

# Solid Oxide Electrolyzer Using Thermodynamics

# Introduction

This example models a solid oxide electrolyzer cell wherein water vapor is reduced to form hydrogen gas on the cathode, and oxygen gas is evolved on the anode. The current distribution in the cell is coupled to the cathode mass transfer of hydrogen and water and momentum transport.

# Model Definition

On the anode, oxygen ions are oxidized to form oxygen gas,

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

whereas on the cathode, water vapor is reduced to form hydrogen gas and oxygen ions:

$$2H_2O(g) + 4e^- \leftrightarrow 2H_2(g) + 2O^{2-}$$
 (2)

Figure 1 shows the model geometry. Since the oxygen is the only gas present in the anode gas chamber, and isobaric conditions are assumed, there is no need to explicitly model the anode gas transport. Four computational domains are hence used in the model: the

cathode gas channels, the cathode gas diffusion electrode, the solid oxide electrolyte layer, and the anode gas diffusion electrode.



Figure 1: Model geometry. From top: Cathode gas channels, cathode gas diffusion electrode, solid oxide electrolyte layer, and anode gas diffusion layer. The positions of the inlet and outlet are indicated in the figure.

The composition of the hydrogen-water vapor mixture will change as a result of the electrochemical reactions. The mass transport of hydrogen and water vapor is modeled in the cathode gas channels and the gas diffusion electrode, coupled to the resulting (laminar) flow of the gas mixture. The mass transport of hydrogen and water is modeled using the Transport of Concentrated Species interface, using Maxwell-Stefan diffusion. The momentum flow is defined in the model using the Brinkman Equations interface for the porous gas diffusion electrodes. The Navier-Stokes equations are used for the nonporous gas channels.

The current distribution is defined assuming a constant conductivity of the solid electrolyte. The Secondary Current Distribution interface is used to define the electrode reactions and the electrolyte charge transport in the porous gas diffusion electrodes and the electrolyte layer.

On the cathode side, the electrode kinetics depends on the local concentration of water and hydrogen according to the law of mass action (and Nernst equation). On the anode side, and a uniform partial pressure of oxygen is assumed and a concentration-independent Butler-Volmer expression is hence used to define the electrode kinetics.

The Thermodynamics and Chemistry nodes are used to automatically define the properties of the cathode gas mixture, as well as the equilibrium potentials of the electrode reactions.

# Results and Discussion

Figure 2 shows the velocity magnitude distribution in the cell. The highest velocities are located close to the inlet and outlet.



Slice: Velocity magnitude (m/s) Streamline: Velocity field

Figure 2: Velocity in the cell.

Figure 3 shows how the density and the dynamic viscosity of the gas relate to the hydrogen and water molar fractions shown in Figure 4. As the hydrogen content of the gas increases toward the outlet, the density and the viscosity both decrease.



Figure 3: Density (left) and dynamic viscosity (right).



Figure 4: Hydrogen (left) and water vapor (right) concentrations.

Figure 5 shows the molar fraction of hydrogen in the gas mixture, and the corresponding hydrogen flux streamlines. The molar fraction is close to zero at the inlet and almost 100% at the outlet.



Streamline: Total flux Volume: Mole fraction (1)

Figure 5: Hydrogen molar fraction (slice) and flux (streamlines).

Finally, Figure 6 shows the cross-sectional electrolyte current density in the middle of the electrolyte between the anode and the cathode. The current density is highest close to the inlet, where the water/hydrogen ratio is high, and decreases toward the outlet.





Figure 6: Electrolyte current density through electrolyte layer.

**Application Library path:** Fuel\_Cell\_and\_Electrolyzer\_Module/Electrolyzers/ soec\_thermodynamics

# Modeling Instructions

This tutorial models the current distribution in a solid oxide electrolyzer. The tutorial comprises two major parts. First, the thermodynamics and the electrode reactions are defined to provide the equilibrium potentials of the anode and the cathode, and a secondary (not concentration dependent) current distribution is modeled. In the second part, mass and momentum transport are added to model a concentration-dependent current distribution of the cell, where the mixture properties of the anode gas depends on the molar fractions of water and hydrogen.

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>

Primary and Secondary Current Distribution>Secondary Current Distribution (cd).

- 3 Click Add.
- 4 Click 🔿 Study.
- 5 In the Select Study tree, select Preset Studies for Selected Physics Interfaces> Stationary with Initialization.
- 6 Click **M** Done.

## GEOMETRY I

The model geometry is available as a parameterized geometry sequence in a separate MPH-file. If you want to build it from scratch, follow the instructions in the section Appendix —Geometry Modeling Instructions. Otherwise load it from file using the following steps.

- 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 soec\_thermodynamics\_geom\_sequence.mph.

**3** In the **Geometry** toolbar, click **H** Build All.



## **GLOBAL DEFINITIONS**

#### **Geometry Parameters**

- 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.

## **Physics Parameters**

Some parameters were imported with the geometry sequence. Import some additional physics parameters from a text file.

- I In the Home toolbar, click **P**; 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 📂 Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file soec\_thermodynamics\_physics\_parameters.txt.

Add a thermodynamic system for the hydrogen/water gas mixture.

5 In the Physics toolbar, click  $\bowtie$  Thermodynamics and choose Thermodynamic System.

#### SELECT SYSTEM

- I Go to the Select System window.
- 2 Click Next in the window toolbar.

## SELECT SPECIES

- I Go to the Select Species window.
- 2 In the Species list, select water (7732-18-5, H2O).
- **3** Click + Add Selected.
- 4 In the Species list, select hydrogen (1333-74-0, H2).
- 5 Click + Add Selected.
- 6 Click Next in the window toolbar.

#### SELECT THERMODYNAMIC MODEL

- I Go to the Select Thermodynamic Model window.
- 2 Click Finish in the window toolbar.

#### **GLOBAL DEFINITIONS**

#### Gas System - H2 and H2O

- In the Model Builder window, under Global Definitions>Thermodynamics click
  Gas System I (ppI).
- **2** In the **Settings** window for **Thermodynamic System**, type Gas System H2 and H20 in the **Label** text field.
- 3 Right-click Global Definitions>Thermodynamics>Gas System H2 and H2O and choose Generate Chemistry.

#### SELECT SPECIES

- I Go to the Select Species window.
- 2 In the list, choose hydrogen and water.
- **3** Click + Add Selected.
- 4 Click Next in the window toolbar.

#### CHEMISTRY SETTINGS

I Go to the Chemistry Settings window.

- 2 From the Mass transfer list, choose Concentrated species.
- 3 Click Finish in the window toolbar.

#### CHEMISTRY - H2 AND H20

- I In the Model Builder window, under Component I (compl) click Chemistry (chem).
- 2 In the Settings window for Chemistry, type Chemistry H2 and H20 in the Label text field.
- **3** Locate the Model Input section. Select the Enable electrode reactions check box.
- **4** From the *E* list, choose **Electrode potential (cd)**.
- 5 Click to expand the Calculate Transport Properties section.

## Electrode Reaction 1

Add the electrode reaction for the cathode. Use the (ads) annotation in the reaction formula to define that the oxygen ions do not belong the main (gas) phase.

- I In the Physics toolbar, click 🔚 Domains and choose Electrode Reaction.
- In the Model Builder window, expand the Component I (compl)>Chemistry H2 and H2O (chem) node, then click Electrode Reaction I.
- 3 In the Settings window for Electrode Reaction, locate the Reaction Formula section.
- 4 In the Formula (written as reduction) text field, type H20+2e<=>H2+0(ads).
- 5 Click Apply.
- 6 Locate the Equilibrium Potential section. From the list, choose Automatic.
- 7 Locate the **Electrode Kinetics** section. In the  $i_{0,ref}(T)$  text field, type i0\_H2.

For the first computation we will assume constant mass fractions (concentrations) for the species.

- 8 In the Model Builder window, under Component I (compl) click Chemistry -H2 and H2O (chem).
- 9 In the Settings window for Chemistry, locate the Species Matching section.

10 Find the Bulk species subsection. In the table, enter the following settings:

Species	Туре	Mass fraction	Value (I)	From Thermodynamics
H2	Variable	User defined	0.5	H2
H2O	Variable	User defined	0.5	H2O

II Find the Surface species subsection. In the table, enter the following settings:

Species	Species concentration type	Surface concentration (mol/m <sup>2</sup> )
O(ads)	Variable	1e-5[mol/m^2]

## GLOBAL DEFINITIONS

Now add a second thermodynamics system for the anode oxygen gas.

In the Physics toolbar, click  $\bowtie$  Thermodynamics and choose Thermodynamic System.

## SELECT SYSTEM

- I Go to the Select System window.
- 2 Click Next in the window toolbar.

## SELECT SPECIES

- I Go to the Select Species window.
- 2 In the Species list, select oxygen (7782-44-7, 02).
- **3** Click + Add Selected.
- 4 Click **Next** in the window toolbar.

## SELECT THERMODYNAMIC MODEL

- I Go to the Select Thermodynamic Model window.
- 2 Click **Finish** in the window toolbar.

## GLOBAL DEFINITIONS

#### Gas System - O2

- I In the Model Builder window, under Global Definitions>Thermodynamics click Gas System I (pp2).
- 2 In the Settings window for Thermodynamic System, type Gas System 02 in the Label text field.
- 3 Right-click Global Definitions>Thermodynamics>Gas System 02 and choose Generate Chemistry.

#### SELECT SPECIES

- I Go to the Select Species window.
- 2 In the list, select oxygen.
- **3** Click + Add Selected.

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

#### CHEMISTRY SETTINGS

- I Go to the Chemistry Settings window.
- 2 Click **Finish** in the window toolbar.

#### CHEMISTRY - 02

- I In the Model Builder window, under Component I (compl) click Chemistry 2 (chem2).
- 2 In the Settings window for Chemistry, type Chemistry 02 in the Label text field.
- 3 Locate the Model Input section. Select the Enable electrode reactions check box.
- **4** From the *E* list, choose **Electrode potential (cd)**.

#### Electrode Reaction 1

- I In the Physics toolbar, click 🔚 Domains and choose Electrode Reaction.
- 2 In the Settings window for Electrode Reaction, locate the Reaction Formula section.
- 3 In the Formula (written as reduction) text field, type 02+4e<=>20(ads).
- 4 Click Apply.
- 5 Locate the Equilibrium Potential section. From the list, choose Automatic.
- **6** Locate the **Electrode Kinetics** section. In the  $i_{0,ref}(T)$  text field, type i0\_02.
- **7** In the  $\alpha_a$  text field, type **3.5**.
- 8 In the Model Builder window, under Component I (compl) click Chemistry 02 (chem2).
- 9 In the Settings window for Chemistry, locate the Species Matching section.

**IO** Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Туре	Mass fraction	Value (I)	From Thermodynamics
O2	Variable	User defined	1	O2

II Find the Surface species subsection. In the table, enter the following settings:

Species	Species concentration type	Surface concentration (mol/m^2)
O(ads)	Variable	1e-5[mol/m^2]

## SECONDARY CURRENT DISTRIBUTION (CD)

Now define the current distribution in the gas diffusion electrodes and the electrolyte.

- I In the Model Builder window, under Component I (comp1) click Secondary Current Distribution (cd).
- **2** In the **Settings** window for **Secondary Current Distribution**, locate the **Domain Selection** section.
- 3 Click Telear Selection.
- 4 Select Domains 1–3 only.

#### Electrolyte I

- I In the Model Builder window, under Component I (compl)> Secondary Current Distribution (cd) click Electrolyte I.
- 2 In the Settings window for Electrolyte, locate the Electrolyte section.
- **3** From the  $\sigma_l$  list, choose **User defined**. In the associated text field, type sigma\_1.

Porous Electrode - H2 and H2O (Cathode)

- I In the Physics toolbar, click 🔚 Domains and choose Porous Electrode.
- 2 In the Settings window for Porous Electrode, type Porous Electrode H2 and H20 (Cathode) in the Label text field.
- 3 Locate the Domain Selection section. From the Selection list, choose Cathode.
- 4 Locate the Electrolyte Current Conduction section. From the  $\sigma_l$  list, choose User defined. In the associated text field, type sigma\_1.
- **5** In the  $\varepsilon_l$  text field, type por\_1.
- $\label{eq:stability} \begin{array}{l} \textbf{6} \ \ Locate \ the \ \textbf{Electrode Current Conduction} \ section. \ From \ the \ \sigma_s \ list, \ choose \ \textbf{User defined}. \\ In \ the \ associated \ text \ field, \ type \ \texttt{sigmas}. \end{array}$
- 7 In the  $\varepsilon_s$  text field, type 1-por\_1.

#### Porous Electrode Reaction I

Couple the electrode reaction current density to the chemistry interface for the cathode as follows.

- I In the Model Builder window, click Porous Electrode Reaction I.
- **2** In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.
- 3 In the  $E_{eq}$  text field, type chem.Eeq\_er1.
- 4 Locate the Electrode Kinetics section. From the i<sub>loc,expr</sub> list, choose User defined. In the associated text field, type chem.iloc\_er1.
- **5** Locate the **Active Specific Surface Area** section. In the  $a_v$  text field, type S.

#### Porous Electrode - O2 (Anode)

- I In the Model Builder window, right-click Porous Electrode H2 and H2O (Cathode) and choose Duplicate.
- 2 In the Settings window for Porous Electrode, type Porous Electrode 02 (Anode) in the Label text field.
- 3 Locate the Domain Selection section. From the Selection list, choose Anode.

#### Porous Electrode Reaction 1

- I In the Model Builder window, expand the Porous Electrode O2 (Anode) node, then click Porous Electrode Reaction I.
- **2** In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.
- 3 In the  $E_{eq}$  text field, type chem2.Eeq\_er1.
- 4 Locate the Electrode Kinetics section. In the  $i_{loc.expr}$  text field, type chem2.iloc\_er1.

#### Electric Ground 1

- I In the Physics toolbar, click 🔚 Boundaries and choose Electric Ground.
- 2 In the Settings window for Electric Ground, locate the Boundary Selection section.
- **3** From the Selection list, choose Cathode Current Collector.

#### Electrode Current I

- I In the Physics toolbar, click 📄 Boundaries and choose Electrode Current.
- 2 In the Settings window for Electrode Current, locate the Boundary Selection section.
- **3** From the Selection list, choose Anode Current Collector.
- 4 Locate the Electrode Current section. From the list, choose Average current density.
- **5** In the  $i_{s,average}$  text field, type I\_avg.

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

#### MESH I

The physics settings for the first part of the tutorial are now complete. Add a user-defined mesh.

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, click to expand the Element Size Parameters section.
- **3** Locate the **Element Size** section. Click the **Custom** button.
- 4 Locate the Element Size Parameters section.
- 5 Select the Maximum element size check box. In the associated text field, type H\_ch\*0.8.

#### Swept 1

- I In the Mesh toolbar, click As Swept.
- 2 In the Settings window for Swept, locate the Domain Selection section.
- 3 From the Geometric entity level list, choose Domain.
- **4** Select Domains 5–7 only.
- 5 Click 🖷 Build Selected.



6 Click 🖷 Build Selected.

#### Boundary Layers 1

Also add boundary layer mesh nodes at this stage. These are actually not needed for the first calculation, but will improve the accuracy and convergence of the solution for the second part of the tutorial when mass transport and convection has been added.

- 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** Select Domains 5–7 only.

## 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 Click Paste Selection.
- 4 In the Paste Selection dialog box, type 21-23, 25, 28-30, 32, 35-37, 39 in the Selection text field.
- 5 Click OK.
- 6 In the Settings window for Boundary Layer Properties, locate the Layers section.
- 7 In the Number of layers text field, type 2.
- 8 In the Stretching factor text field, type 1.3.
- 9 From the Thickness specification list, choose First layer.
- **IO** In the **Thickness** text field, type H\_Ch/10.
- II Click 🖷 Build Selected.

## Free Tetrahedral I

- I In the Mesh toolbar, click 🧄 Free Tetrahedral.
- 2 In the Settings window for Free Tetrahedral, locate the Domain Selection section.
- 3 From the Geometric entity level list, choose Domain.
- **4** Select Domains 4 and 8 only.

## 5 Click 🖷 Build Selected.



#### Boundary Layers 2

- I In the Model Builder window, under Component I (comp1)>Mesh I right-click Boundary Layers I and choose Duplicate.
- 2 In the Settings window for Boundary Layers, locate the Geometric Entity Selection section.
- **3** Click Clear Selection.
- **4** Select Domains 4 and 8 only.

#### Boundary Layer Properties

- I In the Model Builder window, expand the Boundary Layers 2 node, then click Boundary Layer Properties.
- **2** In the Settings window for Boundary Layer Properties, locate the Boundary Selection section.
- **3** Click **Clear Selection**.
- 4 Click **Paste Selection**.
- 5 In the Paste Selection dialog box, type 14-18, 24, 31, 38, 41, 43-45, 47, 49, 51, 52 in the Selection text field.
- 6 Click OK.

## Boundary Layers 2

In the Model Builder window, right-click Boundary Layers 2 and choose Build Selected.

## Free Triangular 1

- I In the Mesh toolbar, click  $\bigwedge$  Boundary and choose Free Triangular.
- 2 In the Settings window for Free Triangular, locate the Boundary Selection section.
- 3 From the Selection list, choose Cathode Current Collector.
- 4 Click 🖷 Build Selected.



# Swept 2

In the Mesh toolbar, click A Swept.

#### Distribution I

- I Right-click Swept 2 and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 Click Clear Selection.
- **4** Select Domain 3 only.
- 5 Locate the Distribution section. From the Distribution type list, choose Predefined.
- 6 In the Element ratio text field, type 2.
- 7 Select the **Reverse direction** check box.

## Distribution 2

- I In the Model Builder window, right-click Swept 2 and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 Click Clear Selection.
- **4** Select Domain 2 only.
- **5** Locate the **Distribution** section. In the **Number of elements** text field, type **2**.

#### Distribution 3

- I In the Model Builder window, under Component I (comp1)>Mesh 1>Swept 2 right-click Distribution I and choose Duplicate.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 Click Clear Selection.
- **4** Select Domain 1 only.
- 5 Locate the Distribution section. Clear the Reverse direction check box.
- 6 Click 📗 Build All.



# **STUDY I** The problem is now ready for solving.

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

## RESULTS

Electrode Potential with Respect to Ground (cd)

- I In the Model Builder window, under Results click Electrode Potential with Respect to Ground (cd).
- 2 In the Electrode Potential with Respect to Ground (cd) toolbar, click Inspect the potential plot. The plot should look as follows:

Multislice: Electric potential (V) Arrow Volume: Electrode current density vector



#### COMPONENT I (COMPI)

Now start with the second part of the tutorial which adds a reacting flow interface to the cathode side of the model, and couples the distribution of hydrogen and water vapor to the electrochemistry.

## ADD PHYSICS

- I 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 Chemical Species Transport>Reacting Flow in Porous Media> Transport of Concentrated Species.

- 4 Click Add to Component I in the window toolbar.
- 5 In the Home toolbar, click 🙀 Add Physics to close the Add Physics window.

## MULTIPHYSICS

Reacting Flow 1 (nirf1)

- I In the Model Builder window, under Component I (compl)>Multiphysics click Reacting Flow I (nirfl).
- 2 In the Settings window for Reacting Flow, locate the Temperature section.
- **3** In the *T* text field, type T.

#### MATERIALS

Note that a **Porous Material** node has been created automatically when adding an entry from the **Reacting Flow in Porous Media** branch of the **Add Physics** window.

Porous Material I (pmat1)

- I In the Model Builder window, expand the Component I (comp1)>Materials node, then click Porous Material I (pmat1).
- 2 In the Settings window for Porous Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Cathode.
- **4** Locate the **Porosity** section. In the  $\varepsilon_p$  text field, type por.
- **5** Locate the **Homogenized Properties** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Permeability	kappa_iso ; kappaii = kappa_iso,	kappa	m²	Basic
	kappaij = 0			

#### **BRINKMAN EQUATIONS (BR)**

- I In the Model Builder window, under Component I (compl) click Brinkman Equations (br).
- 2 Select Domains 3–8 only.
- 3 In the Settings window for Brinkman Equations, locate the Domain Selection section.
- 4 Click har Create Selection.
- 5 In the Create Selection dialog box, type Gas domains in the Selection name text field.
- 6 Click OK.

- 7 In the Settings window for Brinkman Equations, locate the Physical Model section.
- 8 Clear the Neglect inertial term (Stokes flow) check box.

#### Fluid Properties 1

- I In the Physics toolbar, click 🔚 Domains and choose Fluid Properties.
- 2 In the Settings window for Fluid Properties, locate the Domain Selection section.
- **3** From the Selection list, choose Channel Domains.

#### Inlet I

- I 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 **Inlet**.
- 4 Locate the Boundary Condition section. From the list, choose Mass flow.
- 5 Locate the Mass Flow section. In the *m* text field, type Mflux\_in.

#### Outlet I

- I 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 Outlet.
- 4 Locate the Pressure Conditions section. Select the Normal flow check box.

#### TRANSPORT OF CONCENTRATED SPECIES IN POROUS MEDIA (TCS)

- I In the Model Builder window, under Component I (comp1) click Transport of Concentrated Species in Porous Media (tcs).
- 2 In the Settings window for Transport of Concentrated Species in Porous Media, locate the Domain Selection section.
- 3 From the Selection list, choose Gas domains.
- 4 Locate the Transport Mechanisms section. From the Diffusion model list, choose Maxwell-Stefan.
- **5** Click to expand the **Dependent Variables** section. In the **Mass fractions** table, enter the following settings:

wH2 wH20

#### Species Molar Masses I

I In the Model Builder window, under Component I (compl)>

Transport of Concentrated Species in Porous Media (tcs) click Species Molar Masses I.

- 2 In the Settings window for Species Molar Masses, locate the Molar Mass section.
- 3 From the  $M_{\rm wH2}$  list, choose Molar mass (chem/H2).
- 4 From the  $M_{\rm wH2O}$  list, choose Molar mass (chem/H2O).

#### Fluid I

I In the Model Builder window, under Component I (compl)>

#### Transport of Concentrated Species in Porous Media (tcs)>Porous Medium 1 click Fluid 1.

- 2 In the Settings window for Fluid, locate the Diffusion section.
- **3** In the table, enter the following settings:

Species I	Species 2	Diffusivity	Diffusion coefficient (m^2/ s)
wH2	wH2O	Maxwell-Stefan diffusivity , H2-H2O (chem)	comp1.chem.D_H2_H2O

4 From the Effective diffusivity model list, choose Bruggeman model.

#### Porous Electrode Coupling 1

- I In the Physics toolbar, click 📄 Domains and choose Porous Electrode Coupling.
- **2** In the **Settings** window for **Porous Electrode Coupling**, locate the **Domain Selection** section.
- 3 From the Selection list, choose Cathode.

#### Reaction Coefficients I

- I In the Model Builder window, expand the Porous Electrode Coupling I node, then click Reaction Coefficients I.
- 2 In the Settings window for Reaction Coefficients, locate the Model Inputs section.
- **3** From the  $i_v$  list, choose Local current source, Porous Electrode Reaction I (cd/pcel/perl).
- **4** Locate the **Stoichiometric Coefficients** section. In the *n* text field, type **2**.
- **5** In the  $v_{wH2}$  text field, type 1.
- **6** In the  $v_{wH2O}$  text field, type -1.

#### Inflow I

- I In the Physics toolbar, click 🔚 Boundaries and choose Inflow.
- 2 In the Settings window for Inflow, locate the Boundary Selection section.

- **3** From the **Selection** list, choose **Inlet**.
- 4 Locate the Inflow section. From the Mixture specification list, choose Mass flow rates.
- **5** In the  $J_{\text{in.wH2O}}$  text field, type Mflux\_in.

## Outflow I

- I 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 **Outlet**.

Transport Properties 1

- I In the Physics toolbar, click 🔚 Domains and choose Transport Properties.
- 2 In the Settings window for Transport Properties, locate the Domain Selection section.
- **3** From the Selection list, choose Channel Domains.
- **4** Locate the **Diffusion** section. In the table, enter the following settings:

Species I	Species 2	Diffusivity	Diffusion coefficient (m^2/ s)
wH2	wH2O	Maxwell-Stefan diffusivity , H2-H2O (chem)	comp1.chem.D_H2_H2O

Initial Values 1

- I In the Model Builder window, click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** From the Mixture specification list, choose Mole fractions.
- 4 In the  $x_{0.\text{wH2O}}$  text field, type 0.95\*(1-x/(W\_cell\*stoich)).

#### CHEMISTRY - H2 AND H20 (CHEM)

- In the Model Builder window, under Component I (comp1) click Chemistry -H2 and H20 (chem).
- 2 In the Settings window for Chemistry, locate the Species Matching section.
- 3 From the Species solved for list, choose Transport of Concentrated Species in Porous Media.

Species	Туре	Mass fraction	Value (I)	From Thermodynamics
H2	Variable	wH2	Solved for	H2
H2O	Variable	wH2O	Solved for	H2O

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

## STUDY I

The concentration-dependent model is now ready for solving. Use a sequence of study steps, solving for the secondary current distribution first, then the flow, and finally the fully coupled problem. By solving for only one set of physics at a time in individual steps, suitable initial values automatically propagate to the final study step where the complete problem is solved.

Step 1: Current Distribution Initialization

- I In the Model Builder window, under Study I click Step I: Current Distribution Initialization.
- **2** In the Settings window for Current Distribution Initialization, locate the **Physics and Variables Selection** section.
- **3** In the table, clear the **Solve for** check boxes for **Brinkman Equations (br)** and **Transport of Concentrated Species in Porous Media (tcs)**.
- 4 In the table, clear the Solve for check box for Reacting Flow I (nirfl).

Step 2: Stationary

- I In the Model Builder window, click Step 2: Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- **3** In the table, enter the following settings:

Physics interface	Solve for	Equation form
Secondary Current Distribution (cd)	$\checkmark$	Automatic (Stationary)
Brinkman Equations (br)		Automatic (Stationary)
Transport of Concentrated Species in Porous Media (tcs)		Automatic (Stationary)

4 In the table, clear the Solve for check box for Reacting Flow I (nirfl).

## Stationary 2

I In the Study toolbar, click 🔁 Study Steps and choose Stationary>Stationary.

- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- **3** In the table, clear the Solve for check boxes for Secondary Current Distribution (cd) and Transport of Concentrated Species in Porous Media (tcs).
- 4 In the table, clear the Solve for check box for Reacting Flow I (nirfl).

#### Stationary 3

I In the Study toolbar, click 🔁 Study Steps and choose Stationary>Stationary.

Remove the old study sequence and generate a new one.

## Solver Configurations

In the Model Builder window, under Study I right-click Solver Configurations and choose Delete Configurations.

#### Solution 1 (soll)

- I In the Study toolbar, click **The Show Default Solver**.
- 2 In the Model Builder window, expand the Solution I (soll) node.
- 3 In the Model Builder window, expand the Study I>Solver Configurations> Solution I (soll)>Stationary Solver 4 node.
- 4 Right-click Stationary Solver 4 and choose Fully Coupled.
- **5** In the **Study** toolbar, click **= Compute**.

The problem should solve in about two minutes.

## RESULTS

Start the postprocessing of the solution by inspecting and polishing the default plot for the velocity field.

Slice

I In the Model Builder window, expand the Results>Velocity (br) node, then click Slice.

- 2 In the Settings window for Slice, locate the Plane Data section.
- 3 From the Plane list, choose xy-planes.
- 4 From the Entry method list, choose Coordinates.
- **5** In the **z-coordinates** text field, type H\_cell-H\_ch/2.
- 6 In the Velocity (br) toolbar, click 💽 Plot.

#### Streamline 1

I In the Model Builder window, right-click Velocity (br) and choose Streamline.

- 2 In the Settings window for Streamline, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (comp1)>
  Brinkman Equations>Velocity and pressure>u,v,w Velocity field.
- 3 Locate the Selection section. From the Selection list, choose Inlet.
- 4 Locate the Coloring and Style section. Find the Point style subsection. From the Type list, choose Arrow.
- **5** From the **Arrow distribution** list, choose **Equal inverse time**.
- 6 From the Color list, choose Black.
- 7 In the Velocity (br) toolbar, click **O** Plot.





#### Density

The density of the gas mixture will change as water is replaced by hydrogen in the gas stream. Plot the density as follows:

- I In the Home toolbar, click 🚛 Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Density in the Label text field.

#### Surface 1

I Right-click **Density** and choose **Surface**.

- 2 In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
  Brinkman Equations>Material properties>br.rho Density kg/m<sup>3</sup>.
- **3** In the **Density** toolbar, click **I** Plot.



## Viscosity

Also, the viscosity will change in the gas stream.

- I In the Home toolbar, click 🚛 Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Viscosity in the Label text field.

#### Surface 1

- I Right-click **Viscosity** and choose **Surface**.
- In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
  Brinkman Equations>Material properties>br.mu Dynamic viscosity Pa·s.
- **3** In the **Viscosity** toolbar, click **I** Plot.



## Concentration, H2, Surface (tcs)

Default plots where created for the hydrogen and water concentrations.



Concentration, H2O, Surface (tcs)

Species H2O: Molar concentration (mol/m<sup>3</sup>)



#### Molar Fraction and Flux, H2

Create a plot for the hydrogen molar fraction and flux as follows:

- I In the Home toolbar, click 🚛 Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Molar Fraction and Flux, H2 in the Label text field.
- 3 Locate the Plot Settings section. Clear the Plot dataset edges check box.

#### Streamline 1

- I Right-click Molar Fraction and Flux, H2 and choose Streamline.
- 2 In the Settings window for Streamline, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Transport of Concentrated Species in Porous Media>Species wH2>Fluxes>tcs.tflux\_wH2x, ...,tcs.tflux\_wH2z - Total flux.
- 3 Locate the Streamline Positioning section. In the Number text field, type 30.

- 4 Locate the Selection section. From the Selection list, choose Outlet.
- 5 Locate the Coloring and Style section. Find the Point style subsection. From the Type list, choose Arrow.
- 6 From the Arrow distribution list, choose Equal inverse time.
- 7 From the Color list, choose Black.

#### Selection 1

- 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 Channel Domains.

Volume 1

- I In the Model Builder window, right-click Molar Fraction and Flux, H2 and choose Volume.
- In the Settings window for Volume, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
  Transport of Concentrated Species in Porous Media>Species wH2>tcs.x\_wH2 Mole fraction.

Selection 1

- I Right-click Volume I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.
- **3** From the **Selection** list, choose **Cathode**.
- **4** Click the **Show Grid** button in the **Graphics** toolbar.

## 5 In the Molar Fraction and Flux, H2 toolbar, click 💿 Plot.

Streamline: Total flux Volume: Mole fraction (1)



#### Cross-Sectional Electrolyte Current Density

Finally, plot the current distribution across the electrolyte layer as follows:

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

#### Slice 1

- I Right-click Cross-Sectional Electrolyte Current Density and choose Slice.
- 2 In the Settings window for Slice, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (comp1)> Secondary Current Distribution>Electrolyte current density vector - A/m<sup>2</sup>>cd.llz - Electrolyte current density vector, z-component.
- 3 Locate the Plane Data section. From the Plane list, choose xy-planes.
- 4 From the Entry method list, choose Coordinates.
- 5 In the z-coordinates text field, type H\_gde+H\_el/2.



Appendix —Geometry 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 Click **M** Done.

## GLOBAL DEFINITIONS

## **Geometry Parameters**

- 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.

- 3 Locate the Parameters section. Click 📂 Load from File.
- 4 Browse to the model's Application Libraries folder and double-click the file soec\_thermodynamics\_geom\_parameters.txt.

## GEOMETRY I

#### Anode

- I In the **Geometry** toolbar, click 🗍 **Block**.
- 2 In the Settings window for Block, type Anode in the Label text field.
- 3 Locate the Size and Shape section. In the Width text field, type W\_cell.
- 4 In the **Depth** text field, type D\_cell.
- 5 In the **Height** text field, type H\_gde.
- **6** Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

## Electrolyte

- I Right-click Anode and choose Duplicate.
- 2 In the Settings window for Block, type Electrolyte in the Label text field.
- 3 Locate the Position section. In the z text field, type H\_gde.

## Cathode

- I Right-click Electrolyte and choose Duplicate.
- 2 In the Settings window for Block, type Cathode in the Label text field.
- **3** Locate the **Position** section. In the **z** text field, type H\_gde+H\_e1.

Work Plane I (wp1)

- I In the Geometry toolbar, click 🖶 Work Plane.
- 2 In the Settings window for Work Plane, locate the Plane Definition section.
- 3 In the z-coordinate text field, type H\_cell-H\_ch.

Work Plane I (wpI)>Plane Geometry

In the Model Builder window, click Plane Geometry.

Work Plane I (wp1)>Rectangle I (r1)

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type W\_ch.
- 4 In the **Height** text field, type N\_ch\*(W\_ch+W\_rib).

- 5 Locate the **Position** section. In the **xw** text field, type W\_rib/2.
- 6 In the yw text field, type W\_rib/2.

Work Plane I (wp1)>Rectangle 2 (r2)

- I Right-click Component I (comp1)>Geometry I>Work Plane I (wp1)>Plane Geometry> Rectangle I (r1) and choose Duplicate.
- 2 In the Settings window for Rectangle, locate the Position section.
- 3 In the **xw** text field, type W\_rib/2+L\_ch+W\_ch.
- 4 In the **yw** text field, type -W\_rib/2.

Work Plane 1 (wp1)>Rectangle 3 (r3)

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type L\_Ch.
- 4 In the **Height** text field, type W\_ch.
- 5 Locate the **Position** section. In the **xw** text field, type W\_rib/2+W\_ch.
- 6 In the **yw** text field, type W\_rib/2.

Work Plane I (wp1)>Array I (arr1)

- I In the Work Plane toolbar, click 💭 Transforms and choose Array.
- 2 Select the object r3 only.
- 3 In the Settings window for Array, locate the Size section.
- **4** In the **yw size** text field, type N\_ch.
- 5 Locate the Displacement section. In the yw text field, type W\_ch+W\_rib.
- 6 In the Work Plane toolbar, click 🟢 Build All.

#### Channel Domains

- I In the Model Builder window, right-click Geometry I and choose Extrude.
- 2 In the Settings window for Extrude, type Channel Domains in the Label text field.
- 3 Locate the **Distances** section. In the table, enter the following settings:

#### Distances (m)

H\_ch

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

## Form Union (fin)

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

#### Inlet

- I In the Geometry toolbar, click 🝖 Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Inlet 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 19 only.

#### Outlet

- I In the Geometry toolbar, click 🔓 Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Outlet 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 42 only.

## Cathode Current Collector

- I In the Geometry toolbar, click 🝖 Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Cathode Current Collector 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 10, 26, 33, and 40 only.

## Anode Current Collector

- I In the Geometry toolbar, click 🐚 Selections and choose Explicit Selection.
- 2 In the Settings window for Explicit Selection, type Anode Current Collector 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 3 only.