

# Shunt Currents in an Alkaline Electrolyzer Stack

# Introduction

In an alkaline electrolyzer stack, all cells share the same electrolyte. As a result of all cells being in ionic contact, parasitic shunt currents flow between the cells through the manifolds and the electrolyte channels, on both the inlet and outlet side.

This example models a secondary current distribution in a stack comprising 20 cells. The electricity-to-hydrogen coulombic and energy efficiencies for the stack are computed, as well as the individual shunt currents entering or exiting each cell.





Figure 1: Model stack geometry.

Figure 1 shows the full model geometry. The stack consists of two end plates and 20 repeating unit cells, shown in Figure 2.



Figure 2: Repeating cell unit. Scaled ten times in the x direction.

The endplates and the bipolar plates are made of steel. The electrolyte is 6 M KOH.

The model is set up using the **Water Electrolyzer** interface. The electrode surfaces are modeled using Butler–Volmer kinetics and ohmic losses both in the electrode and electrolyte phases are included, but and 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, with the stack set to operate at 85°C.

The effective electrolyte conductivity in the electrolyte compartment on each side of the separate is set to depend on the electrolyte volume fraction according to

$$\sigma_{l,\,\text{eff}} = \varepsilon_l^{3/2} \sigma_{l,\,\text{bulk}} \tag{1}$$

where  $\sigma_{l,\text{bulk}}$  is the bulk conductivity of 6.0 KOH. Due to gas evolution in the cell electrolyte compartments, the electrolyte volume fraction  $\varepsilon_l$  is defined to vary linearly with z from 100% at the bottom of the electrode active surface area to 50% at the exit to the upper manifolds.

The model is solved using an auxiliary sweep, sweeping the average cell voltage from 1.3 V to 1.8 V.

# Results and Discussion

Figure 3 shows the electric potential in the end plates and bipolar plates of the stack for an average cell voltage of 1.8 V.



Figure 3: Electrode phase potential.

Figure 4 and Figure 5 show the electrolyte phase potential in the stack, and the corresponding electrolyte current streamlines in the inlet/outlet channels and manifolds, for an average cell voltage of 1.8 V, respectively.



Figure 4: Electrolyte phase potential.



E\_cell(6)=1.8 V Streamline: Electrolyte current density vector Streamline Color: Electrolyte potential (V)

Figure 5: Current streamlines in the inlet and outlet channels and manifolds.



Figure 6: Entering or exiting shunt current per cell at an average cell voltage of 1.3 V.



Figure 7: Entering or exiting shunt current per cell at an average cell voltage of 1.8 V.

#### 6 | SHUNT CURRENTS IN AN ALKALINE ELECTROLYZER STACK

The shunt current streamlines in Figure 5 can be integrated over the internal boundary between each manifold and the corresponding electrolyte compartment to compute the individual entry/exit shunt currents of each cell. This is shown in Figure 6 and Figure 7 for the average cell voltages of 1.3 and 1.8 V. The lower effective electrolyte conductivity in the upper channels, due to lower electrolyte volume fraction (Equation 1) results in lower shunt currents for the outlet channels compared to the inlet channels. It is also seen that the shunt currents are more pronounced toward the end of the stack. The higher stack voltage results in generally higher shunt currents in Figure 7, compared to Figure 6.

Figure 8 shows a polarization plot for the stack, where the total current on the x-axis was computed by integrating the current density over one of the end plates of the stack. The plot also show the open circuit and thermoneutral cell voltage for the operating conditions. The thermoneutral cell voltage is of particular interest since additional heat would be required to heat the stack when operating the electrolyzer below this voltage.



Figure 8: Polarization plot for the stack.

We can also compute the coloumbic efficiency for hydrogen production in the stack. This efficiency measure is defined as the total hydrogen evolution current density in all cells, divided by the stack current times the number of cells. The coloumbic efficiency is plotted in Figure 9. The interplay between different polarization effects results in the efficiency being lower at lower stack currents.



Figure 9: Current-to-hydrogen coloumbic efficiency.

Finally, we can also have a look at the energy efficiency of the stack for different current levels in Figure 10. For a system of this kind there are various ways of defining the energy efficiency. Here we base the efficiency measure on the Gibbs free energy of the produced hydrogen, and define the efficiency as the maximum possible energy (per time unit) which would be possible to produce in a fuel cell operating at the same conditions  $(I_{112} \times E_{eq})$ , divided by the electrical energy required to produce it in the stack  $(I_{stack} \times E_{stack})$ . The energy efficiency first increases, as a result of the increasing coloumbic efficiency (Figure 9), to reach at maximum around 1400 A. The decrease seen after 1400 A is due to an increasing stack voltage at higher currents (Figure 8).



Figure 10: Electrical energy-to-hydrogen energy (Gibbs) efficiency.

Notes About the COMSOL Implementation

A **Global Evaluation Sweep** is used to compute the table values plotted in Figure 6 and Figure 7. To update these plots and the corresponding table after recomputing the model, the global evaluation sweep needs to be reevaluated.

**Application Library path:** Fuel\_Cell\_and\_Electrolyzer\_Module/Electrolyzers/ aec\_shunt\_currents

# Modeling Instructions

From the File menu, choose New.

# NEW

In the New window, click **Model Wizard**.

# MODEL WIZARD

I In the Model Wizard window, click 间 3D.

- 2 In the Select Physics tree, select Electrochemistry>Water Electrolyzers> Hydroxide Exchange (we).
- 3 Click Add.
- 4 Click  $\bigcirc$  Study.
- 5 In the Select Study tree, select Preset Studies for Selected Physics Interfaces> Stationary with Initialization.
- 6 Click 🗹 Done.

# GEOMETRY I

Load the geometry sequence from a file.

- I 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 aec\_shunt\_currents\_geom\_sequence.mph.
- 3 In the Geometry toolbar, click 📗 Build All.



4 In the Model Builder window, collapse the Geometry I node.

# DEFINITIONS

The stack geometry has a high aspect ratio, with the cell thicknesses being very small in relation to the cross-sectional area. To facilitate setting up the physics, add a view with scaling in the x direction as follows:

# View 20

- I In the Model Builder window, expand the Component I (compl)>Definitions node.
- 2 Right-click **Definitions** and choose **View**.

# Camera

- I In the Model Builder window, expand the View 20 node, then click Camera.
- 2 In the Settings window for Camera, locate the Camera section.
- 3 From the View scale list, choose Manual.
- 4 In the x scale text field, type 10.
- 5 Click 🚺 Update.



You can now toggle between the two views at any time.

- 6 Click the  $\sqrt{-}$  Go to Default View button in the Graphics toolbar.
- 7 In the Graphics window toolbar, click ▼ next to ↓ Go to Default View, then choose Go to View I.
- 8 In the Graphics window toolbar, click ▼ next to ↓ Go to Default View, then choose Go to View 20.

# GLOBAL DEFINITIONS

#### **Geometry Parameters**

Some parameters were loaded with the geometry sequence.

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, type Geometry Parameters in the Label text field.

Add some more parameters from a text file.

**Physics Parameters** 

- I In the Home toolbar, click Pi Parameters and choose Add>Parameters.
- 2 In the Settings window for Parameters, type Physics Parameters in the Label text field.
- **3** Locate the **Parameters** section. Click *b* Load from File.
- 4 Browse to the model's Application Libraries folder and double-click the file aec\_shunt\_currents\_physics\_parameters.txt.

# ADD MATERIAL

I In the Home toolbar, click 👬 Add Material to open the Add Material window.

This model uses the **Materials** node to define the properties of the bipolar plates, end plates, and electrolyte.

- 2 Go to the Add Material window.
- 3 In the tree, select Built-in>Steel AISI 4340.
- 4 Right-click and choose Add to Component I (compl).
- 5 In the tree, select Fuel Cell and Electrolyzer>Aqueous Alkali>Potassium Hydroxide, KOH.
- 6 Right-click and choose Add to Component I (compl).
- 7 In the Home toolbar, click 🙀 Add Material to close the Add Material window.

# MATERIALS

Steel AISI 4340 (mat1)

- I In the Settings window for Material, locate the Geometric Entity Selection section.
- 2 From the Selection list, choose Current Conductors.

Potassium Hydroxide, KOH (mat2)

- I In the Model Builder window, click Potassium Hydroxide, KOH (mat2).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- **3** From the Selection list, choose Electrolyte Compartments.

## DEFINITIONS

#### Variables I

I In the Model Builder window, under Component I (compl) right-click Definitions and choose Variables.

Add some variable expressions from a text file. Most of these will be used during postprocessing of the solution.

- 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\_shunt\_currents\_variables.txt.

Note that some expressions are marked in orange, indicating unknown operators. Add these operators as follows:

# Integration 1 (intop1)

- I In the Definitions toolbar, click 🖉 Nonlocal Couplings and choose Integration.
- 2 In the Settings window for Integration, type intop\_point\_h2 in the Operator name text field.
- 3 Locate the Source Selection section. From the Geometric entity level list, choose Point.
- 4 Select Point 15 only.

#### Integration 2 (intop2)

- I In the Definitions toolbar, click A Nonlocal Couplings and choose Integration.
- 2 In the Settings window for Integration, type intop\_point\_02 in the Operator name text field.
- 3 Locate the Source Selection section. From the Geometric entity level list, choose Point.
- **4** Select Point 57 only.

#### Integration 3 (intop3)

- I In the Definitions toolbar, click 🖉 Nonlocal Couplings and choose Integration.
- 2 In the Settings window for Integration, type intop\_h2\_electrodes in the Operator name text field.
- **3** Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 From the Selection list, choose H2 Electrodes.

Integration 4 (intop4)

- I In the Definitions toolbar, click *A* Nonlocal Couplings and choose Integration.
- 2 In the Settings window for Integration, type intop\_cc in the Operator name text field.
- **3** Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 1 only.

#### Integration 5 (intop5)

- I In the Definitions toolbar, click *N* Nonlocal Couplings and choose Integration.
- 2 In the Settings window for Integration, type intop\_upper in the Operator name text field.
- **3** Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 From the Selection list, choose Upper Manifold Active Cell Boundaries.

#### Integration 6 (intop6)

- I In the Definitions toolbar, click 🖉 Nonlocal Couplings and choose Integration.
- 2 In the Settings window for Integration, type intop\_lower in the Operator name text field.
- **3** Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 From the Selection list, choose Lower Manifold Active Cell Boundaries.

#### Variables I

All variable expressions should now have turned black.

# WATER ELECTROLYZER (WE)

You are now ready to start defining the physics.

- I In the Model Builder window, under Component I (compl) click Water Electrolyzer (we).
- 2 In the Settings window for Water Electrolyzer, locate the H2 Gas Mixture section.
- 3 Clear the **H20** check box.
- **4** Find the **Reactions** subsection. Select the **Include H2O(I)** in reaction stoichiometry check box.
- 5 Locate the O2 Gas Mixture section. Clear the H2O check box.
- 6 Select the Include H2O(I) in reaction stoichiometry check box.

#### Separator 1

- I 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 Separators.
- **4** Locate the **Effective Electrolyte Charge Transport** section. In the ε<sub>1</sub> text field, type epsl\_sep.

Current Collector I

- I In the Physics toolbar, click 🔚 Domains and choose Current Collector.
- 2 In the Settings window for Current Collector, locate the Domain Selection section.
- **3** From the Selection list, choose Current Conductors.
- **4** Locate the **Electrode Charge Transport** section. From the  $\sigma_s$  list, choose **From material**.

#### H2 Gas-Electrolyte Compartment I

- I 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 H2 Gas Electrolyte Compartments.
- **4** Locate the **Effective Electrolyte Charge Transport** section. In the  $\varepsilon_1$  text field, type eps1.

#### O2 Gas-Electrolyte Compartment I

- I In the Physics toolbar, click 🔚 Domains and choose 02 Gas-Electrolyte Compartment.
- **2** In the **Settings** window for **02 Gas-Electrolyte Compartment**, locate the **Domain Selection** section.
- 3 From the Selection list, choose Oxygen Gas Electrolyte Compartments.
- **4** Locate the **Effective Electrolyte Charge Transport** section. In the  $\varepsilon_1$  text field, type eps1.

# Internal H2 Electrode Surface I

- I In the Physics toolbar, click 🔚 Boundaries and choose Internal H2 Electrode Surface.
- 2 In the Settings window for Internal H2 Electrode Surface, locate the Boundary Selection section.
- 3 From the Selection list, choose H2 Electrodes.

#### H2 Electrode Reaction I

- I In the Model Builder window, click H2 Electrode Reaction I.
- **2** In the Settings window for H2 Electrode Reaction, locate the Stoichiometric Coefficients section.

- **3** In the  $v_{\text{H2O}(1)}$  text field, type -1.
- 4 Locate the Electrode Kinetics section. From the Exchange current density type list, choose Lumped multistep.
- **5** In the  $i_{0,ref}(T)$  text field, type i0\_ref\_h2.
- 6 From the Pressure dependence list, choose Cathodic reaction orders.
- **7** In the  $\xi_{c,H2}$  text field, type 1.

Internal O2 Electrode Surface I

- I In the Physics toolbar, click 🔚 Boundaries and choose Internal O2 Electrode Surface.
- **2** In the **Settings** window for **Internal O2 Electrode Surface**, locate the **Boundary Selection** section.
- **3** From the Selection list, choose **02** Electrodes.

O2 Electrode Reaction 1

- I In the Model Builder window, click O2 Electrode Reaction I.
- **2** In the **Settings** window for **O2 Electrode Reaction**, locate the **Stoichiometric Coefficients** section.
- **3** In the  $v_{\text{H2O}(1)}$  text field, type -1.
- 4 Locate the Electrode Kinetics section. From the Exchange current density type list, choose Lumped multistep.
- **5** In the  $i_{0,ref}(T)$  text field, type i0\_ref\_02.
- 6 From the Pressure dependence list, choose Anodic reaction orders.
- **7** In the  $\xi_{a,O2}$  text field, type 1.

#### Electronic Conducting Phase I

In the Model Builder window, under Component I (compl)>Water Electrolyzer (we) click Electronic Conducting Phase I.

# Electric Ground 1

- I In the Physics toolbar, click 层 Attributes and choose Electric Ground.
- **2** Select Boundary 1 only.

#### Electronic Conducting Phase 1

In the Model Builder window, click Electronic Conducting Phase I.

# Electric Potential 1

- I In the Physics toolbar, click 📃 Attributes and choose Electric Potential.
- **2** Select Boundary 1610 only.

- 3 In the Settings window for Electric Potential, locate the Electric Potential section.
- **4** In the  $\phi_{s,bnd}$  text field, type E\_stack.

# Electrolyte Phase I

The electrolyte properties need input from the physics with regards to the electrolyte concentration and the temperature.

- I In the Model Builder window, under Component I (compl)>Water Electrolyzer (we) click Electrolyte Phase I.
- 2 In the Settings window for Electrolyte Phase, locate the Model Input section.
- **3** From the *c* list, choose **User defined**.

The model input variables can be defined locally on this node or as a **Common model** input. In the associated text field, type c\_KOH.

# **GLOBAL DEFINITIONS**

#### Default Model Inputs

- I 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.
- Find the Expression for remaining selection subsection. In the Temperature text field, type T.

Also, the pressure needs to be set since the equilibrium potentials of the electrode reactions depend on the pressure.

- 5 In the tree, select General>Pressure (Pa) minput.pA.
- 6 In the **Pressure** text field, type p\_abs.

# MESH I

This model requires a manual mesh. The geometry has been set up in such a way that it can easily be swept in the x direction. For good accuracy when computing the shunt currents, a more well-resolved mesh is needed in the manifolds and channels.

## Size 1

I In the Model Builder window, under Component I (comp1) right-click Mesh I and choose Size.

- 2 In the Settings window for Size, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Boundary.

**4** From the **Selection** list, choose **Upper**/

#### Lower Manifold and Active Area Boundaries (for Meshing).

5 Locate the Element Size section. From the Predefined list, choose Extra fine.

## Size 2

- I In the Model Builder window, right-click Mesh I and choose Size.
- 2 In the Settings window for Size, locate the Geometric Entity Selection section.
- **3** From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Channels.
- 5 Locate the Element Size section. From the Predefined list, choose Finer.

#### Swept I

In the **Mesh** toolbar, click A Swept.

# Distribution I

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- **3** From the Selection list, choose H2 Gas Electrolyte Compartments.

#### Distribution 2

- I In the Model Builder window, right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- **3** From the Selection list, choose Current Conductors.
- 4 Locate the Distribution section. In the Number of elements text field, type 1.

#### Distribution 3

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- **3** From the Selection list, choose Oxygen Gas Electrolyte Compartments.

#### Distribution 4

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- **3** From the **Selection** list, choose **Separators**.
- 4 Locate the Distribution section. In the Number of elements text field, type 2.

Swept 1 Right-click Swept 1 and choose Build Selected.



# Boundary Layers 1

The local current densities on the electrode surfaces are higher in the regions close to the manifolds. Add boundary layer meshes there in order to improve the shunt current accuracy further.

- I In the Mesh toolbar, click Boundary Layers.
- 2 In the Settings window for Boundary Layers, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Active Cell Volume.
- **5** Click to expand the **Transition** section. Clear the **Smooth transition to interior mesh** check box.

#### Boundary Layer Properties

- I 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 Upper/Lower Active Area Boundaries (for Meshing).
- 4 Locate the Layers section. In the Number of layers text field, type 5.
- 5 From the Thickness specification list, choose First layer.

6 In the **Thickness** text field, type D\_02/3.

# Boundary Layers 2

- I In the Mesh toolbar, click Boundary Layers.
- 2 In the Settings window for Boundary Layers, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Manifolds.
- 5 Locate the Transition section. Clear the Smooth transition to interior mesh check box.

Boundary Layer Properties

- I 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 Manifold Active Cell Boundaries.
- 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 D\_02/3.
- 7 Click 📗 Build All.



The model is now ready for solving. Use an auxiliary sweep for sweeping the average cell voltage from 1.3 to 1.8 V.

# STUDY I

Step 2: Stationary

- I In the Model Builder window, under Study I click Step 2: Stationary.
- 2 In the Settings window for Stationary, click to expand the Study Extensions section.
- **3** Select the **Auxiliary sweep** check box.
- 4 Click + Add.
- **5** In the table, click to select the cell at row number 1 and column number 3.
- 6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E_cell (Cell voltage (varied in	range(1.3,0.1,1.8)	V
sweep))		

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

# RESULTS

Electrode Potential with Respect to Ground

Reproduce the plots from the Results and Discussion section as follows.

- I In the **Settings** window for **3D Plot Group**, type Electrode Potential with Respect to Ground in the **Label** text field.
- **2** In the **Model Builder** window, expand the **Electrode Potential with Respect to Ground** node.

Arrow Volume 1, Multislice 1

- In the Model Builder window, under Results>Electrode Potential with Respect to Ground, Ctrl-click to select Multislice I and Arrow Volume I.
- 2 Right-click and choose Disable.

# Surface 1

- I In the Model Builder window, right-click Electrode Potential with Respect to Ground and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- 3 In the **Expression** text field, type we.phis.
- 4 In the Electrode Potential with Respect to Ground toolbar, click 🗿 Plot.
- 5 In the Graphics window toolbar, click ▼ next to ↓ Go to Default View, then choose Go to View 1.

#### Electrode Potential with Respect to Ground

- I In the Model Builder window, click Electrode Potential with Respect to Ground.
- 2 In the Settings window for 3D Plot Group, locate the Plot Settings section.
- **3** Clear the **Plot dataset edges** check box.
- **4** In the **Electrode Potential with Respect to Ground** toolbar, click **O** Plot.



#### **Electrolyte Potential**

- I In the Model Builder window, under Results click Electrolyte Potential (we).
- 2 In the Settings window for 3D Plot Group, type Electrolyte Potential in the Label text field.
- **3** Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.
- 4 In the Model Builder window, expand the Electrolyte Potential node.

# Arrow Volume 1, Multislice 1

- I In the Model Builder window, under Results>Electrolyte Potential, Ctrl-click to select Multislice I and Arrow Volume I.
- 2 Right-click and choose **Disable**.

# Surface 1

I In the Model Builder window, right-click Electrolyte Potential and choose Surface.

**2** In the **Electrolyte Potential** toolbar, click **OM Plot**.



# Shunt Current Streamlines

- I In the Home toolbar, click 🚛 Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Shunt Current Streamlines in the Label text field.
- 3 Locate the Plot Settings section. Clear the Plot dataset edges check box.

#### Streamline 1

- I Right-click Shunt Current Streamlines and choose Streamline.
- 2 In the Settings window for Streamline, locate the Streamline Positioning section.
- **3** In the **Number** text field, type 100.
- 4 Locate the Selection section. From the Selection list, choose Manifold Active Cell Boundaries.
- 5 Locate the Coloring and Style section. Find the Point style subsection. From the Type list, choose Arrow.

# Selection I

- I Right-click Streamline I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Channels and Manifolds.

#### Color Expression 1

- I In the Model Builder window, right-click Streamline I and choose Color Expression.
- 2 In the Settings window for Color Expression, click to expand the Title section.
- 3 From the Title type list, choose Automatic.
- **4** Locate the **Coloring and Style** section. Click **Change Color Table**.
- 5 In the Color Table dialog box, select Aurora>AuroraBorealis in the tree.
- 6 Click OK.

## Surface 1

- I In the Model Builder window, right-click Shunt Current Streamlines and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- **3** In the **Expression** text field, type **1**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

#### Material Appearance 1

Right-click Surface I and choose Material Appearance.

## Surface 2

- I In the Model Builder window, right-click Shunt Current Streamlines and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- **3** In the **Expression** text field, type **1**.
- 4 Locate the Title section. From the Title type list, choose None.

# Material Appearance 1

- I Right-click Surface 2 and choose Material Appearance.
- 2 In the Settings window for Material Appearance, locate the Appearance section.
- 3 From the Material list, choose Potassium Hydroxide, KOH (mat2).

#### Transparency 1

- I In the Model Builder window, right-click Surface 2 and choose Transparency.
- 2 In the Settings window for Transparency, locate the Transparency section.
- **3** Set the **Transparency** value to **0.9**.

**4** In the Shunt Current Streamlines toolbar, click **I** Plot.

E\_cell(6)=1.8 V Streamline: Electrolyte current density vector Streamline Color: Electrolyte potential (V)



# Polarization Plot

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the **Settings** window for **ID Plot Group**, type Polarization Plot in the **Label** text field.

#### Global I

- I Right-click Polarization Plot and choose Global.
- 2 In the Settings window for Global, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Global definitions>Parameters>E\_cell Cell voltage (varied in sweep) V.
- 3 Click Add Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (comp1)>Definitions>Variables>Eeq\_cell Cell equilibrium voltage V.
- 4 Click Add Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (compl)>Definitions>Variables>Etherm\_cell Cell thermoneutral voltage V.
- 5 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 6 Click Replace Expression in the upper-right corner of the x-Axis Data section. From the menu, choose Component I (compl)>Definitions>Variables>I\_stack Stack current A.

- 7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.
- 8 Click to expand the Legends section. From the Legends list, choose Manual.
- **9** In the table, enter the following settings:

#### Legends

E<sub>cell</sub>

E<sub>ocv</sub>

E<sub>therm</sub>

Polarization Plot

- I In the Model Builder window, click Polarization Plot.
- 2 In the Settings window for ID Plot Group, locate the Legend section.
- 3 From the Position list, choose Upper left.
- 4 Locate the Plot Settings section.
- 5 Select the y-axis label check box. In the associated text field, type Voltage (V).
- 6 Click to expand the Title section. From the Title type list, choose None.
- 7 In the Polarization Plot toolbar, click 💽 Plot.



Coulombic Efficiency I In the Home toolbar, click I Add Plot Group and choose ID Plot Group.

2 In the Settings window for ID Plot Group, type Coulombic Efficiency in the Label text field.

# Global I

- I Right-click Coulombic Efficiency and choose Global.
- In the Settings window for Global, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (compl)>Definitions> Variables>Eff\_coulombic Current-to-hydrogen coloumbic efficiency.
- 3 Locate the y-Axis Data section. In the table, enter the following settings:

Expression	Unit	Description
Eff_coulombic	9 <sub>0</sub>	Current-to-hydrogen coloumbic efficiency

- 4 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 5 Click Replace Expression in the upper-right corner of the x-Axis Data section. From the menu, choose Component I (compl)>Definitions>Variables>I\_stack Stack current A.
- 6 Locate the Legends section. Clear the Show legends check box.

Coulombic Efficiency

- I In the Model Builder window, click Coulombic Efficiency.
- 2 In the Settings window for ID Plot Group, locate the Title section.
- **3** From the **Title type** list, choose **None**.



# Energy Efficiency

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Energy Efficiency in the Label text field.

## Global I

- I Right-click Energy Efficiency and choose Global.
- In the Settings window for Global, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (compl)>Definitions> Variables>Eff\_energy Electrical energy-to-hydrogen energy efficiency.
- 3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description	
Eff_energy	0,0	Electrical energy-to-hydrogen energy efficiency	

- 4 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 5 Click Replace Expression in the upper-right corner of the x-Axis Data section. From the menu, choose Component I (compl)>Definitions>Variables>I\_stack Stack current A.
- 6 Locate the Legends section. Clear the Show legends check box.

# Energy Efficiency

- I In the Model Builder window, click Energy Efficiency.
- 2 In the Settings window for ID Plot Group, locate the Title section.
- 3 From the Title type list, choose None.
- **4** In the **Energy Efficiency** toolbar, click **I** Plot.



# Global Evaluation Sweep 1

- I In the Results toolbar, click <sup>8,85</sup><sub>e-12</sub> More Derived Values and choose Other> Global Evaluation Sweep.
- 2 In the Settings window for Global Evaluation Sweep, locate the Data section.
- 3 From the Parameter value (E\_cell (V)) list, choose 1.3.
- 4 Locate the Parameters section. In the table, enter the following settings:

Parameter name	Parameter value list
Cell	<pre>range(1,1,N_cells)</pre>

- **5** Locate the **Expressions** section. Click *b* Load from File.
- 6 Browse to the model's Application Libraries folder and double-click the file aec\_shunt\_currents\_global\_sweep\_evaluation\_expressions.txt.
- 7 Click **=** Evaluate.

Shunt Currents per Cell

- I In the Results toolbar, click  $\sim$  ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Shunt Currents in the Label text field.
- 3 In the Label text field, type Shunt Currents per Cell.

#### Table Graph I

- I Right-click Shunt Currents per Cell and choose Table Graph.
- 2 In the Settings window for Table Graph, click to expand the Legends section.
- **3** Select the **Show legends** check box.
- **4** In the **Shunt Currents per Cell** toolbar, click **I** Plot.
- **5** Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.
- 6 Find the Line markers subsection. From the Marker list, choose Cycle.

#### Shunt Currents per Cell

- I In the Model Builder window, click Shunt Currents per Cell.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 3 Select the y-axis label check box. In the associated text field, type Current (A).
- 4 Locate the Legend section. From the Position list, choose Upper left.
- 5 In the Shunt Currents per Cell toolbar, click 🗿 Plot.



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Global Evaluation Sweep 1

- I In the Model Builder window, under Results>Derived Values click Global Evaluation Sweep I.
- 2 In the Settings window for Global Evaluation Sweep, locate the Data section.
- 3 From the Parameter value (E\_cell (V)) list, choose 1.8.
- 4 Click **= Evaluate**.

Table Graph I

I In the Model Builder window, under Results>Shunt Currents per Cell click Table Graph I.



2 In the Shunt Currents per Cell toolbar, click 💽 Plot.