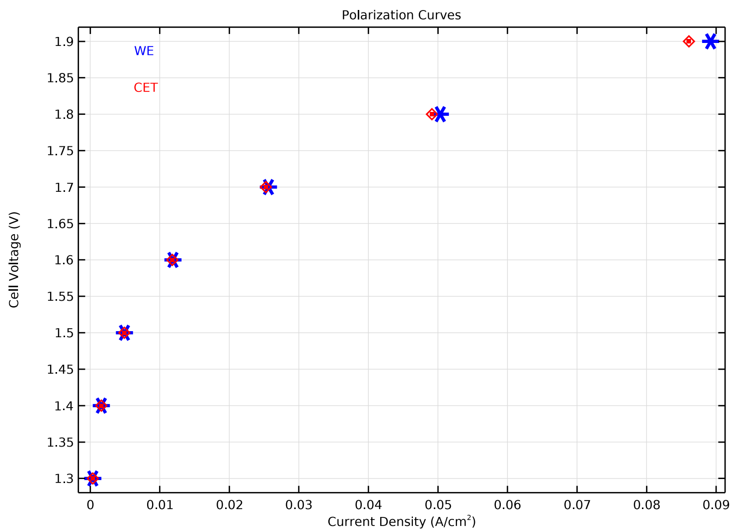
2 In the **Settings** window for **Annotation**, locate the **Annotation** section.

3 In the **Text** text field, type `CET`.

4 Locate the **Position** section. In the **Y** text field, type `1.85`.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Red**.

6 In the **Polarization Curves** toolbar, click **Plot**.



Concentration, K (cet)

1 In the **Model Builder** window, under **Results** click **Concentration, K (cet)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** checkbox.

5 In the **Graphics** window toolbar, click ▾ next to **Go to Default View**, then choose **Go to View 2**.

Surface 1

1 In the **Model Builder** window, expand the **Concentration, K (cet)** 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 **Ranitomeya**.

Streamline 1

In the **Model Builder** window, right-click **Streamline 1** and choose **Disable**.

Concentration, K (cet)

Right-click **Results** > **Concentration, K (cet)** > **Streamline 1** and choose **Arrow Surface**.

Arrow Surface 1

1 In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Concentrated Electrolyte Transport** > **Fluxes** > **cet.tflux_Kx,cet.tflux_Ky - Total flux, K**.

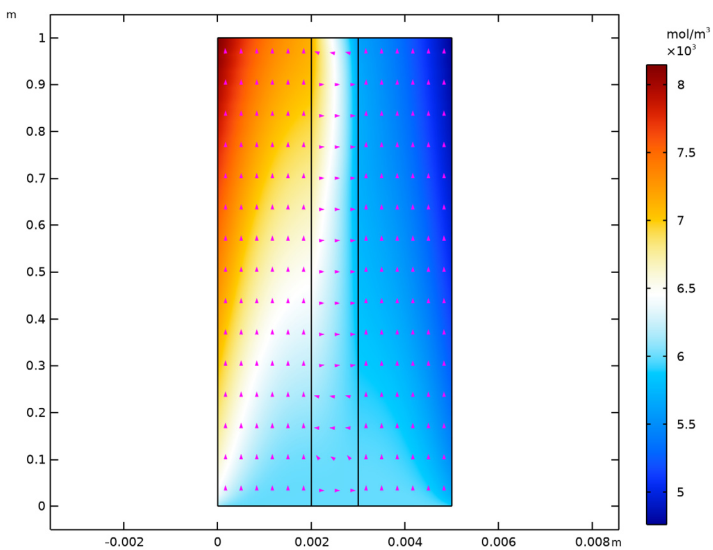
2 Locate the **Coloring and Style** section. From the **Arrow type** list, choose **Arrowhead**.

3 From the **Arrow length** list, choose **Normalized**.

4 Select the **Scale factor** checkbox. In the associated text field, type `0.004`.

5 From the **Color** list, choose **Magenta**.

6 In the **Concentration, K (cet)** toolbar, click **Plot**.



Concentration, H2O (cet)

1 In the **Model Builder** window, under **Results** click **Concentration, H2O (cet)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** checkbox.

5 In the **Graphics** window toolbar, click ▾ next to **Go to Default View**, then choose **Go to View 2**.

Surface 1

1 In the **Model Builder** window, expand the **Concentration, H2O (cet)** node, then click **Surface 1**.

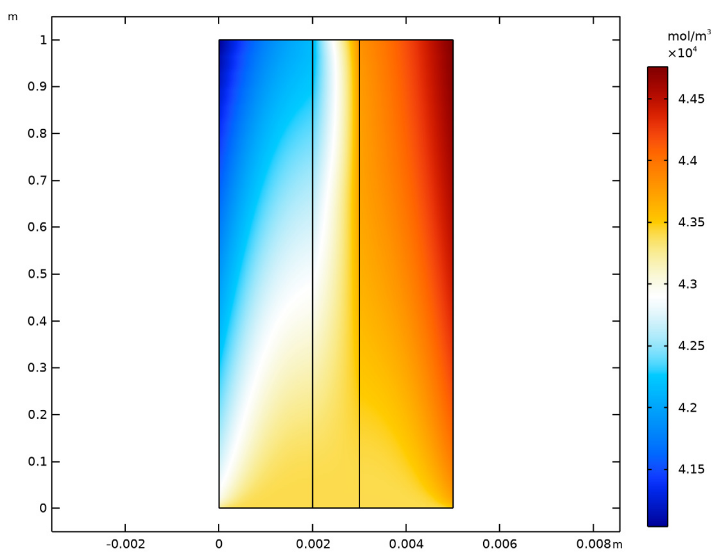
2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **Ranitomeya**.

Streamline 1

1 In the **Model Builder** window, right-click **Streamline 1** and choose **Disable**.

2 In the **Concentration, H2O (cet)** toolbar, click **Plot**.



Cut Line 2D 1

Here, add two cut lines, one for each study, to compare how key properties change as a function of x.

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

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

3 In row **Point 2**, set **X** to `0.005`.

4. In row **Point 1**, set **Y** to 0.85.
5. In row **Point 2**, set **Y** to 0.85.

Cut Line 2D 2

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 - Using CET/Solution 3 (sol3)**.
4. Locate the **Line Data** section. In row **Point 2**, set **x** to 0.005.
5. In row **Point 1**, set **y** to 0.85.
6. In row **Point 2**, set **y** to 0.85.

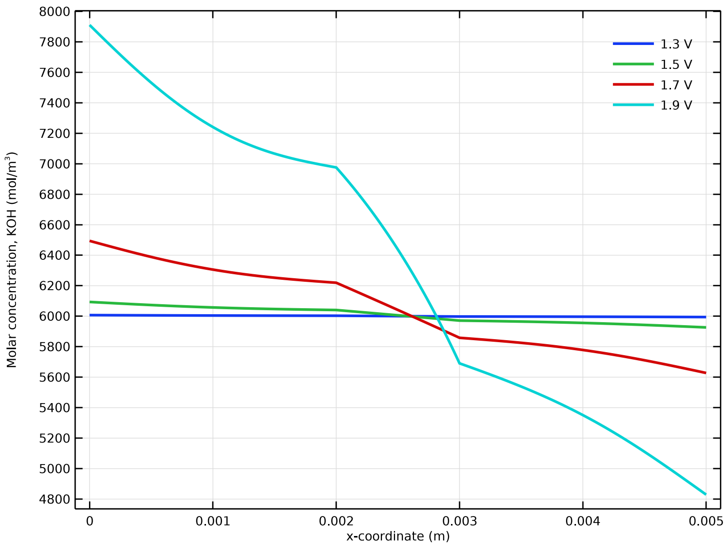
Concentration of KOH

1. In the **Results** toolbar, click **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.
3. From the **Title type** list, choose **None**.
4. Locate the **Plot Settings** section.
5. Select the **y-axis label** checkbox. In the associated text field, type Molar concentration, KOH (mol/m³).
6. In the **Label** text field, type Concentration of KOH.
7. Locate the **Legend** section. Clear the **Background** checkbox.

Line Graph 1

1. In the **Concentration of KOH** toolbar, click **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Data** section.
3. From the **Dataset** list, choose **Cut Line 2D 2**.
4. From the **Parameter selection (E_cell)** list, choose **From list**.
5. In the **Parameter values (E_cell (V))** list, choose **1.3**, **1.5**, **1.7**, and **1.9**.
6. Locate the **y-Axis Data** section. In the **Expression** text field, type cet.c_K_OH.
7. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
8. In the **Expression** text field, type x.
9. Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
10. Click to expand the **Legends** section. Select the **Show legends** checkbox.

11 In the **Concentration of KOH** toolbar, click **Plot**.



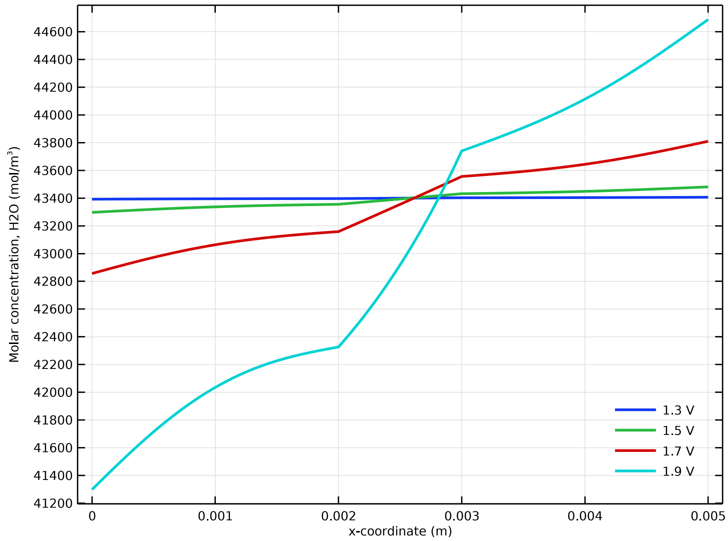
Concentration of H2O

1. In the **Model Builder** window, right-click **Concentration of KOH** and choose **Duplicate**.
2. In the **Model Builder** window, click **Concentration of KOH 1**.
3. In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.
4. Clear the **y-axis label** checkbox.
5. In the **Label** text field, type `Concentration of H2O`.
6. Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Line Graph 1

1. In the **Model Builder** window, click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3. In the **Expression** text field, type `cet.c_H2O`.

4 In the **Concentration of H2O** toolbar, click **Plot**.



Fluid Density

1 In the **Model Builder** window, right-click **Concentration of KOH** and choose **Duplicate**.

2 In the **Model Builder** window, click **Concentration of KOH 1**.

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

4 Clear the **y-axis label** checkbox.

5 In the **Label** text field, type `Fluid Density`.

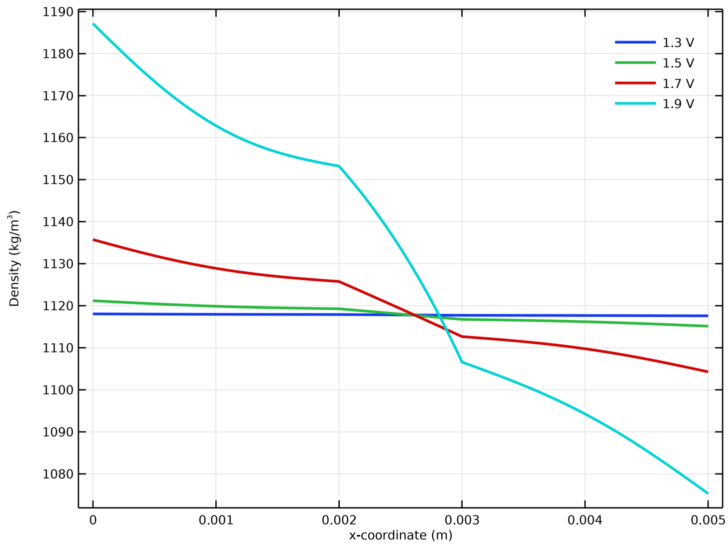
Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

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

3 In the **Expression** text field, type `cet.rho`.

4 In the **Fluid Density** toolbar, click **Plot**.



Electrolyte Conductivity

1 In the **Model Builder** window, right-click **Concentration of KOH** and choose **Duplicate**.

2 In the **Model Builder** window, click **Concentration of KOH 1**.

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

4 Clear the **y-axis label** checkbox.

5 In the **Label** text field, type `Electrolyte Conductivity`.

6 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

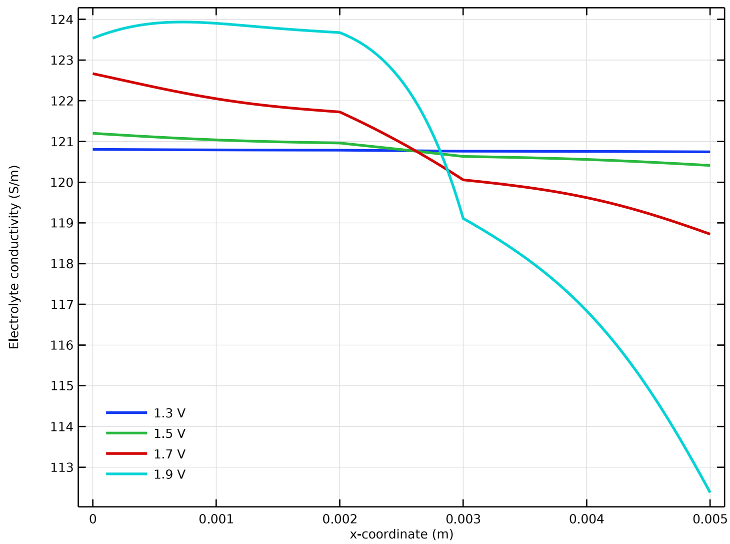
Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

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

3 In the **Expression** text field, type `cet.sigmal`.

4 In the **Electrolyte Conductivity** toolbar, click **Plot**.



Velocity, Y-direction

1 In the **Model Builder** window, right-click **Concentration of KOH** and choose **Duplicate**.

2 In the **Model Builder** window, click **Concentration of KOH 1**.

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

4 Clear the **y-axis label** checkbox.

5 In the **Label** text field, type `Velocity, Y-direction`.

6 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Using CET/ Solution 3 (sol3)**.

7 From the **Parameter selection (E_cell)** list, choose **From list**.

8 In the **Parameter values (E_cell (V))** list, choose **1.3** and **1.9**.

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

Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

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

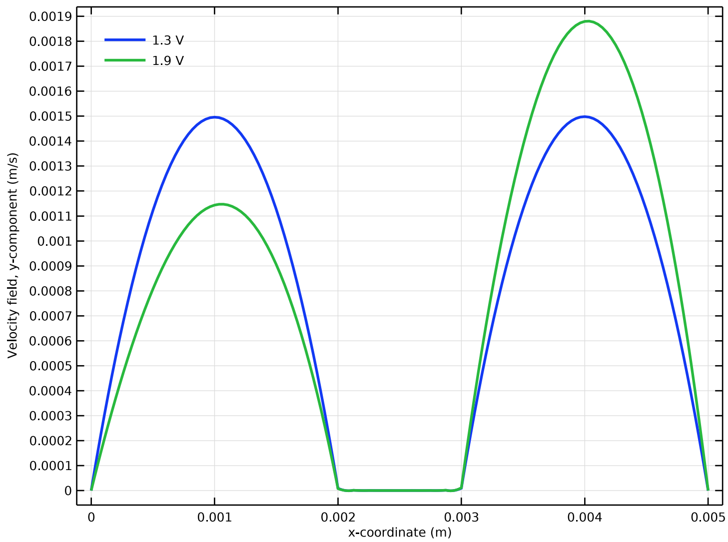
3 From the **Dataset** list, choose **From parent**.

4 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.

5 Select Boundaries 3, 6, and 9 only.

6 Locate the **y-Axis Data** section. In the **Expression** text field, type `v`.

7 In the **Velocity, Y-direction** toolbar, click **Plot**.



Fluid Viscosity

1 In the **Model Builder** window, right-click **Concentration of KOH** and choose **Duplicate**.

2 In the **Model Builder** window, click **Concentration of KOH 1**.

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

4 Clear the **y-axis label** checkbox.

5 In the **Label** text field, type `Fluid Viscosity`.

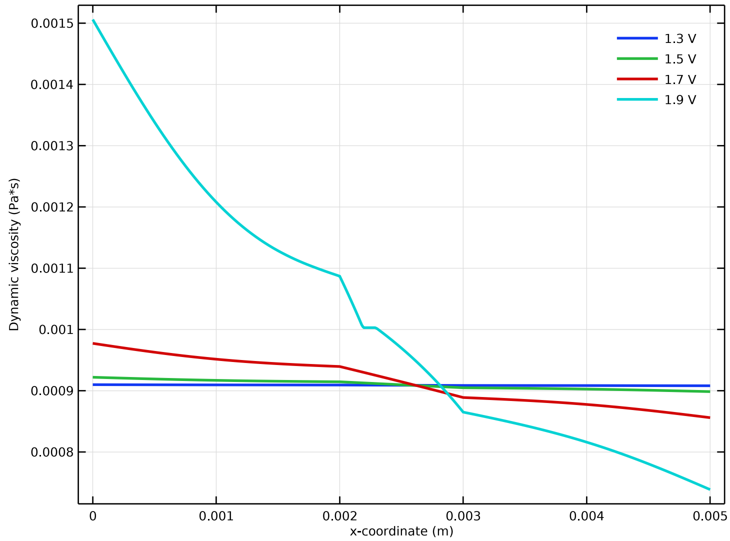
Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

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

3 In the **Expression** text field, type `fp.mu`.

4 In the **Fluid Viscosity** toolbar, click **Plot**.



Electrolyte Potential

1. In the **Model Builder** window, right-click **Fluid Viscosity** and choose **Duplicate**.
2. In the **Settings** window for **1D Plot Group**, type `Electrolyte Potential` in the **Label** text field.
3. Locate the **Plot Settings** section.
4. Select the **y-axis label** checkbox. In the associated text field, type `Electrolyte Potential (V)`.
5. Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Line Graph 1

1. In the **Model Builder** window, expand the **Electrolyte Potential** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **Data** section.
3. From the **Dataset** list, choose **Cut Line 2D 1**.
4. Locate the **y-Axis Data** section. In the **Expression** text field, type `we.phil`.
5. Locate the **Data** section. From the **Parameter selection (E_cell)** list, choose **Last**.
6. Locate the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
WE

Line Graph 2

1 Right-click **Results > Electrolyte Potential > Line Graph 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Cut Line 2D 2**.

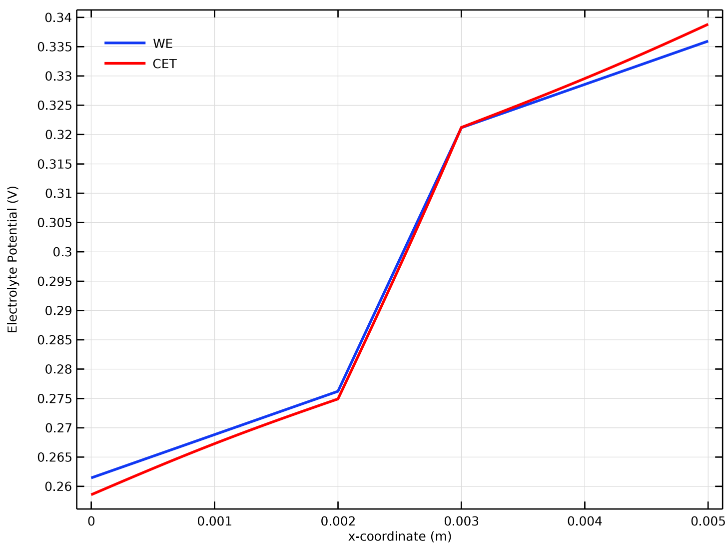
4 Locate the **y-Axis Data** section. In the **Expression** text field, type `cet.phil`.

5 Locate the **Legends** section. In the table, enter the following settings:

Legends
CET

6 Locate the **Coloring and Style** section. From the **Color** list, choose **Red**.

7 In the **Electrolyte Potential** toolbar, click **Plot**.



STUDY 1 - WE ONLY

Finally, disable the **Concentrated Electrolyte Transport** and **Free and Porous Media Flow, Brinkman** interfaces and the CET variables in Study 1 to ensure that it can still be solved.

Step 1: Current Distribution Initialization

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

2 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Definitions** > **Variables - KOH Properties, CET**.

5 Right-click and choose **Disable**.

6 In the tree, select **Component 1 (comp1)** > **Concentrated Electrolyte Transport (cet)**.

7 Right-click and choose **Disable in Model**.

8 In the tree, select **Component 1 (comp1)** > **Free and Porous Media Flow, Brinkman (fp)**.

9 Right-click and choose **Disable in Model**.

Step 2: Stationary

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

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Definitions** > **Variables - KOH Properties, CET**.

5 Right-click and choose **Disable**.

6 In the tree, select **Component 1 (comp1)** > **Concentrated Electrolyte Transport (cet)**.

7 Right-click and choose **Disable in Model**.

8 In the tree, select **Component 1 (comp1)** > **Free and Porous Media Flow, Brinkman (fp)**.

9 Right-click and choose **Disable in Model**.