

Polymer Electrolyte Membrane Electrolyzer

Introduction

In a polymer electrolyte membrane electrolyzer cell (PEMEC), the two electrode compartments are separated by a polymer membrane, coated by porous gas diffusion electrodes. Liquid water is fed to the anode side, forming oxygen gas on the anode side and hydrogen gas on the cathode side.

The respective designs of the flow field patterns are important in order to obtain a uniform distribution of flow, in combination with low pressure drops, during operation.

In this example, the mixture model is used to model the two-phase fluid dynamics on the anode side of a PEMEC.

The model geometry and operating condition were taken from Ref. 1, with added gravity and zero tangential (no slip) conditions for all channel walls. The single-phase results for a 60 ml/min flow rate were verified versus Ref. 2.

Model Definition

Figure 1 shows the model geometry. From the circular inlet (located at the top boundary of the cylinder), liquid water is led into a manifold, which in turn distributes the flow over 23 channels. Oxygen gas is produced at the anode electrode, located below the

23 channels. The two-phase oxygen gas/liquid water mixture exits the cell through the exit manifold.

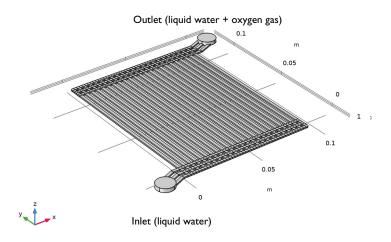


Figure 1: Geometry of the anode flow field.

The model is set up using the Mixture Model, Laminar Flow interface, with liquid water defining the continuous phase and the oxygen gas bubbles the dispersed phase. Incompressible and isothermal conditions are assumed.

The inlet flow rate of liquid water is 260 ml/min. This is defined using an Inlet boundary condition.

At the electrode surface/channel boundaries liquid water is consumed, and oxygen gas is produced according to

$$2H_2O(l) \rightarrow O_2(g) + 4H^+ + 4e^-$$

The protons are transported through the polymer membrane, dividing the two electrode compartments, over to the cathode side of the electrolyzer cell. In addition to the oxygen gas produced, there is hence a net mass outflux due to the proton transport at the electrode surface/channel boundaries.

The combined oxygen gas production/total mass outflux is defined using an Inlet boundary condition node, assuming a total oxygen production of 5 mg/s.

A pressure condition is used at the outlet boundaries. No-slip wall conditions are set for all other boundaries.

Finally, the buoyancy effects due to gravity are included in the model using a Gravity node, with the gravity vector pointing downward in the z direction.

The model is solved in two steps. First the single-phase (pure liquid water, no oxygen production) stationary flow is computed using a stationary solver. This solution is then used as initial conditions for a 10 s time-dependent simulation, where the oxygen production is ramped up to full production from 0 during the first second.

Results and Discussion

Figure 2 shows a slice plot of the mass-averaged velocity magnitude.

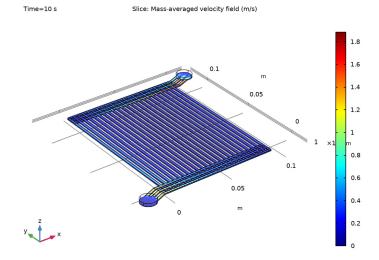


Figure 2: Slice plot of the velocity magnitude at t = 10 s.

The highest velocities are found in the inlet/outlet manifold channels. A good practice when assuming laminar flow is to check the Reynolds number of the computed results.

The Reynolds number Re is defined as

$$Re = \frac{\rho u D}{u}$$

where ρ is the density, u the velocity, μ the dynamic viscosity and D the characteristic length.

Given that the width of the channels, 2 mm, is larger than the height, 0.889 mm, we choose the doubled height (an approximation valid for a wide duct) as the characteristic length D. At the inlet, where we have pure water and the density-to-dynamic viscosity is the highest, the maximum velocity is about 1.3 m/s.

The Reynolds number for the inlet manifold channels becomes (all parameter values using the corresponding SI units)

$$Re = \frac{\rho uD}{\mu} \approx \frac{10^3 \times 1.3 \times (2 \times 0.889 \times 10^{-3})}{10^{-3}} \approx 2300$$

A similar calculation for the outlet renders lower values. Reynolds numbers in the range of 2300 and lower, indicates that turbulence should not have to be considered for the given geometry and flow rates.

Figure 3 shows the gas volume fraction due to evolved oxygen in the cell at 10 s.

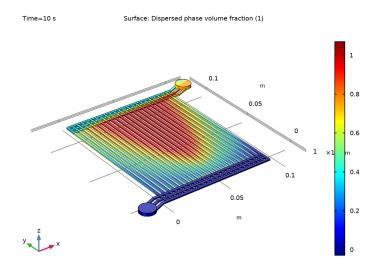


Figure 3: Gas volume fraction in the cell at t = 10 s.

The gas volume fraction approaches 100% at the end of the electrode flow channels.

Figure 4 and Figure 5 show the pressure drop in the anode flow field at t = 0 and t = 10 s, respectively. The pressure drop is significantly reduced as a result of the oxygen gas production.

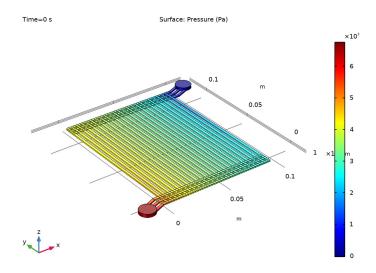


Figure 4: Pressure drop in the cell at t = 0 s.

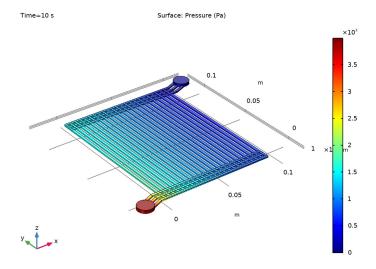


Figure 5: Pressure drop in the cell at t = 10 s.

Finally, shows the velocity magnitudes at half the length (y direction) and half in the height (z direction) of the electrode channels at various times. This plot is important since it indicates the uniformness of the flow distribution over the individual channels. As can be seen, the flow distribution not particularly uniform for pure water (t=0 s). However, the distribution becomes somewhat more uniform at two-phase conditions (t=10 s) due to the right-most channels lowering their velocities. It is also seen that the flow field distribution does not change significantly between 2 s and 10 s. This indicates that a stationary flow

distribution is established in less than a second after full oxygen production has been reached at 1 s.

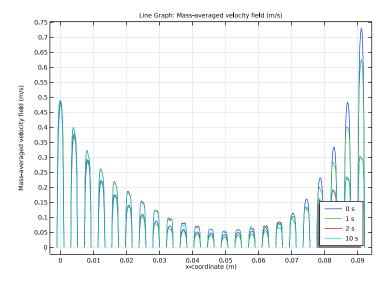


Figure 6: Individual channel velocities at various times.

Notes About the COMSOL Implementation

The local oxygen flux is multiplied by a smoothed step function, going from 1 to 0 when the volume fraction of oxygen approaches 1. The smoothing improves convergence.

Reference

- 1. J. Nie and Y. Chen, "Numerical modeling of three-dimensional two-phase gas-liquid flow in the field plate of a PEM electrolysis cell," Int. J. Hydrogen Energy, vol. 35, pp. 3183-3197, 2010.
- 2. J. Nie, Y. Chen, S. Cohen, B. Carter, and R. Boehm, "Numerical and experimental study of three-dimensional fluid flow in the bipolar plate of a PEM electrolysis cell," Int. J. Thermal Sciences, vol. 48, pp. 1914-1922, 2009.

Application Library path: CFD Module/Multiphase Flow/pem electrolyzer

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

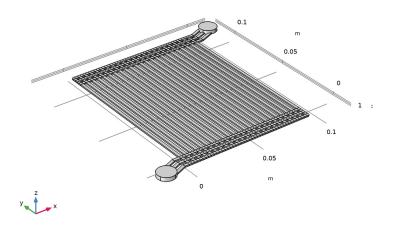
- I In the Model Wizard window, click **3D**.
- 2 In the Select Physics tree, select Fluid Flow>Multiphase Flow>Mixture Model> Mixture Model, Laminar Flow (mm).
- 3 Click Add.
- 4 Click 🗪 Study.
- 5 In the Select Study tree, select General Studies>Time Dependent.
- 6 Click **Done**.

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 with the following steps.

- I In the Geometry toolbar, click Insert Sequence.
- 2 Browse to the model's Application Libraries folder and double-click the file pem_electrolyzer_geom_sequence.mph.

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



GLOBAL DEFINITIONS

Use the parameterization to reduce the number of channels and the channel lengths when setting up the model. It is often a good practice to start a modeling project on a reduced geometry size (or dimension). This saves time and computational resources while troubleshooting.

Parameters 1

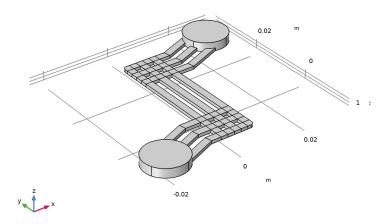
- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
N_ch	3	3	Number of electrode channels
L_ch	118*h_a/5	0.02098 m	Electrode channel lenghts

GEOMETRY I

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

2 Click the Zoom Extents button in the Graphics toolbar.



GLOBAL DEFINITIONS

Load some more physics parameters and variables from text files. Note that parameters and variables defining the oxygen and water flows are scaled with the geometric parameters.

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 pem_electrolyzer_parameters.txt.

DEFINITIONS

Variables 1

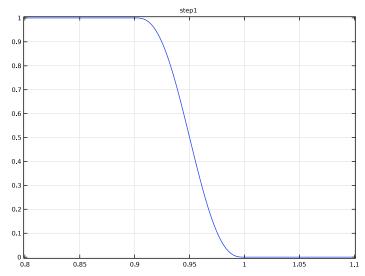
- I In the Model Builder window, under Component I (compl) right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, locate the Variables section.
- 3 Click Load from File.

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

The variables make use of a step and a ramp function. These have not yet been defined, hence some of the loaded variable expressions are marked in orange. Define the missing functions as follows:

Step I (step I)

- I In the Home toolbar, click f(x) Functions and choose Local>Step.
- 2 In the Settings window for Step, locate the Parameters section.
- 3 In the Location text field, type 0.95.
- **4** In the **From** text field, type 1.
- 5 In the To text field, type 0.
- 6 Click to expand the Smoothing section. In the Size of transition zone text field, type 0.1.
- 7 Click **Tollick** Plot.

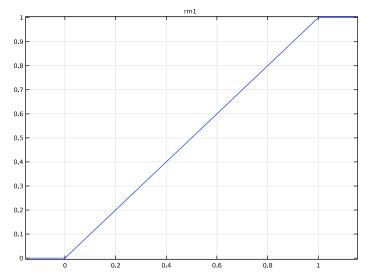


The step function is used to set the oxygen flux to zero locally when the gas volume fraction approaches 1. Smoothing is important in order to avoid discrete jumps in the flux. We will decrease the smoothing later when solving for the full model.

Ramb I (rm I)

- I In the Home toolbar, click f(X) Functions and choose Local>Ramp.
- 2 In the Settings window for Ramp, locate the Parameters section.

- **3** Select the **Cutoff** check box.
- 4 Click Plot.



The ramp function is used to ramp up the oxygen flux from zero when the timedependent solver starts. This shortens the computational time.

DEFINITIONS

In the Model Builder window, collapse the Component I (compl)>Definitions node.

ADD MATERIAL

- I In the Home toolbar, click **Add Material** to open the Add Material window. Add liquid water and oxygen gas from the Material Library. Note that the order is important - Add water first.
- 2 Go to the Add Material window.
- 3 In the tree, select Built-in>Water, liquid.
- 4 Click Add to Component I (compl).
- 5 In the tree, select Liquids and Gases>Gases>Oxygen.
- 6 Click Add to Component I (compl).

7 In the Home toolbar, click 👯 Add Material to close the Add Material window.

The oxygen node under Materials should now have a small warning symbol in the Model Builder Tree. This is because the selection of this node is zero. This is expected at this point.

Since the water node was added first, it got assigned to all domains by default.

MIXTURE MODEL, LAMINAR FLOW (MM)

- I In the Settings window for Mixture Model, Laminar Flow, locate the Physical Model section.
- 2 From the Dispersed phase list, choose Liquid droplets/bubbles.
- 3 From the Slip model list, choose Schiller-Naumann. In this model, water is the continuous phase, and oxygen the dispersed phase.

Mixture Properties 1

- I In the Model Builder window, under Component I (compl)>Mixture Model, Laminar Flow (mm) click Mixture Properties I.
- 2 In the Settings window for Mixture Properties, locate the Materials section.
- 3 From the Continuous phase list, choose Water, liquid (mat I).
- 4 From the Dispersed phase list, choose Oxygen (mat2).
- 5 Locate the Dispersed Phase Properties section. From the ρ_d list, choose User defined. In the associated text field, type rho02.
- **6** In the d_d text field, type D_bubbles.
- 7 Locate the Mixture Model section. From the Mixture viscosity model list, choose Volume averaged.

Inlet - Liauid Water

- I In the Physics toolbar, click **Boundaries** and choose **Inlet**.
- 2 In the Settings window for Inlet, type Inlet Liquid Water in the Label text field.
- 3 Locate the Boundary Selection section. From the Selection list, choose Inlet.
- **4** Locate the **Velocity** section. In the J_0 text field, type Flow_rate/(pi*R_in^2).

Inlet - Electrode Surface Oxygen Evolution

- I In the Physics toolbar, click **Boundaries** and choose **Inlet**.
- 2 In the Settings window for Inlet, type Inlet Electrode Surface Oxygen Evolution in the Label text field.
- 3 Locate the Boundary Selection section. From the Selection list, choose Electrode Surface.

- **4** Locate the **Velocity** section. In the J_0 text field, type mixture_flow.
- 5 Locate the Dispersed Phase Boundary Condition section. From the Dispersed phase boundary condition list, choose Dispersed phase flux.
- **6** In the $N_{\rm od}$ text field, type disp_flow.

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.

Gravity I

- I In the **Physics** toolbar, click **Domains** and choose **Gravity**. The cell is oriented so that the *z* direction points upward.
- 2 In the Settings window for Gravity, locate the Domain Selection section.
- 3 From the Selection list, choose All domains.
- **4** Locate the **Gravity** section. Specify the **g** vector as

0	x
0	у
-g_const	z

MESH I

Manual meshing is required for a geometry of this complexity. Use a swept mesh along the electrode channels, and free tetraheadal meshing for the remaining domains.

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 2 In the Settings window for Mesh, locate the Mesh Settings section.
- 3 From the Sequence type list, choose Physics-controlled mesh.

Swebt I

Right-click Component I (compl)>Mesh I and choose Swept.

Size

- I In the Settings window for Size, locate the Element Size section.
- 2 From the Predefined list, choose Finer.

Swept 1

I In the Model Builder window, click Swept I.

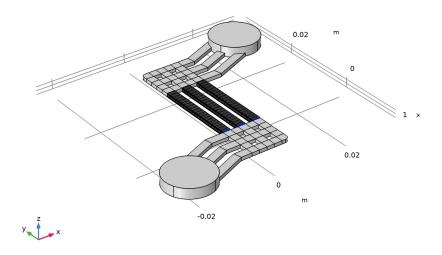
- 2 In the Settings window for Swept, locate the Domain Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Channels Above Electrode Surface.
- 5 Click to expand the Source Faces section. From the Selection list, choose Inlets to Electrode Channels .
- 6 Click to expand the **Destination Faces** section. From the **Selection** list, choose **Outlets from Electrode Channels.**

Distribution 1

- 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 Channels Above Electrode Surface.
- 4 Locate the Distribution section. In the Number of elements text field, type floor (L ch/ $(0.5*w_ch)$.

Size 1

- I Right-click Swept I and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** Click the **Custom** button.
- 4 Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Boundary.
- 5 From the Selection list, choose Inlets to Electrode Channels .
- 6 Locate the Element Size Parameters section. Select the Maximum element size check box.
- 7 In the associated text field, type h a/4.

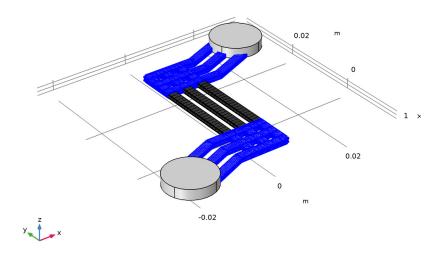


Free Tetrahedral I

- I In the Model Builder window, right-click Mesh I and choose 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 From the Selection list, choose Manifolds.
- 5 Click to expand the Scale Geometry section. In the z-direction scale text field, type 2.

Size 1

- I Right-click Free Tetrahedral I and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** Click the **Custom** button.
- 4 Locate the Element Size Parameters section. Select the Maximum element size check box.
- 5 In the associated text field, type w_ch/4.

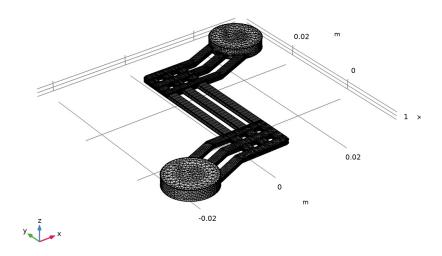


Free Tetrahedral 2

- I In the Model Builder window, right-click Mesh I and choose Free Tetrahedral.
- 2 In the Settings window for Free Tetrahedral, locate the Scale Geometry section.
- 3 In the z-direction scale text field, type 2.

Size 1

- I Right-click Free Tetrahedral 2 and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** Click the **Custom** button.
- 4 Locate the Element Size Parameters section. Select the Maximum element size check box.
- **5** In the associated text field, type h_a.



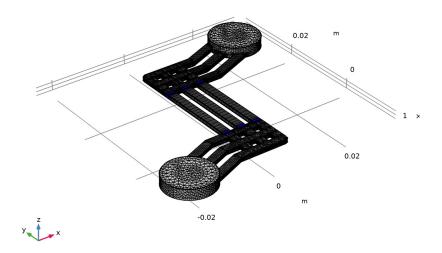
Boundary Layers 1

Add boundary layer meshing to resolve steep velocity gradients at the inlet and outlet regions to the electrode channels and along the walls..

- I In the Model Builder window, right-click Mesh I and choose 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 Channels Above Electrode Surface.

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 Inlets and Outlets to Electrode Channels.
- 4 Locate the Boundary Layer Properties section. In the Number of boundary layers text field, type 4.
- 5 From the Thickness of first layer list, choose Manual.
- 6 In the Thickness text field, type w_ch/15.

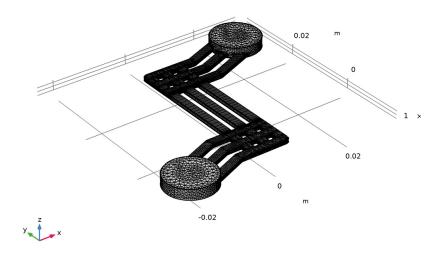


Boundary Layers 2

- I In the Model Builder window, right-click Mesh I and choose 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 Electrode Channels and Manifolds.

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 Layer Properties section.
- 3 In the Number of boundary layers text field, type 2.
- 4 From the Thickness of first layer list, choose Manual.
- 5 In the Thickness text field, type h_a/8.



STUDY I

The problem is now ready for solving. Add a Stationary study step to first solve for the velocity and pressure fields for pure liquid water. This solution will then be used as initial values for the time-dependent simulation.

Stationary

- I In the Study toolbar, click study Steps and choose Stationary>Stationary.
- 2 Right-click Study I>Step 2: Stationary and choose Move Up.

Step 2: Time Dependent

- I In the Model Builder window, click Step 2: Time Dependent.
- 2 In the Settings window for Time Dependent, locate the Study Settings section.
- 3 In the Output times text field, type 0 1 2 10.

Solution I (soll)

- I In the Study toolbar, click Show Default Solver.
- 2 In the Model Builder window, expand the Solution I (soll) node, then click Dependent Variables I.
- 3 In the Settings window for Dependent Variables, locate the General section.

- 4 From the Defined by study step list, choose User defined.
- 5 In the Model Builder window, expand the Study I>Solver Configurations> Solution I (soll)>Dependent Variables I node, then click Volume fraction, dispersed phase (compl.phid).
- 6 In the Settings window for Field, locate the General section.
- 7 Clear the Solve for this field check box.
- 8 In the Model Builder window, click Squared slip velocity (compl.slipvel).
- **9** In the **Settings** window for **Field**, locate the **General** section.
- 10 Clear the Solve for this field check box.

By using manual scales for the volume fraction of the dispersed phase and the slip velocity, the computation time can be reduced. (Suitable values for the slip velocity was derived by solving the problem using automatic scales first, and then evaluating the solution. This is another reason for why it makes sense to start with a small geometry first.)

- II In the Model Builder window, expand the Study I>Solver Configurations> Solution I (soll)>Dependent Variables 2 node, then click Volume fraction, dispersed phase (compl.phid).
- 12 In the Settings window for Field, locate the Scaling section.
- 13 From the Method list, choose Manual.
- 14 In the Model Builder window, click Squared slip velocity (compl.slipvel).
- **15** In the **Settings** window for **Field**, locate the **Scaling** section.
- 16 From the Method list, choose Manual.
- 17 In the Scale text field, type 1e-4.
- **18** In the **Model Builder** window, click **Study 1**.
- 19 In the Settings window for Study, locate the Study Settings section.
- **20** Clear the **Generate default plots** check box.
- 21 In the Study toolbar, click **Compute**.

The model should take about half an hour to solve.

RESULTS

Create plots for the pressure, velocity and gas volume fraction as follows:

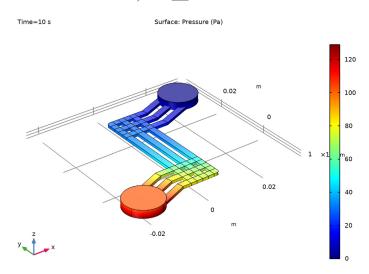
Pressure

I In the Home toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the Settings window for 3D Plot Group, type Pressure in the Label text field.

Surface I

- I Right-click Pressure 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)>Mixture Model, Laminar Flow>VelAndPressure>p - Pressure - Pa.
- 3 In the Pressure toolbar, click Plot.



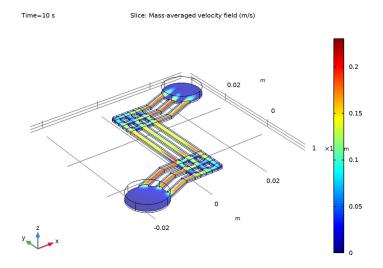
Velocity

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

Slice 1

- I Right-click **Velocity** 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 (compl)>Mixture Model, Laminar Flow>VelAndPressure>mm.U - Mass-averaged velocity field - m/s.
- 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 a/2.

6 In the Velocity toolbar, click Plot.



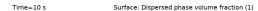
Gas Volume Fraction

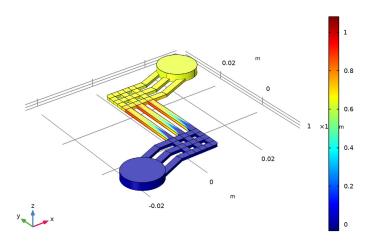
- I In the Home toolbar, click In Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Gas Volume Fraction in the Label text field.

Surface I

I Right-click Gas Volume Fraction and choose Surface.

2 In the Gas Volume Fraction toolbar, click Plot.





Cut Line 3D I

- I In the Results toolbar, click Cut Line 3D.
- 2 In the Settings window for Cut Line 3D, locate the Line Data section.
- 3 In row Point I, set x to -w_ch/2.
- 4 In row Point I, set y to L_ch/2.
- 5 In row Point 1, set z to h a/2.
- 6 In row Point 2, set x to N ch*w ch*2-3*w ch/2.
- 7 In row Point 2, set y to L_ch/2.
- 8 In row Point 2, set z to h a/2.

Velocity in Electrode Channels

- I In the Results toolbar, click \(\subseteq ID \) Plot Group.
- 2 In the Settings window for ID Plot Group, type Velocity in Electrode Channels in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Cut Line 3D 1.

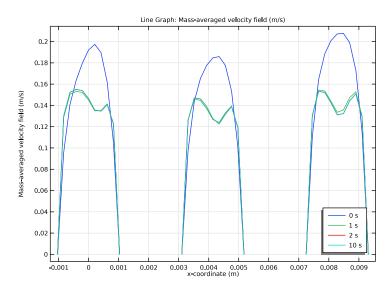
Line Graph I

I Right-click Velocity in Electrode Channels and choose Line Graph.

- 2 In the Settings window for Line Graph, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (compl)>Mixture Model, Laminar Flow>VelAndPressure>mm.U - Mass-averaged velocity field - m/s.
- 3 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- **4** In the **Expression** text field, type x.
- **5** Click to expand the **Legends** section. Select the **Show legends** check box.

Velocity in Electrode Channels

- I In the Model Builder window, click Velocity in Electrode Channels.
- 2 In the Settings window for ID Plot Group, locate the Legend section.
- 3 From the Position list, choose Lower right.
- 4 In the Velocity in Electrode Channels toolbar, click **1** Plot.



GLOBAL DEFINITIONS

Now model the full geometry. Go back and set the number of channels and the cell length to their original values.

Parameters 1

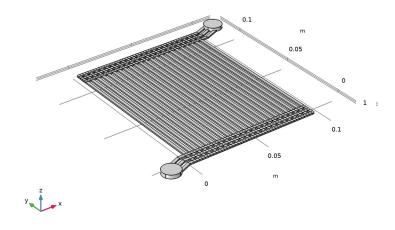
- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
N_ch	23	23	Number of electrode channels
L_ch	118*h_a	0.1049 m	Electrode channel lenghts

GEOMETRY I

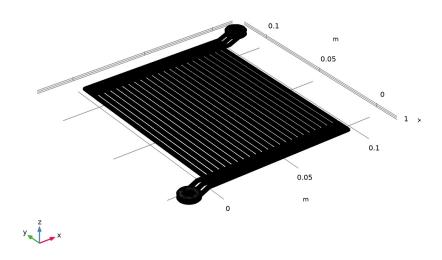
- I In the Home toolbar, click | Build All.
- 2 Click the Zoom Extents button in the Graphics toolbar.



MESH I

Inspect the mesh after the geometry change.

In the Model Builder window, under Component I (compl) right-click Mesh I and choose **Build All.**



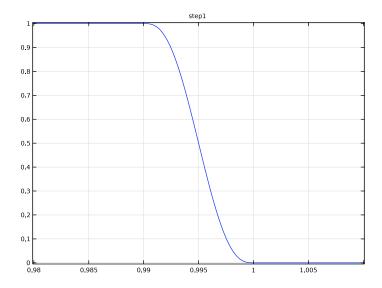
DEFINITIONS

Step I (step I)

Decrease the smoothing of the step function.

- I In the Model Builder window, under Component I (compl)>Definitions click Step I (step I).
- 2 In the Settings window for Step, locate the Parameters section.
- 3 In the Location text field, type 0.995.
- 4 Locate the Smoothing section. In the Size of transition zone text field, type 0.01.

5 Click Plot.



STUDY I

Solution I (soll)

Before solving, make a copy of the solution for the small geometry to keep it for future reference.

I In the Model Builder window, under Study I>Solver Configurations right-click Solution I (soll) and choose Solution>Copy.

Solution - Small Geometry

- In the Model Builder window, under Study 1>Solver Configurations click Solution 1 -Copy 1 (sol3).
- 2 In the **Settings** window for **Solution**, type Solution Small Geometry in the **Label** text field.

Solver Configurations

Reset the solver sequence in order to obtain the default solver for the new problem size.

Solution I (soll)

- I In the Model Builder window, right-click Solver Configurations and choose Reset Solver to Default.
- 2 In the Settings window for Dependent Variables, locate the General section.

- 3 From the Defined by study step list, choose User defined.
- 4 In the Model Builder window, expand the Study I>Solver Configurations> Solution I (soll)>Dependent Variables I node, then click Volume fraction, dispersed phase (compl.phid).
- 5 In the Settings window for Field, locate the General section.
- 6 Clear the Solve for this field check box.
- 7 In the Model Builder window, click Squared slip velocity (compl.slipvel).
- 8 In the Settings window for Field, locate the General section.
- **9** Clear the **Solve for this field** check box.
- 10 In the Model Builder window, expand the Study 1>Solver Configurations> Solution I (soll)>Dependent Variables 2 node, then click Volume fraction, dispersed phase (compl.phid).
- II In the Settings window for Field, locate the Scaling section.
- 12 From the Method list, choose Manual.
- 13 In the Model Builder window, click Squared slip velocity (compl.slipvel).
- 14 In the Settings window for Field, locate the Scaling section.
- 15 From the Method list, choose Manual.
- 16 In the Scale text field, type 1e-5.

Step 2: Time Dependent

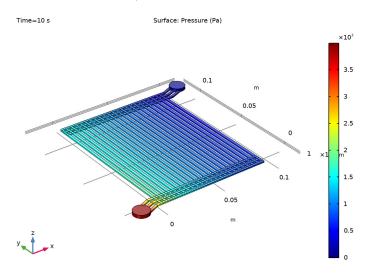
The problem will take several hours to solve. Plot the gas volume fraction while solving in order to monitor the solution process.

- I In the Model Builder window, click Step 2: Time Dependent.
- 2 In the Settings window for Time Dependent, click to expand the Results While Solving section.
- **3** Select the **Plot** check box.
- 4 From the Plot group list, choose Gas Volume Fraction.
- 5 From the Update at list, choose Time steps taken by solver. The full problem is now ready for solving.
- 6 In the Home toolbar, click **Compute**.

RESULTS

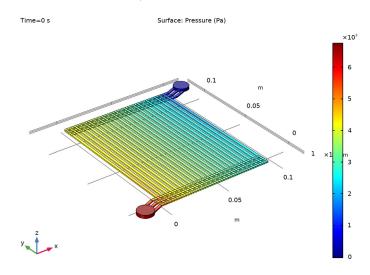
Pressure

I In the Pressure toolbar, click Plot.



- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Time (s) list, choose 0.

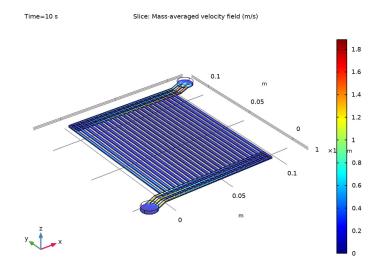
4 In the Pressure toolbar, click Plot.



5 From the **Time (s)** list, choose **10**.

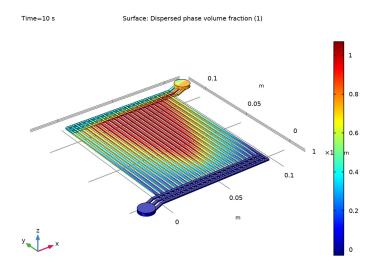
Velocity

- I In the Model Builder window, click Velocity.
- 2 In the **Velocity** toolbar, click **Plot**.



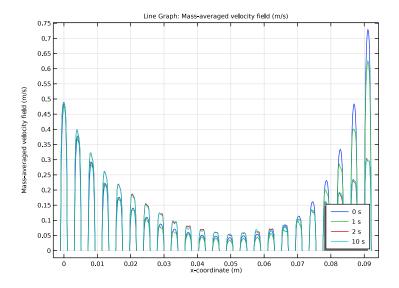
Gas Volume Fraction

- I In the Model Builder window, click Gas Volume Fraction.
- 2 In the Gas Volume Fraction toolbar, click Plot.



Velocity in Electrode Channels

I In the Model Builder window, click Velocity in Electrode Channels.



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 **1** 3D.
- 2 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 pem_electrolyzer_geom_sequence_parameters.txt.

GEOMETRY I

Work Plane I (wpl) In the Geometry toolbar, click Swork Plane. Work Plane I (wp I)>Plane Geometry In the Model Builder window, click Plane Geometry. Work Plane I (wpl)>Circle I (cl) I In the Work Plane toolbar, click • Circle. 2 In the Settings window for Circle, locate the Size and Shape section. 3 In the Radius text field, type R_in. 4 Click | Build Selected. 5 Click the Zoom Extents button in the Graphics toolbar. Work Plane I (wp I)>Rectangle I (r I) 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 inout*3/4. 4 In the **Height** text field, type w_ch. 5 Locate the Position section. In the yw text field, type -w ch*2.5. 6 Click | Build Selected. Work Plane I (wp I)>Rectangle 2 (r2) 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 inout*1/4. 4 In the **Height** text field, type w ch. **5** Locate the **Position** section. In the **xw** text field, type L_inout*3/4. 6 In the yw text field, type -w ch*2.5. 7 Click Pauld Selected. 8 Click the **Zoom Extents** button in the **Graphics** toolbar. Work Plane I (wpl)>Array I (arrl) I In the Work Plane toolbar, click Transforms and choose Array. 2 Select the objects r1 and r2 only.

3 In the Settings window for Array, locate the Size section.

- 4 In the yw size text field, type 3.
- 5 Locate the Displacement section. In the yw text field, type 2*w_ch.
- 6 Click Pauld Selected.

Work Plane I (wpl)>Polygon I (poll)

- I In the Work Plane toolbar, click / Polygon.
- 2 In the Settings window for Polygon, locate the Coordinates section.
- **3** In the table, enter the following settings:

xw (m)	yw (m)
L_inout*3/4	2*w_ch*1.25
L_inout*3/4	-2*w_ch*1.25
L_inout*3/4-5*w_ch*tan(ang_inout/2)	-2*w_ch*1.25

4 Click | Build Selected.

Work Plane I (wbl)>Difference I (difl)

- I In the Work Plane toolbar, click Booleans and Partitions and choose Difference.
- 2 Select the object arr1(1,3,1) only.
- 3 In the Settings window for Difference, locate the Difference section.
- 4 Click Clear Selection.
- 5 Select the objects arr1(1,1,1), arr1(1,2,1), and arr1(1,3,1) only.
- **6** Find the **Objects to subtract** subsection. Select the **Activate Selection** toggle button.
- **7** Select the objects **cl** and **poll** only.
- 8 Click | Build Selected.

Work Plane I (wp I) > Polygon 2 (pol2)

- I In the Work Plane toolbar, click / Polygon.
- 2 In the Settings window for Polygon, locate the Coordinates section.
- **3** In the table, enter the following settings:

xw (m)	yw (m)
L_inout*3/4	2*w_ch*1.25
L_inout*3/4	-2*w_ch*1.25
L_inout*3/4+5*w_ch*tan(ang_inout/2)	-2*w_ch*1.25

4 Click | Build Selected.

Work Plane I (wp I)>Difference 2 (dif2)

- I In the Work Plane toolbar, click Booleans and Partitions and choose Difference.
- 2 Select the objects arr1(1,1,2), arr1(1,2,2), and arr1(1,3,2) only.
- 3 In the Settings window for Difference, locate the Difference section.
- 4 Find the Objects to subtract subsection. Select the Activate Selection toggle button.
- **5** Select the object **pol2** only.
- 6 Click Pauld Selected.

Work Plane I (wpl)>Rotate I (rot1)

- I In the Work Plane toolbar, click Transforms and choose Rotate.
- 2 Select the object difl only.
- 3 In the Settings window for Rotate, locate the Rotation section.
- 4 In the Angle text field, type ang_inout.
- 5 Locate the Center of Rotation section. In the xw text field, type L_inout*3/4.
- 6 In the yw text field, type 2*w_ch*1.25.
- 7 Click | Build Selected.

Work Plane I (wpl)>Union I (unil)

- I In the Work Plane toolbar, click Booleans and Partitions and choose Union.
- 2 Click in the **Graphics** window and then press Ctrl+A to select both objects.
- 3 In the Settings window for Union, click | Build Selected.

Work Plane I (wpl)>Move I (movl)

- I In the Work Plane toolbar, click Transforms and choose Move.
- 2 Select the object unil only.
- 3 In the Settings window for Move, locate the Displacement section.
- 4 In the xw text field, type -L inout-w ch*0.5.
- 5 In the yw text field, type -w_ch*2.5.
- 6 Click | Build Selected.
- 7 Click the Zoom Extents button in the Graphics toolbar.

Work Plane I (wp I)>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 w ch.

- 4 In the Height text field, type L_ch+10*w_ch.
- 5 Locate the Position section. In the xw text field, type -w_ch/2.
- 6 In the yw text field, type -5*w ch.
- 7 Click | Build Selected.

Work Plane I (wpl)>Array 2 (arr2)

- I In the Work Plane toolbar, click Transforms and choose Array.
- 2 Click the **Zoom Extents** button in the **Graphics** toolbar.
- **3** Select the object **r3** only.
- 4 In the Settings window for Array, locate the Size section.
- 5 In the xw size text field, type N_ch.
- 6 Locate the **Displacement** section. In the xw text field, type w ch*2.
- 7 Click | Build Selected.

Work Plane I (wp I)>Rectangle 4 (r4)

- 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 (N ch-0.5)*(2*w ch).
- 4 In the **Height** text field, type w ch.
- 5 Locate the Position section. In the xw text field, type -w ch/2.
- 6 In the yw text field, type -w ch*5.

Work Plane I (wpI)>Array 3 (arr3)

- I In the Work Plane toolbar, click Transforms and choose Array.
- 2 Select the object **r4** only.
- 3 In the Settings window for Array, locate the Size section.
- **4** In the **yw size** text field, type **3**.
- **5** Locate the **Displacement** section. In the **yw** text field, type w ch*2.
- 6 Click | Build Selected.

Work Plane I (wpl)>Copy I (copyl)

- I In the Work Plane toolbar, click Transforms and choose Copy.
- 2 Click the **Zoom Extents** button in the **Graphics** toolbar.
- 3 Select the objects arr3(1,1), arr3(1,2), and arr3(1,3) only.
- 4 In the Settings window for Copy, locate the Displacement section.

- 5 In the yw text field, type L_ch+5*w_ch.
- 6 Click | Build Selected.

Work Plane I (wp I)>Rotate 2 (rot2)

- I In the Work Plane toolbar, click Transforms and choose Rotate.
- 2 Select the object mov! only.
- 3 In the Settings window for Rotate, locate the Rotation section.
- 4 In the Angle text field, type 180.
- 5 Locate the Center of Rotation section. In the xw text field, type (N ch-1)*w ch.
- 6 In the yw text field, type L ch/2.
- 7 Locate the Input section. Select the Keep input objects check box.
- 8 Click | Build Selected.

Work Plane I (wp I)>Union 2 (uni2)

- I In the Work Plane toolbar, click Booleans and Partitions and choose Union.
- 2 Click the Select Box button in the Graphics toolbar.
- 3 Click in the **Graphics** window and then press Ctrl+A to select all objects.

Fillet Selection 1

- I In the Work Plane toolbar, click \(\frac{1}{2} \) Selections and choose Box Selection.
- 2 In the Settings window for Box Selection, type Fillet Selection 1 in the Label text field.
- 3 Locate the Geometric Entity Level section. From the Level list, choose Point.
- 4 Locate the **Box Limits** section. In the xw maximum text field, type 0.
- 5 In the yw minimum text field, type L ch+w ch*4.5.
- 6 Click **Pauld Selected**.

Fillet Selection 2

- I In the Work Plane toolbar, click Selections and choose Box Selection.
- 2 In the Settings window for Box Selection, type Fillet Selection 2 in the Label text field.
- 3 Locate the Geometric Entity Level section. From the Level list, choose Point.
- 4 Locate the Box Limits section. In the xw minimum text field, type 2*w ch*(N ch-1).
- 5 In the yw maximum text field, type -w_ch*4.5.
- 6 Click | Build Selected.

Work Plane I (wpl)>Fillet I (fill)

- I In the Work Plane toolbar, click Fillet.
- 2 In the Settings window for Fillet, locate the Points section.
- 3 From the Vertices to fillet list, choose Fillet Selection 1.
- 4 Locate the Radius section. In the Radius text field, type w_ch/2.
- 5 Click | Build Selected.

Work Plane I (wb I)>Fillet 2 (fil2)

- I Right-click Component I (compl)>Geometry I>Work Plane I (wpl)>Plane Geometry> Fillet I (fill) and choose Duplicate.
- 2 In the Settings window for Fillet, locate the Points section.
- **3** Find the **Vertices to fillet** subsection. Select the **Metivate Selection** toggle button.
- 4 From the Vertices to fillet list, choose Fillet Selection 2.
- 5 Click **Pail Build Selected**.

Extrude I (extI)

- I In the Model Builder window, right-click Geometry I and choose Extrude.
- 2 In the Settings window for Extrude, locate the Distances section.
- **3** In the table, enter the following settings:

Distances (m) h_a

4 Click | Build Selected.

Cylinder I (cyl1)

- I In the Geometry toolbar, click Cylinder.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type R in.
- 4 In the Height text field, type 3*h a.
- 5 Click **Pail Build Selected**.

Rotate I (rot1)

- I In the Geometry toolbar, click Transforms and choose Rotate.
- **2** Select the object **cyll** only.
- 3 In the Settings window for Rotate, locate the Rotation section.
- 4 In the Angle text field, type ang_inout.

- 5 Locate the Point on Axis of Rotation section. In the x text field, type L_inout*3/4.
- 6 In the y text field, type 2*w_ch*1.25.
- 7 Click **Build Selected**.

Move I (movI)

- I In the Geometry toolbar, click Transforms and choose Move.
- 2 Select the object rot1 only.
- 3 In the Settings window for Move, locate the Displacement section.
- 4 In the x text field, type -L inout-w ch*0.5.
- 5 In the y text field, type -w ch*2.5.
- 6 Click | Build Selected.

Rotate 2 (rot2)

- I In the Geometry toolbar, click Transforms and choose Rotate.
- **2** Select the object **mov1** only.
- 3 In the Settings window for Rotate, locate the Input section.
- 4 Select the Keep input objects check box.
- 5 Locate the Rotation section. In the Angle text field, type 180.
- 6 Locate the Point on Axis of Rotation section. In the x text field, type (N ch-1) *w ch.
- 7 In the y text field, type L_ch/2.
- 8 Click Pauld Selected.

Form Union (fin)

- I In the Model Builder window, click Form Union (fin).
- 2 In the Settings window for Form Union/Assembly, click | Build Selected.
- 3 Click the Zoom Extents button in the Graphics toolbar.

Inlet Manifold

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Box Selection.
- 2 In the Settings window for Box Selection, type Inlet Manifold in the Label text field.
- 3 Locate the Box Limits section. In the x minimum text field, type -L inout.
- 4 In the y maximum text field, type w ch/2.
- 5 Locate the Output Entities section. From the Include entity if list, choose Entity inside box.
- 6 Click | Build Selected.

Outlet Manifold

- I In the Geometry toolbar, click **Selections** and choose Box Selection.
- 2 In the Settings window for Box Selection, type Outlet Manifold in the Label text field.
- 3 Locate the Box Limits section. In the x maximum text field, type N_ch*w_ch*2+ L_inout-w_ch.
- 4 In the y minimum text field, type L ch-w ch/2.
- 5 Locate the Output Entities section. From the Include entity if list, choose Entity inside box.

Channels Above Electrode Surface

- I In the Geometry toolbar, click 🔓 Selections and choose Box Selection.
- 2 In the Settings window for Box Selection, type Channels Above Electrode Surface in the Label text field.
- 3 Locate the Box Limits section. In the y minimum text field, type -w ch/2.
- 4 In the y maximum text field, type L ch+w ch/2.
- 5 Locate the Output Entities section. From the Include entity if list, choose Entity inside box.

Electrode Surface

- I In the Geometry toolbar, click **Selections** and choose Box Selection.
- 2 In the Settings window for Box Selection, type Electrode Surface in the Label text field.
- 3 Locate the Geometric Entity Level section. From the Level list, choose Boundary.
- 4 Locate the Box Limits section. In the y minimum text field, type -w ch/2.
- 5 In the y maximum text field, type L_ch+w_ch/2.
- 6 In the z maximum text field, type h_a/2.
- 7 Locate the Output Entities section. From the Include entity if list, choose Entity inside box.

Inlet

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Box Selection.
- 2 In the Settings window for Box Selection, type Inlet in the Label text field.
- 3 Locate the Geometric Entity Level section. From the Level list, choose Boundary.
- 4 Locate the **Box Limits** section. In the x maximum text field, type 0.
- 5 In the z minimum text field, type h a*2.

6 Locate the Output Entities section. From the Include entity if list, choose Entity inside box.

Outlet

- I In the Geometry toolbar, click **Selections** and choose Box Selection.
- 2 In the Settings window for Box Selection, locate the Geometric Entity Level section.
- 3 From the Level list, choose Boundary.
- 4 In the Label text field, type Outlet.
- 5 Locate the Box Limits section. In the x minimum text field, type N ch*w ch*2.
- 6 In the z minimum text field, type h a*2.
- 7 Locate the Output Entities section. From the Include entity if list, choose Entity inside box.

Exterior Boundaries to Electrode Channels

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Adjacent Selection.
- 2 In the Settings window for Adjacent Selection, type Exterior Boundaries to Electrode Channels in the Label text field.
- 3 Locate the Input Entities section. Click + Add.
- 4 In the Add dialog box, select Channels Above Electrode Surface in the Input selections list.
- 5 Click OK.

Exteror Boundaries to Inlet Manifold

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Adjacent Selection.
- 2 In the Settings window for Adjacent Selection, type Exteror Boundaries to Inlet Manifold in the Label text field.
- 3 Locate the Input Entities section. Click + Add.
- 4 In the Add dialog box, select Inlet Manifold in the Input selections list.
- 5 Click OK.

Inlets to Electrode Channels

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Intersection Selection.
- 2 In the Settings window for Intersection Selection, type Inlets to Electrode Channels in the Label text field.
- 3 Locate the Geometric Entity Level section. From the Level list, choose Boundary.
- **4** Locate the **Input Entities** section. Click + **Add**.

- 5 In the Add dialog box, in the Selections to intersect list, choose Exterior Boundaries to Electrode Channels and Exteror Boundaries to Inlet Manifold.
- 6 Click OK.

Manifolds

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Union Selection.
- 2 In the Settings window for Union Selection, type Manifolds in the Label text field.
- 3 Locate the Input Entities section. Click + Add.
- 4 In the Add dialog box, in the Selections to add list, choose Inlet Manifold and Outlet Manifold.
- 5 Click OK.

Exterior Boundaries to Manifolds

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Adjacent Selection.
- 2 In the Settings window for Adjacent Selection, type Exterior Boundaries to Manifolds in the Label text field.
- 3 Locate the **Input Entities** section. Click + Add.
- 4 In the Add dialog box, select Manifolds in the Input selections list.
- 5 Click OK.

Inlets and Outlets to Electrode Channels

- I In the Geometry toolbar, click Selections and choose Intersection Selection.
- 2 In the Settings window for Intersection Selection, type Inlets and Outlets to Electrode Channels in the Label text field.
- 3 Locate the Geometric Entity Level section. From the Level list, choose Boundary.
- **4** Locate the **Input Entities** section. Click + **Add**.
- 5 In the Add dialog box, in the Selections to intersect list, choose Exterior Boundaries to Electrode Channels and Exterior Boundaries to Manifolds.
- 6 Click OK.

Electrode Channels and Manifolds

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Union Selection.
- 2 In the Settings window for Union Selection, type Electrode Channels and Manifolds in the **Label** text field.
- 3 Locate the Input Entities section. Click + Add.

- 4 In the Add dialog box, in the Selections to add list, choose Inlet Manifold, Outlet Manifold, and Channels Above Electrode Surface.
- 5 Click OK.

Exteror Boundaries to Outlet Manifold

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Adjacent Selection.
- 2 In the Settings window for Adjacent Selection, type Exteror Boundaries to Outlet Manifold in the Label text field.
- 3 Locate the Input Entities section. Click + Add.
- 4 In the Add dialog box, select Outlet Manifold in the Input selections list.
- 5 Click OK.

Outlets from Electrode Channels

- I In the Geometry toolbar, click \(\frac{1}{2} \) Selections and choose Intersection Selection.
- 2 In the Settings window for Intersection Selection, type Outlets from Electrode Channels in the Label text field.
- 3 Locate the Geometric Entity Level section. From the Level list, choose Boundary.
- 4 Locate the Input Entities section. Click + Add.
- 5 In the Add dialog box, in the Selections to intersect list, choose Exterior Boundaries to Electrode Channels and Exteror Boundaries to Outlet Manifold.
- 6 Click OK.