Created in COMSOL Multiphysics 6.1

Fuel Cell Cathode with Liquid Water

Introduction

In low-temperature fuel cells, the produced water can condensate as liquid water if the partial pressure of vapor exceeds the (equilibrium) vapor pressure. The produced liquid water can flood the gas diffusion electrodes, gas diffusion layers, and/or the flow channels and manifolds, resulting in decreased fuel cell performance.

This tutorial expands the model defined in the Mass Transport and Electrochemical Reaction in a Fuel Cell Cathode tutorial to include also the effects liquid water formation in the porous gas diffusion electrode.

Model Definition

Liquid water is produced in the extended model using a user-defined expression for vapor condensation, depending on the relative humidity level in the gas phase:

$$R = k(p_{\mathrm{H2O}} - p_{\mathrm{vap}}) \tag{1}$$

where k is a rate constant, p_{H2O} is the partial pressure of water vapor, and p_{vap} the vapor pressure.

The porous gas diffusion electrode is assumed to be hydrophobic. The capillary pressure, p_c, is defined as

$$p_c = p_l - p_g \tag{2}$$

where p_l and p_g are the phase pressures, with the subscripts l and g referring to the liquid and gas phases, respectively.

The capillary pressure depends on the liquid saturation s_l in the porous media as depicted in Figure 1. (Note: The capillary pressure curve originally stems from Ref. 1 for measurements on a gas diffusion layer, that is, not a gas diffusion electrode, and is used here solely for tutorial purposes.)

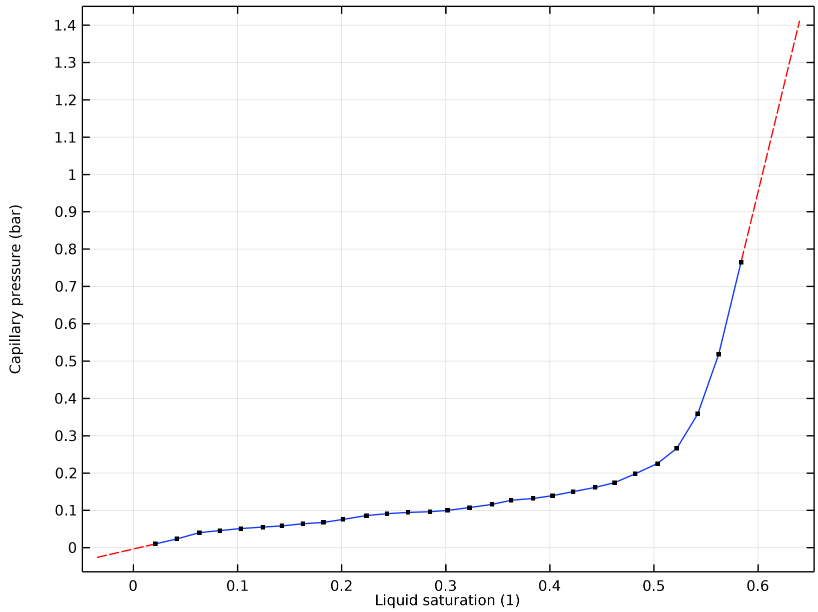


Figure 1: Capillary pressure versus liquid saturation.

The momentum transfer in the liquid phase is modeled using Darcy's law according to

$$\nabla \cdot (\rho_l \mathbf{u}_l) = R \tag{3}$$

with the volume averaged velocity $\mathbf{u}_i$ in the liquid fluid phase of index l defined as

$$\mathbf{u}_l = -\frac{\kappa_{r,l}}{\mu_l}\kappa\nabla p_l \tag{4}$$

where μ_l is the dynamic viscosity of the fluid and κ the absolute permeability of the porous media.

$\kappa_{r,l}$ in the above equation is the relative permeability, which is defined to depend on the fluid saturation level according to

$$\kappa_{r,l} = s_l^2 \tag{5}$$

A similar correlation is used for Darcy's law in the gas phase, solved for by the fuel cell interface, i.e

$$\kappa_{r,g} = s_g^2 \tag{6}$$

The Phase Transport in Porous Media interface is used to set up the flow formulation of the liquid water, based on Darcy's law, solving for s_l, to the model.

As boundary conditions for the liquid phase transport model, a liquid water saturation according to a capillary pressure of 0 Pa is set at the inlet.

The model is solved in a stationary study consisting of four study steps. In order to facilitate convergence, the potential variables, the pressure and gas phase species, and the liquid saturation are solved for in individual study steps first for a cell voltage of 1 V. The fully coupled problem is then solved in the last study step, using an auxiliary sweep to ramp the voltage from 1 to 0.5 V.

Results and Discussion

Figure 2 compares the relative humidity level in the cell at 0.5 V when and when not including water condensation and liquid water transport in the model. When not including water condensation, the air mixture gets significantly oversaturated to about 160% relative humidity. When including condensation, the relative humidity stays close to 100% throughout the cathode.

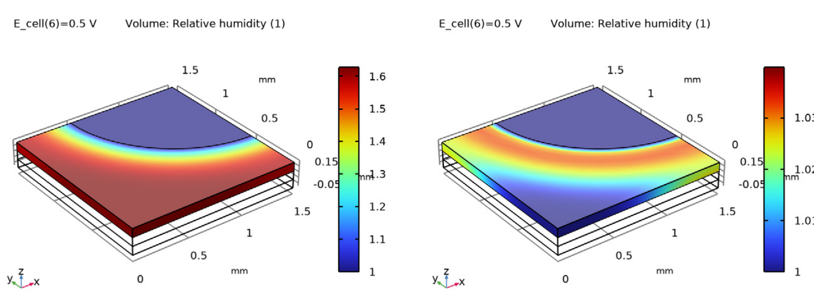


Figure 2: Relative humidity assuming no water condensation (left) and when including condensation and water transport (right).

Figure 3 shows the liquid saturation level and the corresponding capillary pressure level when including liquid water transport. Liquid water now forms in the electrode and is transported out toward the inlet hole mainly by the capillary pressure gradient. The water saturation level in the pores does not exceed 10%.

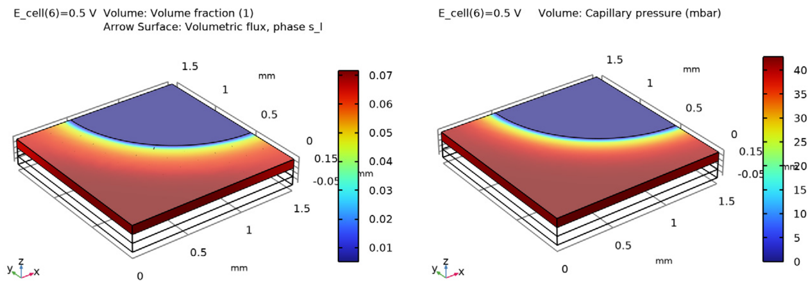


Figure 3: Liquid water saturation level and liquid water flux (left) and corresponding capillary pressure distribution (right).

Finally, the polarization curves for the two cases are compared in Figure 4. Introducing liquid water transport in the model slightly increases the current levels for a given voltage especially for lower voltages. This may seem counterintuitive, but the reason for this is that the condensation of water vapor results in an increased partial pressure of oxygen, which has a positive effect on the cathode potential. The small volume (<10%) of liquid water has only a minor detrimental effect on the overall gas transport rate.

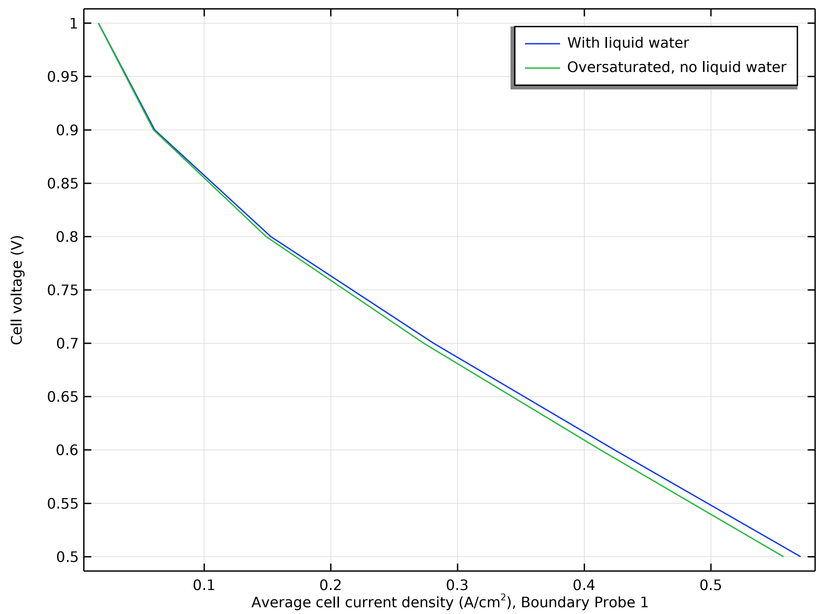


Figure 4: Comparisons of polarization plots when, and when not, considering liquid water formation and transport in the cathode.

Reference

1. E.C. Kumbur, K.V. Sharp, and M.M. Mench, "Validated Leverett Approach for Multiphase Flow in PEFC Diffusion Media, I. Hydrophobicity Effect," *Journal of The Electrochemical Society*, vol. 154, no. 12, pp. B1295–B1304, 2007.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/fuel_cell_cathode_with_liquid_water`

Modeling Instructions

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

2 In the **Application Libraries** window, select **Fuel Cell and Electrolyzer Module>Fuel Cells>fuel_cell_cathode** in the tree.

3 Click **Open**.

First, make a simulation for an inlet relative humidity of 100%.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
RH	100[%]	1	Relative humidity

STUDY 1

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

RESULTS

Make a plot of the relative humidity as follows:

Relative Humidity

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

2 In the **Settings** window for **3D Plot Group**, type `Relative Humidity` in the **Label** text field.

Volume 1

1 Right-click **Relative Humidity** and choose **Volume**.

2 In the **Settings** window for **Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Hydrogen Fuel Cell>fc.RH - Relative humidity**.

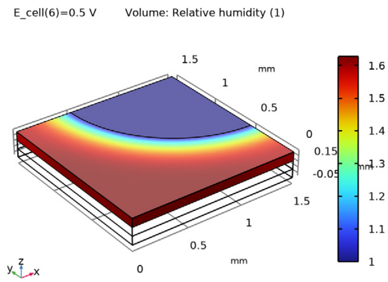
Selection 1

1 Right-click **Volume 1** and choose **Selection**.

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

3 From the **Selection** list, choose **Cathode Gas Diffusion Electrode**.

4 In the **Relative Humidity** toolbar, click **Plot**.



Probe Table 1

Store the probe table containing the polarization data for later comparisons.

Oversaturated, no liquid water transport

1 In the **Model Builder** window, expand the **Results>Tables** node.

2 Right-click **Probe Table 1** and choose **Duplicate**.

3 In the **Settings** window for **Table**, type `Oversaturated, no liquid water transport` in the **Label** text field.

COMPONENT 1 (COMP1)

Now set up the liquid transport model.

ADD PHYSICS

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

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

3 In the tree, select **Fluid Flow>Multiphase Flow>Phase Transport>Phase Transport in Porous Media (phtr)**.

4 Click to expand the **Dependent Variables** section. In the **Volume fractions** table, enter the following settings:

s_g
s_l

5 Click **Add to Component 1** in the window toolbar.

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

GLOBAL DEFINITIONS

The gas volume fraction will be a variable in the modified model, depending on the liquid saturation level. Locate and change the `eps_gas` parameter name and description as follows:

Parameters 1

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
eps_pores	0.4	0.4	Pore volume fraction in porous electrode

Also, add a parameter `kce` to define the condensation evaporation rate constant.

4 In the table, enter the following settings:

Name	Expression	Value	Description
kce	5.62e4[mol/m^3/s]	56200 mol/(m³·s)	Condensation evaporation rate constant

DEFINITIONS

Load some variable expressions from a file:

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** 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 `fuel_cell_cathode_with_liquid_water_variables.txt`.

The `pc` variable will be marked in orange since the capillary pressure function has not yet been defined. Define the function as follows:

Interpolation 1 (int1)

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

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

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

6 Click **Import**.

7 In the **Function name** text field, type `pc`.

8 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

9 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
t	1

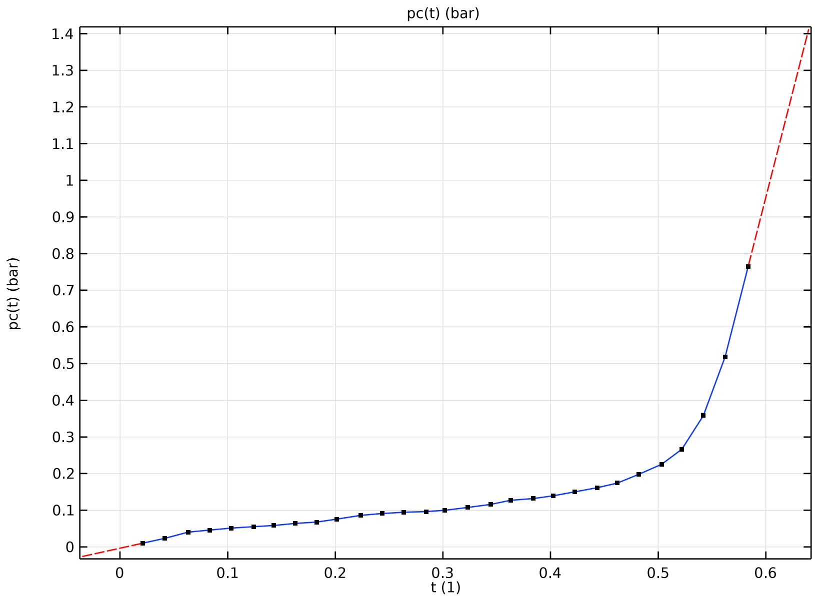
10 In the **Function** table, enter the following settings:

Function	Unit
pc	bar

11 Click to expand the **Related Functions** section. Select the **Define inverse function** check box.

12 In the **Inverse function name** text field, type `s_l`.

13 Click **Plot**.



Variables 1

Now go back and check so that there are no variable marked in orange in the list.

If there are variables marked in orange it could be that you missed setting the dependent variables to `s_g` and `s_l` when adding **Phase Transport In Porous Media**, or that you missed setting the Function name to `pc` when adding the **Interpolation** function, or missed renaming `eps_gas` to `eps_pores` in **Parameters**.

HYDROGEN FUEL CELL (FC)

Enable liquid water stoichiometry as follows:

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** node, then click **Hydrogen Fuel Cell (fc)**.

2 In the **Settings** window for **Hydrogen Fuel Cell**, locate the **O2 Gas Mixture** section.

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

O2 Gas Phase 1

Add the condensation reaction as follows:

In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** click **O2 Gas Phase 1**.

Water Condensation-Evaporation 1

1. In the **Physics** toolbar, click **Attributes** and choose **Water Condensation-Evaporation**.
2. In the **Settings** window for **Water Condensation-Evaporation**, locate the **Condensation-Evaporation Rate** section.
3. In the k_{ce} text field, type `kce`.

O2 Gas Diffusion Electrode 1

Due to the presence of liquid water in the cathode, update the permeability as follows:

1. In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** click **O2 Gas Diffusion Electrode 1**.
2. In the **Settings** window for **O2 Gas Diffusion Electrode**, locate the **Gas Transport** section.
3. In the κ_g text field, type `perm_eff_gas`.

PHASE TRANSPORT IN POROUS MEDIA (PHTR)

Now set up the phase transport as follows:

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Phase Transport in Porous Media (phtr)**.
2. In the **Settings** window for **Phase Transport in Porous Media**, locate the **Domain Selection** section.
3. From the **Selection** list, choose **Cathode Gas Diffusion Electrode**.

Phase and Porous Media Transport Properties 1

1. In the **Model Builder** window, under **Component 1 (comp1)> Phase Transport in Porous Media (phtr)** click **Phase and Porous Media Transport Properties 1**.
2. In the **Settings** window for **Phase and Porous Media Transport Properties**, locate the **Model Input** section.
3. In the p_A text field, type `fc.pA`.
4. Locate the **Capillary Pressure** section. In the p_{csl} text field, type `pc`.

   The Hydrogen Fuel Cell interface declares and announces density and viscosity variables for both the gas mixture and liquid water. Define the corresponding properties in the Phase Transport interface to make use of these variables as follows:
5. Locate the **Phase 1 Properties** section. From the ρ_{sg} list, choose **Density of gas phase (fc)**.

6 From the μ_{sg} list, choose **Dynamic viscosity of gas phase (fc)**.

7 Locate the **Phase 2 Properties** section. From the ρ_{sl} list, choose **Density of liquid water (fc)**.

8 From the μ_{sl} list, choose **Dynamic viscosity of liquid water (fc)**.

9 Locate the **Matrix Properties** section. From the ε_p list, choose **User defined**. In the associated text field, type `eps_gas`.

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

Volume Fraction 1

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

At the inlet boundary, the liquid saturation corresponds to a zero capillary pressure.

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

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

4 Locate the **Volume Fraction** section. Select the **Phase s_l** check box.

5 In the $s_{0,sl}$ text field, type `s_l(0)`.

If `s_l(0)` gets marked in orange you probably missed defining the inverse function on the **Interpolation** function.

Initial Values 1

Use the same expression for the initial volume fraction.

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $s_{0,sl}$ text field, type `s_l(0)`.

Mass Source 1

Add the mass source for the liquid phase, stemming from the fuel cell reactions, as follows:

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

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

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

4 Locate the **Mass Source** section. From the qs_{sl} list, choose **Mass source, liquid phase (fc/o2gasph1)**.

STUDY 1

Use a study sequence consisting of four steps to solve the model. The stepwise approach improves convergence. Modify the existing study as follows:

Stationary - Excluding Phase Transport

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

2 In the **Settings** window for **Stationary**, type `Stationary - Excluding Phase Transport` in the **Label** text field.

3 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Phase Transport in Porous Media (phtr)**.

Step 2: Stationary - Excluding Phase Transport

Right-click **Study 1>Step 3: Stationary - Excluding Phase Transport** and choose **Move Up**.

Stationary - Phase Transport Only

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

2 In the **Settings** window for **Stationary**, type `Stationary - Phase Transport Only` in the **Label** text field.

3 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Hydrogen Fuel Cell (fc)**.

Step 3: Stationary - Phase Transport Only

Right-click **Study 1>Step 4: Stationary - Phase Transport Only** and choose **Move Up**.

Stationary - All Physics

1 In the **Model Builder** window, click **Step 4: Stationary**.

2 In the **Settings** window for **Stationary**, type `Stationary - All Physics` in the **Label** text field.

The study should now contain four steps, in the following order: Step 1: Current Distribution Initialization, Step 2: Stationary - Excluding Phase Transport, Step 3: Stationary - Phase Transport Only, Step 4: Stationary - All Physics.

Solution 1 (sol1)

1 In the **Model Builder** window, right-click **Solver Configurations** and choose **Reset Solver to Default**.

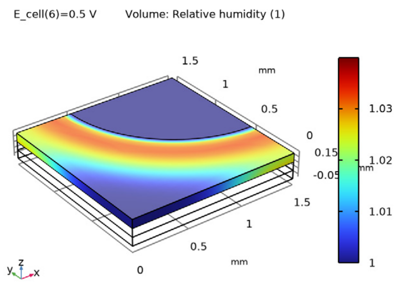
2 In the **Study** toolbar, click **Compute**.

RESULTS

Inspect the relative humidity plot.

Relative Humidity

In the **Relative Humidity** toolbar, click **Plot**.



Liquid Water Saturation

Create a plot of the liquid saturation level as follows:

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

2 In the **Settings** window for **3D Plot Group**, type `Liquid Water Saturation` in the **Label** text field.

Volume 1

1 Right-click **Liquid Water Saturation** and choose **Volume**.

2 In the **Settings** window for **Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Phase Transport in Porous Media>s_l - Volume fraction**.

3 In the **Liquid Water Saturation** toolbar, click **Plot**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Liquid Water Saturation** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Phase Transport in Porous Media>phtr.ux_s_l,...,phtr.uz_s_l - Volumetric flux, phase s_l**.

3 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type `50`.

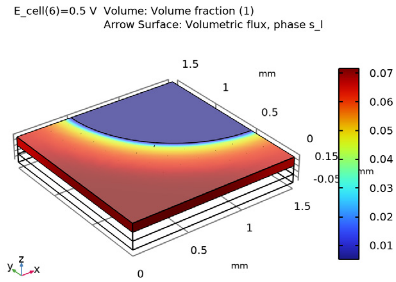
4 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

Selection 1

1 Right-click **Arrow Surface 1** and choose **Selection**.

2 Select Boundary 10 only.

3 In the **Liquid Water Saturation** toolbar, click **Plot**.



Capillary Pressure

Create a plot of the capillary pressure as follows:

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

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

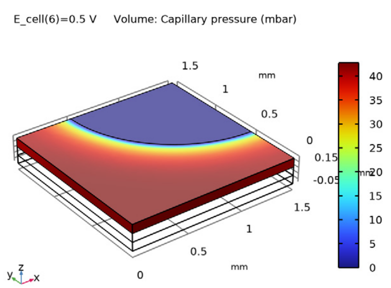
Volume 1

1 Right-click **Capillary Pressure** and choose **Volume**.

2 In the **Settings** window for **Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>pc - Capillary pressure - Pa**.

3 Locate the **Expression** section. From the **Unit** list, choose **mbar**.

4 In the **Capillary Pressure** toolbar, click **Plot**.



Polarization Curve

Finally, compare the polarization plots of the oversaturated and liquid water models as follows:

Probe Table Graph: Limited O2 gas phase transport

1 In the **Model Builder** window, expand the **Polarization Curve** node, then click **Probe Table Graph: Limited O2 gas phase transport**.

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

3 In the table, enter the following settings:

Legends
`With liquid water`

Probe Table Graph: Unlimited O2 gas phase transport

1 In the **Model Builder** window, click **Probe Table Graph: Unlimited O2 gas phase transport**.

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

3 From the **Table** list, choose **Oversaturated, no liquid water transport**.

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

Legends
`Oversaturated, no liquid water`

5 In the **Polarization Curve** toolbar, click **Plot**.