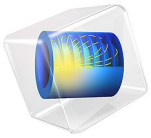


Model created in COMSOL Multiphysics 6.4

Parameter Estimation of a Polymer Electrolyte Membrane Fuel Cell Model

Introduction

This tutorial demonstrates how to use stationary polarization data to perform parameter estimation of a polymer electrolyte membrane fuel cell (PEMFC) model. The model, defining a 5-layer membrane electrode assembly (MEA) is two-dimensional and includes electronic and ionic charge balances, Butler–Volmer kinetics, as well as gas diffusive and convective transport in the oxygen/air gas diffusion layer and electrode (catalytic layer).

Two sets of polarization data, for either a humidified oxygen or air mixture, are used for estimation of four model parameters.

The experimental data and most of the parameters used for defining the model are based on Ref. 1.

Model Definition

Figure 1 shows the model geometry. The geometry consists of five layers: two gas diffusion layers (GDLs), two gas diffusion electrodes (catalytic layers), and one membrane. The left-hand side upper and lower boundaries represent the boundaries facing the ribs of the flow-field plates, acting as current collectors. The right-hand side upper and lower boundaries represent the boundaries facing the gas flow channels, acting as gas inlet/outlets. The upper side of the cell is the oxygen/air side (cathode) side; the lower side is the hydrogen (anode) side.

The two-dimensional geometry can be motivated by assuming that the gases are fed to the cell at high stoichiometry (flow rates) so that partial pressure gradients are negligible along the channels.

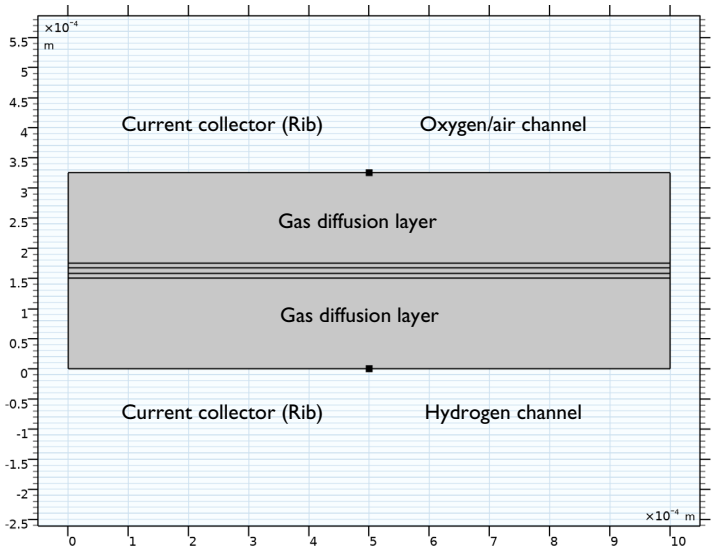


Figure 1: Model geometry of the 5-layer MEA. A membrane, sandwiched between two catalytic layer (gas diffusion electrode) domains, is located between the two gas diffusion layers. The points indicate the intersection between the rib and channels outside the model geometry.

The model is defined using the **Hydrogen Fuel Cell** interface, including the following phenomena:

- Electronic and ionic charge balances using Ohm's law.
- Gas diffusion and convection of the $O_2/N_2/H_2O$ mixture on the oxygen side of the cell in the corresponding GDL and the catalytic layer. (For this cell configuration, hydrogen transport will be fast and it is assumed the partial pressure gradients on the hydrogen side are negligible.)
- Butler–Volmer kinetics in the catalytic layers. On the oxygen side, the kinetics depends on the local partial pressure of oxygen and water vapor. In addition, a local limiting current density is incorporated on the oxygen side representing additional concentration overpotentials due to diffusion through a thin ionomer film covering the catalyst particles.
- Hydrogen permeation through the membrane, giving rise to a small parasitic current on the catalytic layer/membrane boundary on the oxygen side.

For an introduction to fuel cell MEA modeling, see also the Transport Phenomena in a Polymer Electrolyte Fuel Cell Membrane Electrode Assembly tutorial.

PARAMETER ESTIMATION

The **Parameter Estimation** study step is used to fit the model to the experimental polarization data. The stationary polarization data, recorded for both a humidified oxygen and a humidified air oxidant stream, is shown in Figure 2. When using the humidified oxygen as oxidant, the current densities are generally higher.

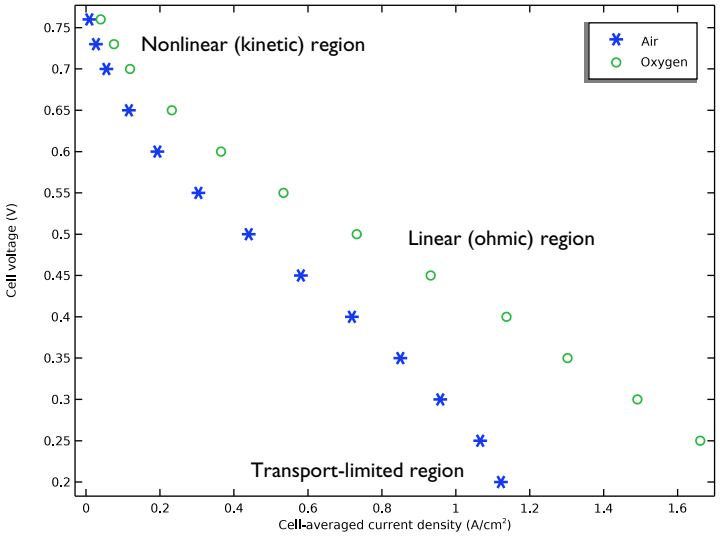


Figure 2: Experimental polarization data.

At high cell voltages, the polarization curves feature a nonlinear voltage dependency on the current density. This nonlinearity is usually associated with kinetic losses, for PEMFCs in particular to the sluggish oxygen reduction reaction (ORR). At intermediate cell voltages, where ohmic voltage losses dominate the polarization behavior, the graphs are more linear. For low voltages, in particular for the air case, the curves bend off downward, approaching a limiting current density, which stems from transport limitations.

In order to achieve a good model fit to the data, we choose a set of fitting parameters that will impact all these three regions of the polarization data. The fitting parameters (also called control variables) are summarized in Table 1.

TABLE 1: FITTING PARAMETERS.

NAME	UNIT	DESCRIPTION
`sigmal_mem`	S/m	Membrane electrolyte conductivity
`log_i0_ref_ORR`	-	Log of oxygen reduction reference exchange current density

TABLE 1: FITTING PARAMETERS.

NAME	UNIT	DESCRIPTION
`alphac_ORR`	-	Cathodic transfer coefficient for oxygen reduction
`ilim_ORR_ref`	A/m^2	Limiting current density for oxygen reduction at 1 atm partial pressure

The parameter `sigmal_mem` defines the electrolyte conductivity of the membrane. This parameter contributes to the linear voltage dependency and will hence affect the slope of the polarization curves in the linear region.

The parameters `log_i0_ref_ORR` and `alphac_ORR` are used in the Butler–Volmer kinetics expression on the oxygen side of the cell, and will mainly affect the upper, nonlinear, region of the polarization plots. Note that we choose to fit the log of the exchange current density, rather than the exchange current density variable directly. In this way, negative values are inherently avoided, and it is also easier to get a good fit if the initial guess of the fitting parameter is off by orders of magnitudes.

The final parameter, `ilim_ORR_ref`, is also used in the kinetics expression on the oxygen side, but will only affect the kinetics expression for large current densities. This parameter will hence affect the lower, transport-limited, part of the polarization curves.

Results and Discussion

Figure 3 shows the results of the fitted model, along with the experimental polarization data.

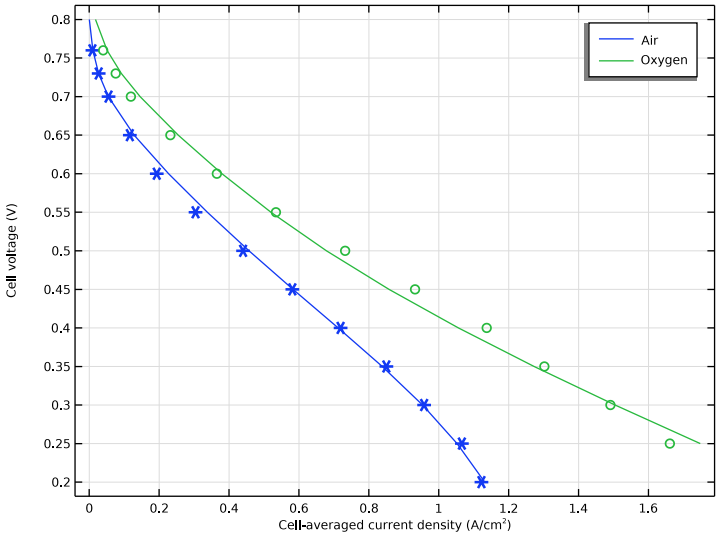


Figure 3: Polarization plots for oxygen (green) and air (blue). Solid lines: fitted model. Markers: experimental data.

The corresponding fitted parameter values are shown in Table 2.

TABLE 2: FITTED PARAMETER VALUES.

NAME	UNIT	INITIAL GUESS	FITTED VALUE
`sigmal_mem`	S/m	10	3.8
`log_i0_ref_ORR`	-	-3	-3.5
`alphac_ORR`	-	0.74	0.91
`ilim_ORR_ref`	A/m^2	3000	2.2e3

Reference

1. M. Butori, B. Eriksson, N. Nikolic, C. Lagergren , G. Lindbergh, and R. Wreland Lindström, "The effect of oxygen partial pressure and humidification in proton exchange membrane fuel cells at intermediate temperature (80–120°C)," *J. Power Sources*, vol. 563, p. 232803, 2023.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pemfc_parameter_estimation`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Electrochemistry** > **Hydrogen Fuel Cells** > **Proton Exchange Membrane (fc)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies** > **Stationary**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Load the model parameters from a text file.

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

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

3 Click **Load from File**.

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

GEOMETRY 1

Draw the gas diffusion layers, the catalyst layers and the membrane of the five-layer fuel cell membrane-electrode-assembly (MEA) as individual rectangles in the geometry. By enabling the **Resulting objects selection**, the resulting domains become available as named selections later on when defining the physics.

Hydrogen GDL

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, type `Hydrogen GDL` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_cell`.

4 In the **Height** text field, type `H_gdl`.

5 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

6 Click **Build Selected**.

Hydrogen Catalyst Layer

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, type `Hydrogen Catalyst Layer` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_cell`.

4 In the **Height** text field, type `H_ct`.

5 Locate the **Position** section. In the **y** text field, type `H_gdl`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

7 Click **Build Selected**.

Membrane

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, type `Membrane` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_cell`.

4 In the **Height** text field, type `H_mem`.

5 Locate the **Position** section. In the **y** text field, type `H_gdl+H_ct`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

7 Click **Build Selected**.

Oxygen Catalyst Layer

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, type `Oxygen Catalyst Layer` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_cell`.

4 In the **Height** text field, type `H_ct`.

5 Locate the **Position** section. In the **y** text field, type `H_gdl+H_ct+H_mem`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

7 Click **Build Selected**.

Oxygen GDL

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, type `Oxygen GDL` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `W_cell`.

4 In the **Height** text field, type `H_gdl`.

5 Locate the **Position** section. In the **y** text field, type `H_gdl+H_ct+H_mem+H_ct`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

7 Click **Build Selected**.

Point 1 (pt1)

Add points to divide the upper and lower boundaries at the intersection between the ribs and the channels.

1 In the **Geometry** toolbar, click **Point**.

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

3 In the **x** text field, type `W_rib/2`.

4 Click **Build Selected**.

Point 2 (pt2)

1 Right-click **Point 1 (pt1)** and choose **Duplicate**.

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

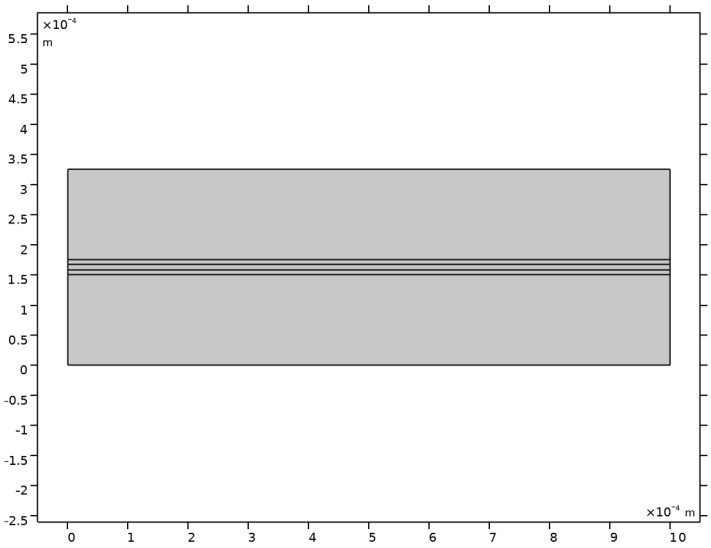
3 In the **y** text field, type `H_cell`.

4 Click **Build Selected**.

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

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

The final geometry should now look as follows:



DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

Load some variable expressions from a text file.

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 `pemfc_parameter_estimation_variables.txt`.

One of the variable expressions indicate an unknown operator or function. Add the missing integration operator as follows:

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

This operator will be used to compute an integral along the top current collector.

2 In the **Settings** window for **Integration**, type `intop_cc` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

View 1

Enable **Show geometry labels** to facilitate boundary selection.

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

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

3 Select the **Show geometry labels** checkbox.

Integration 1 (intop_cc)

1 In the **Model Builder** window, click **Integration 1 (intop_cc)**.

2 Select Boundary 11 only.

Variables 1

If you defined the operator correctly, the indication for the missing operator should now have vanished.

HYDROGEN FUEL CELL (FC)

Now proceed to define the fuel cell model.

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

2 In the **Settings** window for **Hydrogen Fuel Cell**, locate the **H2 Gas Mixture** section.

3 Find the **Transport mechanisms** subsection. Clear the **Include gas phase diffusion** checkbox.

4 Locate the **O2 Gas Mixture** section. Select the **Use Darcy's Law for momentum transport** checkbox.

5 Click to expand the **Electrolyte and Membrane Transport** section. Find the **Crossover species** subsection. Select the **H2** checkbox.

H2 Gas Diffusion Electrode 1

1 In the **Physics** toolbar, click **Domains** and choose **H2 Gas Diffusion Electrode**.

2 In the **Settings** window for **H2 Gas Diffusion Electrode**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Hydrogen Catalyst Layer**.

4 Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_ct`.

5 Locate the **Effective Electrolyte Charge Transport** section. From the **Effective conductivity correction** list, choose **User defined**. In the f_l text field, type `1`.

In this model we will assume the electrolyte conductivity defined on the **Electrolyte Phase** node always refers to the effective electrolyte conductivity. Hence the correction factor is set to unity.

H2 Gas Diffusion Electrode Reaction 1

1 In the **Model Builder** window, click **H2 Gas Diffusion Electrode Reaction 1**.

2 In the **Settings** window for **H2 Gas Diffusion Electrode Reaction**, locate the **Electrode Kinetics** section.

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_HOR`.

4 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_HOR`.

O2 Gas Diffusion Electrode 1

1 In the **Physics** toolbar, click **Domains** and choose **O2 Gas Diffusion Electrode**.

2 In the **Settings** window for **O2 Gas Diffusion Electrode**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Oxygen Catalyst Layer**.

4 Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_ct`.

5 Locate the **Effective Electrolyte Charge Transport** section. From the **Effective conductivity correction** list, choose **User defined**. In the f_l text field, type `1`.

6 Locate the **Gas Transport** section. In the ε_g text field, type `epsg_ct`.

7 In the κ_g text field, type `perm_ct`.

O2 Gas Diffusion Electrode Reaction 1

1 In the **Model Builder** window, click **O2 Gas Diffusion Electrode Reaction 1**.

2 In the **Settings** window for **O2 Gas Diffusion Electrode Reaction**, locate the **Electrode Kinetics** section.

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_ORR`.

4 In the α_a text field, type `alphaa_ORR`.

This models adds a limiting current density, representing the oxygen mass transport limitations in a thin ionomer film, covering the catalytic particles.

5 Select the **Limiting current density** checkbox.

6 In the i_{lim} text field, type `ilim_ORR`.

7 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_ORR`.

H2 Gas Diffusion Layer 1

1 In the **Physics** toolbar, click **Domains** and choose **H2 Gas Diffusion Layer**.

2 In the **Settings** window for **H2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Hydrogen GDL**.

Specify different conductivity values in the x and y directions as follows.

4 Locate the **Electrode Charge Transport** section. From the list, choose **Diagonal**.

5 Specify the σ_s matrix as

`sigmas_gdl_IP`	`0`
`0`	`sigmas_gdl_TP`

O2 Gas Diffusion Layer 1

1 In the **Physics** toolbar, click **Domains** and choose **O2 Gas Diffusion Layer**.

2 In the **Settings** window for **O2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Oxygen GDL**.

4 Locate the **Electrode Charge Transport** section. From the list, choose **Diagonal**.

5 Specify the σ_s matrix as

`sigmas_gdl_IP`	`0`
`0`	`sigmas_gdl_TP`

6 Locate the **Gas Transport** section. In the ε_g text field, type `epsg_gdl`.

7 In the κ_g text field, type `perm_gdl`.

Membrane 1

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

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

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

4 Locate the **Hydrogen Crossover** section. From the Ψ_{H2} list, choose **User defined**. In the associated text field, type `perm_H2`.

Electrolyte Phase 1

Add a second **Electrolyte Phase** node to define the effective conductivity of the membrane. Thereby the default **Electrolyte Phase 1** node will be refer to the catalytic layers only.

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

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

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

Electrolyte Phase 2

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

2 Select Domains 2 and 4 only.

3 In the **Settings** window for **Electrolyte Phase**, locate the **Electrolyte Charge Transport** section.

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

Electronic Conducting Phase 1

In the **Model Builder** window, click **Electronic Conducting Phase 1**.

Electric Ground 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electric Ground**.

2 Select Boundary 2 only.

Electronic Conducting Phase 1

In the **Model Builder** window, click **Electronic Conducting Phase 1**.

Electric Potential 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electric Potential**.

2 Select Boundary 11 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the $\phi_{s,bnd}$ text field, type `E_cell`.

Electronic Conducting Phase 1

Specify the initial electrode phase potential on the oxygen side. This improves convergence.

1 In the **Model Builder** window, click **Electronic Conducting Phase 1**.

Initial Values, O2 Domains 1

1 In the **Physics** toolbar, click **Attributes** and choose **Initial Values, O2 Domains**.

2 In the **Settings** window for **Initial Values, O2 Domains**, locate the **Domain Selection** section.

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

4 Locate the **Initial Values** section. In the ϕ_s text field, type `E_init`.

H2 Gas Phase 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Hydrogen Fuel Cell (fc)** click **H2 Gas Phase 1**.

2 In the **Settings** window for **H2 Gas Phase**, locate the **Composition** section.

3 From the **Mixture specification** list, choose **Humidified mixture**.

4 In the $\mathrm{RH}_{\mathrm{hum}}$ text field, type `RH`.

5 In the T_{hum} text field, type `T`.

Initial Values 1

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

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

3 From the **Mixture specification** list, choose **Humidified mixture**.

4 In the $\mathrm{RH}_{\mathrm{hum}}$ text field, type `RH`.

5 In the T_{hum} text field, type `T`.

O2 Gas Phase 1

In the **Model Builder** window, click **O2 Gas Phase 1**.

O2 Inlet 1

1 In the **Physics** toolbar, click **Attributes** and choose **O2 Inlet**.

2 Select Boundary 13 only.

3 In the **Settings** window for **O2 Inlet**, locate the **Inlet Flow Type** section.

4 From the **Inlet flow type** list, choose **Mixture composition constraint**.

5 Locate the **Mixture Specification** section. From the list, choose **Humidified mixture**.

6 In the $x_{0,\mathrm{N2,dry}}$ text field, type `xN2`.

7 In the $\mathrm{RH}_{\mathrm{hum}}$ text field, type `RH`.

8 In the T_{hum} text field, type `T`.

GLOBAL DEFINITIONS

Default Model Inputs

The temperature defined on the **Default Model Inputs** will be used by all physics nodes.

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

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General** > **Temperature (K) - minput.T**.

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

MESH 1

Define a user-defined mesh as follows:

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

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

4 In the **Mesh** toolbar, click **Clear Sequence**.

Mapped 1

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

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

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domains 2–4 only.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 3 and 15 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Element ratio** text field, type 5.

6 Select the **Reverse direction** checkbox.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 5 and 16 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 In the **Number of elements** text field, type 2.

Distribution 3

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 7 and 17 only.

Free Triangular 1

In the **Mesh** toolbar, click **Free Triangular**.

Size 1

1 Right-click **Free Triangular 1** and choose **Size**.

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

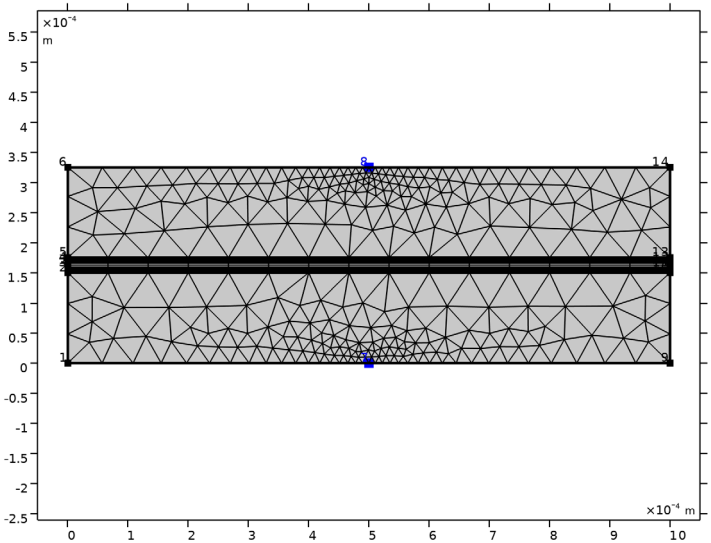
3 From the **Geometric entity level** list, choose **Point**.

4 Select Points 7 and 8 only.

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

6 Click **Build All**.

The finalized mesh should now look as follows:



The problem is now ready for solving. Enable an **Parametric Sweep** to perform polarization sweeps for two different dry inlet nitrogen molar fractions.

STUDY 1

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xN2 (Dry nitrogen molar fraction)	`0.79 0`	1

A dry nitrogen molar fraction of 0.79 corresponds to air, 0 to pure oxygen.

5 In the table, click to select the cell at row number 1 and column number 3.

6 Click to expand the **Advanced Settings** section. From the **Use parametric solver** list, choose **Off**.

Step 1: Stationary

For each nitrogen leve, enable an **Auxiliary Sweep** to perform a sweep of the cell potential.

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

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** checkbox.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E_cell (Cell voltage)	`range(E_init,-0.05,0.25)`	V

Note that **Run continuation for** is set to **Last parameter** by default. This improves convergence since this will result in that, for each nitrogen level, the potential will swept from a higher to a lower value, using the result of the previous computation as initial values for each step.

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

RESULTS

Mole Fraction, O2 (fc)

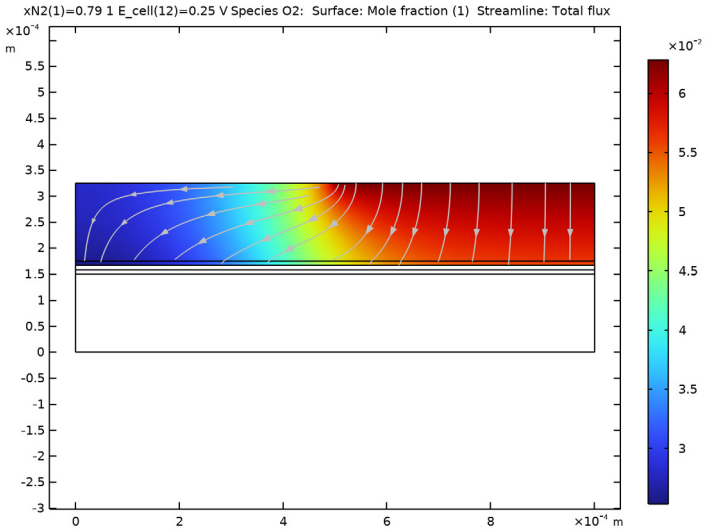
You may now explore the default plots for various nitrogen and cell voltage levels.

1 In the **Model Builder** window, under **Results** click **Mole Fraction, O2 (fc)**.

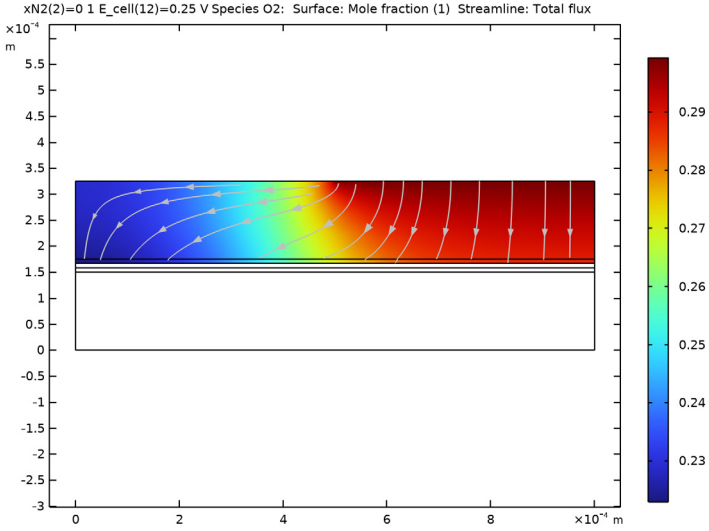
2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Parameter value (xN2)** list, choose **0.79**.

4 In the **Mole Fraction, O2 (fc)** toolbar, click **Plot**.



5 From the **Parameter value (xN2)** list, choose **0**.



6 In the **Mole Fraction, O2 (fc)** toolbar, click **Plot**.

Polarization Plots

Add a polarization plots for air and oxygen as follows:

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

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

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

4 In the **Label** text field, type `Polarization Plots`.

Global 1

1 Right-click **Polarization Plots** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
`E_cell`	`V`	`Cell voltage`

4 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **I_cell_avg - Cell-averaged current density - A/m²**.

5 Locate the **x-Axis Data** section. In the **Unit** field, type `A/cm^2`.

6 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
`Air`
`Oxygen`

Polarization Plots

1 In the **Model Builder** window, click **Polarization Plots**.

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

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

4 In the **Polarization Plots** toolbar, click **Plot**.

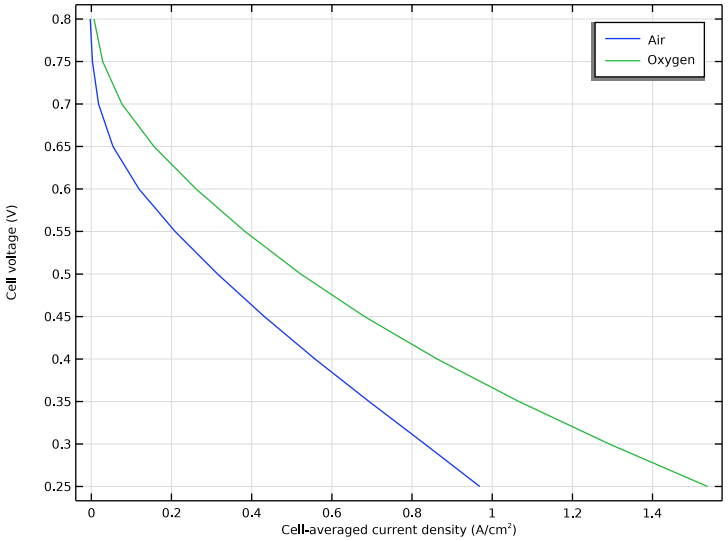


Table 1 - Air Polarization Data

The next step is to compare the computed polarization plots to the corresponding experimental data. Import the polarization data as a table and plot it as follows:

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Table 1 - Air Polarization Data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

Table 2 - O2 Polarization Data

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Table 2 - O2 Polarization Data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `pemfc_parameter_estimation_o2_data.csv`.

Polarization Plots

Enable the x- and y-axis label checkboxes at this point. This will avoid the upcoming table graphs to impact the axis labels.

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

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

3 Select the **x-axis label** checkbox.

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

Table Graph 1

1 Right-click **Polarization Plots** and choose **Table Graph**.

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

3 Find the **Line style** subsection. From the **Line** list, choose **None**.

4 From the **Color** list, choose **Cycle (reset)**.

5 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

Table Graph 2

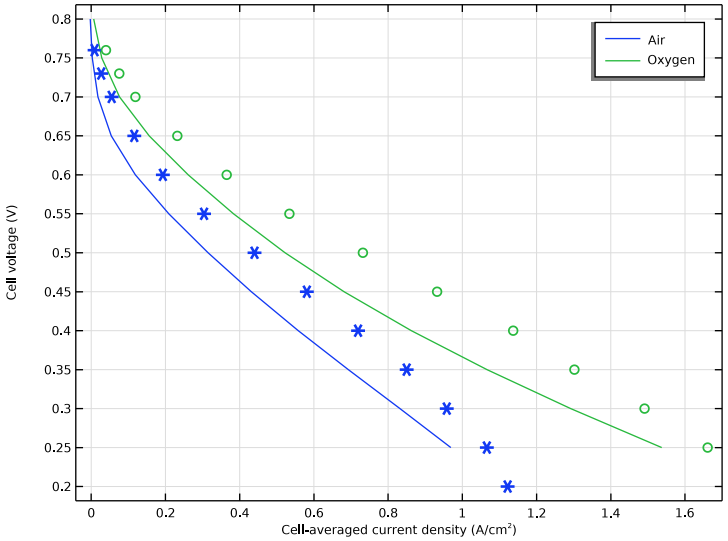
1 Right-click **Table Graph 1** and choose **Duplicate**.

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

3 From the **Table** list, choose **Table 2 - O2 Polarization Data**.

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

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



COMPONENT 1 (COMP1)

The model captures the overall trends in the polarization data, but the model predictivity is poor. In this second part of the tutorial, we will use **Parameter Estimation** to improve the model. **Parameter Estimation** operates by minimizing objective functions using an optimization solver.

Global Least-Squares Objective - Air

The **Least-Squares Objective** nodes will create objective functions based on the data tables, where in this tutorial the columns are defined as either a **Value** or a **Parameter** column. Each objective function is defined as a sum for all rows of the squared differences between experimental data values and the corresponding model variable values, as defined by the **Value** columns and the associated settings. For each row in the data, model parameters may be varied to the values defined in the **Parameter** columns.

Multiple **Least-Squares Objective** nodes may be used, and additional model parameters may be varied for each node, as set by the **Experimental Conditions** section.

How the objective functions are to be minimized will be defined later when we set up the study.

1 In the **Physics** toolbar, click **Optimization** and choose **Parameter Estimation**.

2 In the **Settings** window for **Least-Squares Objective**, type `Global Least-Squares Objective - Air` in the **Label** text field.

3 Locate the **Experimental Data** section. From the **Data source** list, choose **Result table**.

4 Locate the **Data Column Settings** section. In the table, enter the following settings:

Columns	Type	Settings
Current Density (mA/cm^2)	Value	Model expression=I_cell_avg, Column name=col1

5 In the **Model expression** text field, type `I_cell_avg`.

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

7 In the table, enter the following settings:

Columns	Type	Settings
Cell Voltage (V)	Parameter	Name=E_cell

8 From the **Name** list, choose **E_cell (Cell voltage)**.

9 In the **Unit** text field, type `V`.

10 Locate the **Experimental Conditions** section. Click + **Add**.

11 In the table, enter the following settings:

Name	Expression
xN2 (Dry nitrogen molar fraction)	`0.79`

Global Least-Squares Objective - Oxygen

1 Right-click **Global Least-Squares Objective - Air** and choose **Duplicate**.

2 In the **Settings** window for **Least-Squares Objective**, type `Global Least-Squares Objective - Oxygen` in the **Label** text field.

3 Locate the **Experimental Data** section. From the **Result table** list, choose **Table 2 - O2 Polarization Data**.

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

Name	Expression
xN2 (Dry nitrogen molar fraction)	0

ADD STUDY

Add a second study to perform parameter estimation.

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies** > **Stationary**.

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

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

STUDY 2

Parameter Estimation

1 In the **Study** toolbar, click **Optimization** and choose **Parameter Estimation**.

Note that the least-square objectives you defined earlier are now selected by automatically in the **Objective Function** section. This means that the sum of the two least-squares functions will subject to minimization.

In the **Estimated Parameters** section you define what parameters to modify (fit) in order to minimize the objective function, together with (optional) bounds. For this model we will estimate the values of four parameters.

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

3 Click **Add**.

4 In the table, enter the following settings:

Parameter	Initial value	Scale	Lower bound	Upper bound	Unit
sigmal_mem (Membrane electrolyte conductivity)	10[S/m]	1	1	20	S/m

5 Click **Add**.

6 In the table, enter the following settings:

Parameter	Initial value	Scale	Lower bound	Upper bound	Unit
log10_i0_ref_ORR (Log of ORR reference exchange current density (fitting parameter))	-3	1	-6	0	

7 Click **Add**.

8 In the table, enter the following settings:

Parameter	Initial value	Scale	Lower bound	Upper bound	Unit
alphac_ORR (Cathodic transfer coefficient, oxygen reduction)	`log(10)* R_const* T/ (100[mV]* F_const)`	`0.1`	`0.5`	1	1

9 Click + **Add**.

10 In the table, enter the following settings:

Parameter	Initial value	Scale	Lower bound	Upper bound	Unit
ilim_ORR_ref (Limiting current density for oxygen reduction at 1 atm partial pressure)	`3000[A/ m^2]`	1000	1000	5000	A/m^2

11 Locate the **Parameter Estimation Method** section. From the **Least-squares time/ parameter list method** list, choose **Use only least-squares data points**.

Step 1: Stationary

By enabling an **Auxiliary Sweep**, we guide the sweep to start at a high voltage, and then gradually lower the voltage. As in **Study 1**, by running continuation for the cell voltage parameter, this improves convergence.

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

2 In the **Settings** window for **Stationary**, locate the **Study Extensions** section.

3 Select the **Auxiliary sweep** checkbox.

4 From the **Least-squares continuation parameter** list, choose **E_cell (Cell voltage)**.

5 In the **Initial value** text field, type `E_init`.

6 In the **Study** toolbar, click **Get Initial Value**.

Solution 5 (sol5)

1 In the **Model Builder** window, expand the **Study 2** > **Solver Configurations** node.

2 In the **Model Builder** window, expand the **Solution 5 (sol5)** node, then click **Optimization Solver 1**.

3 In the **Settings** window for **Optimization Solver**, locate the **Optimization Solver** section.

4 From the **Gradient method** list, choose **Forward**.

5 In the **Model Builder** window, click **Study 2**.

6 In the **Settings** window for **Study**, locate the **Study Settings** section.

7 Clear the **Generate default plots** checkbox.

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

RESULTS

Objective Probe Table 3

The fitted parameter values should now be shown at the last line of the **Objective Probe Table** created by the study.

Polarization Plots

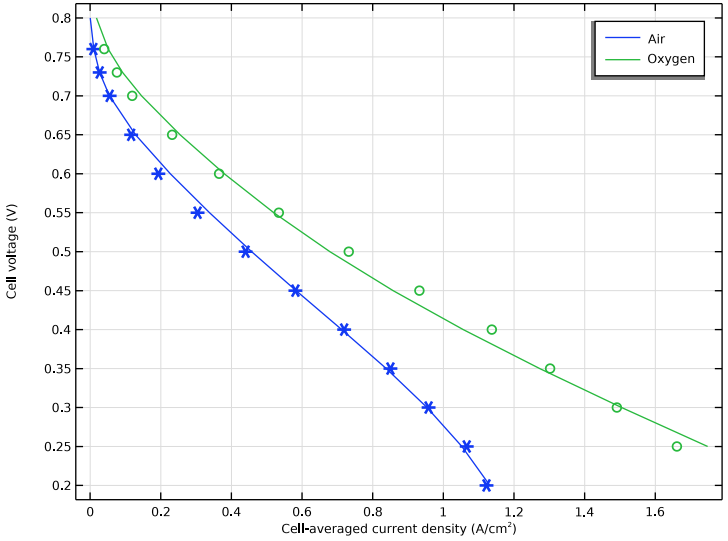
Revisit the **Polarization Plots** plot group and change the data set in order to see the polarization results of the fitted model.

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

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

3 From the **Dataset** list, choose **Study 2/Solution 5 (sol5)**.

4 In the **Polarization Plots** toolbar, click **Plot**.



Follow the instructions below to improve and remove some default plots.

Surface 1

1 In the **Model Builder** window, expand the **Electrode Potential with Respect to Ground (fc)** node, then click **Surface 1**.

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

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

Arrow Surface 1

1 In the **Model Builder** window, click **Arrow Surface 1**.

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

3 Select the **Scale factor** checkbox. In the associated text field, type `1e-9`.

4 From the **Color** list, choose **Yellow**.

Electrolyte Potential (fc)

In the **Model Builder** window, expand the **Results** > **Electrolyte Potential (fc)** node.

Arrow Surface 1

1 In the **Model Builder** window, expand the **Results** > **Electrolyte Potential (fc)** > **Arrow Surface 1** node, then click **Arrow Surface 1**.

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

3 From the **Color** list, choose **Yellow**.

Arrow Surface 1

1 In the **Model Builder** window, expand the **Results** > **Electrode Potential with Respect to Ground (fc) 1** node, then click **Arrow Surface 1**.

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

3 Select the **Scale factor** checkbox. In the associated text field, type `1e-9`.

4 From the **Color** list, choose **Yellow**.

Electrolyte Potential (fc) 1

In the **Model Builder** window, expand the **Results** > **Electrolyte Potential (fc) 1** node.

Arrow Surface 1

1 In the **Model Builder** window, expand the **Results** > **Electrolyte Potential (fc) 1** > **Arrow Surface 1** node, then click **Arrow Surface 1**.

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

3 From the **Color** list, choose **Yellow**.