

ME 370B
Energy Systems II:
Modeling and Advanced Concepts

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Project #9: SOFC Button Cell

Group assignment, due as a PDF file via Canvas, Thursday, March 16, 11 PM

The SOFC is our last project theme for the quarter. It is a double project in that it spans from now until the end of the quarter. The first three parts (Project 9) are due next week and focus on the modeling of a small, uniform element of the cell—a so-called “button cell.” The last parts (Project 10) are not due until the following week, but they involve the build up of a “channel cell” model from your button cell code, and I wanted you to be able to get started on it as soon as you are ready, so I have included Part 1 of that assignment here. (There will be other things to do in Project 10 too, but transitioning from the button to the channel is the essential element.)

The Objectives

- (1) to develop a basic understanding of how high-temperature fuel cells convert chemical-potential energy into electrical-potential energy,
- (2) to extend your understanding of chemical potential to electro-chemical potential,
- (3) to explore how driving restrained processes away from equilibrium (diffusion and reaction at finite rates) leads to losses in efficiency, and
- (4) to see how a complex/coupled problem (such as the channel cell calculation) can be decomposed into simpler problems that are then (relatively) easily reassembled to form a complete analysis.

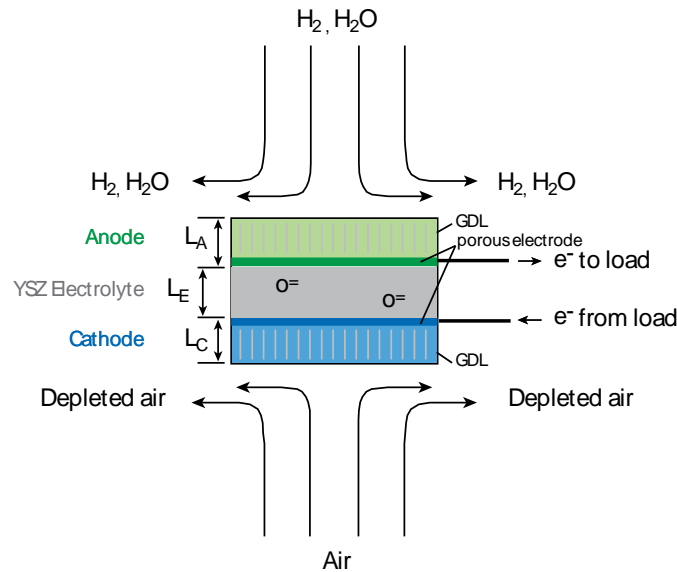
The Assignment

There are three parts to this week’s assignment. The first two can be worked in parallel: One is to generate a basic fuel cell code given specified property values. The other is to work out how those property values vary with temperature, so that you can extend your analysis to other conditions. That extension occurs in the third part of the project, where you incorporate your temperature-dependent properties into your code so as to explore how the choice of operating temperature affects cell performance—a critical factor for SOFCs.

I have also given you the problem statement for the first part of Project 10. In it you incorporate flow channels into your cell, thereby completing the core model of an SOFC. This requires a couple of nontrivial modifications, but they should be pretty straightforward. Beyond that we will exercise your core model, and possibly do some additional analysis (e.g., the exergy distribution).

- (1) 55 Points Analyze the performance of a small element of a fuel cell—referred to as a *button cell*. Shown in the figure below, a button cell consists of an electrolyte layer (yttria-

stabilized zirconia, YSZ) sandwiched between porous electrodes (nickel) and separated from its gas supplies by gas diffusion layers (GDL)—additional layers of porous material that provide support and allow the gases to pass easily to the nickel/YSZ junction. The key difference between such a button cell and a fuel cell is that the gaseous reactants are supplied (and removed) in such a way that there is no accumulation (or depletion) as would occur if it were sharing common supply channels with many similar elements. The problem of analyzing a button cell is just a little bit simpler than doing a fuel cell with channels, but not to worry, we will deal with that next.



Assume that the gas jets impinging on the button are of sufficient velocity that they provide a known boundary condition for gas concentrations at the outer edge of each gas diffusion layer. Also assume that the problem is well modeled as being solely one-dimensional. (This is, in fact, the case if impinging jets are used, as shown.)

Assume that the cell is isothermal at 1000°C (including the gas supplies), and that the pressure in the gas diffusion layers is uniform at 1 bar. Use 15 S/m for the ionic conductivity of YSZ, and assume that the binary diffusivities for $H_2\text{-}H_2O$ and $O_2\text{-}N_2$ are 3.8378×10^{-3} and $2.9417 \times 10^{-4}\text{ m}^2/\text{s}$ respectively. (A *siemen*, S , also known as a *mho*, Ω^{-1} , is the S.I. unit of electrical conductivity. It corresponds to 1 ampere/volt, such that $1\text{ S/m} = 1\text{ (C/m}^2\text{-s)/(V/m)}$.) Assume that the thickness of the electrolyte is $50\text{ }\mu\text{m}$ and the thickness of each gas diffusion layer is 5 mm . You may assume that transport in the GDLs is by ordinary, binary diffusion—the layers are assumed to be sufficiently open that Knudsen-flow effects are negligible. Report all of your results in per-unit-area format such that the actual size of the button is immaterial to your results. (Also, neglect losses due to finite resistance in the electron conductor paths at the anode and cathode. These are typically much, much smaller than any other loss in the cell.)

Assume that the gas fed to the anode side of the cell is humidified hydrogen (3% water vapor by mole), and that the gas supplied to the cathode is engineering air. Use a cathode exchange current density of 1000 A/m^2 and assume that the anode is 100 times more facile than the cathode at performing its reaction. (In plain English, it has an exchange current density that is 100 times that of the cathode.)

Plot the electrical potential vs. area-specific current (a.k.a. *current density*, kA/m^2) over the range of current density from zero to its maximum value. Add a curve showing the power density (kW/m^2) to the plot. Also add curves showing the mole fraction of each relevant species (hydrogen, water, oxygen) at its respective electrode to the plot. (Note that it is depletion of one of these species at its electrode that causes cell operation to terminate at high current densities. Since this occurs because of inadequate diffusive transport, this is referred to as the *diffusion* or *concentration limit* of the cell.)

Make a plot that depicts the losses of electrochemical potential in the cell. This may be done by plotting the loss of electrochemical potential across each region of the cell (input minus output, just like exergy loss) as a function of current density. Show curves corresponding to the combined losses from the two gas diffusion layers (required to drive gas diffusion), the ohmic loss in the YSZ (required to drive O^- from cathode to anode), and the activation loss at each triple junction (required to drive reactants across the transition state). Report each of these losses in units of electron-volts (eV) per reaction so that they are all on a common basis. (FYI: $1\text{eV/rxn} = 96485\text{ J/mol-rxn}$)

Use the losses you computed above to show how each affects the electrochemical potential of the electrons that the cell delivers at its terminals. Starting with the overall affinity of the reactants, subtract each of these losses (at any given current density) from the affinity to build a set of curves depicting the cumulative loss. You should have five curves corresponding to a range from just the reactant affinity to inclusion of all four losses. Since the units being used are eV/rxn, the final curve should match your output electrical potential curve from above, just scaled by a factor of two (since there are two electrons delivered per reaction). If you wish, you can combine this plot with the loss plot to show the losses and their effect jointly.

- (2) 30 Points One of the most important choices in designing a fuel cell is determination of the temperature at which it will operate best. We would like to do that for a solid-oxide cell with YSZ as the electrolyte. Since there are four losses to consider—gas diffusion, ohmic, and two activation losses—we need to know how the operating variables that affect those losses vary with temperature.

Gas diffusion losses depend on the diffusivity of the gas. Since both the anode and cathode GDLs have only two species present (H_2 and H_2O at the anode, O_2 and N_2 at the cathode), only the binary diffusivity of these pairs of gases is needed. Use the expression from Bird, Stewart, and Lightfoot that appears in the lecture notes to plot how the binary diffusivities of these pairs vary with temperature. (Hold off on making the plot for now. We want to put several curves on the same figure.)

The ohmic loss of the cell is determined by the conductivity of YSZ for oxygen ions. Fortunately, the conductivity of high-quality YSZ at 1000°C is well known (15 S/m). So what we need to know is how to scale away from this point for different temperatures. Since oxygen ion conductivity is an activated “jump” process from site to site, it is perhaps not too surprising that the rate of jumps (and therefore the conductivity) follows an Arrhenius form with (absolute) temperature

$$\kappa(T) = A \exp\left(-\frac{E_A}{RT}\right)$$

where E_A is the activation energy—almost exactly 1 eV/particle (96.5 kJ/mol) — and A is a constant. This constant may be eliminated by using the conductivity at any known condition (i.e., κ_o at T_o) such that the expression becomes

$$\kappa(T) = \kappa_o \exp\left[-\frac{E_A}{R}\left(\frac{1}{T} - \frac{1}{T_o}\right)\right]$$

Use this expression to evaluate how the ionic conductivity (and therefore ohmic losses) of YSZ varies with temperature.

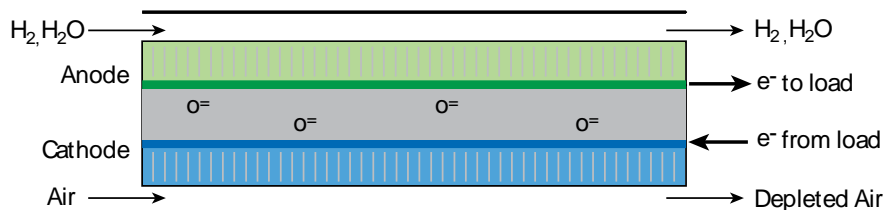
The activation loss for each electrode is determined by its exchange current density (which carries the information for the transition-state energy). It too follows an Arrhenius trend with temperature, with an activation energy that depends upon the choice of both the electrolyte and the metal used for the electrode. Assume a value of 100 kJ/mol for your calculations. Since we have no independent data for the anode exchange current density, continue to assume that it is a factor of 100 higher than that of the cathode. (While this is only approximate, experience has shown that this provides at least a reasonable scaling for this parameter.)

Make a plot that shows how the key parameters of all four loss mechanisms vary with temperature over the range from 600 to 1300°C (for 1 bar reactant pressure). Since the chemical potential of each reactant varies with temperature, also show how the chemical affinity of the overall reaction varies over this range of temperature. In order to make the plot a little more manageable, instead of plotting the actual values, plot each quantity normalized by its value at 1000°C. This will emphasize the effect of changing the temperature away from our base operating condition for Part 1.

- (3) 15 Points Adapt your code from Part 1 to use the temperature-dependent properties from Part 2. Use it to generate a set of electrical potential vs. current density, first-law efficiency (LHV basis) vs. current density, and power density vs. current density curves for a button cell operating at temperatures from 700 to 1200°C in steps of 100°C. Show potential and power density as a family of curves on a single plot vs. current density. Make a second plot showing efficiency and power density vs. current density.

Project 10: (Early notification of Part 1 in case you want to start early given finals, etc.)

- (1) 50 Points Modify your button code by extending it in length and adding gas channels on the outside of the anode and cathode gas diffusion layers. Use a channel width of 10 mm, a height of 5 mm, and a length of 0.5 m. (If you imagine this channel as being folded back and forth 5 times, possibly interleaved with another identical channel, you have the basis for a unit layer of a small fuel cell stack.)



In order to adapt your button cell into such a channel cell, there are two key modifications you will need to make. The first is inclusion of the channels and tracking of the cumulative change in composition in them as the reactants and products flow down the length of the cell. Depletion of reactant concentration and build-up of products in the channels will lead to an additional “channel loss” that will affect the overall performance of the cell.

The second significant modification is imposition of a uniform electrical potential across the length of the channel. This uniform potential occurs because the conductivity of the nickel in the electrodes is high, such that electrons can easily flow along the length of the channel. In the case of the button cell, there was no need to impose this externally since the one-dimensional nature of the cell and its reactant streams precluded development of an electrical potential gradient along the surface of the cell. That is not true with channels. You can imagine that the upstream portion of the cell, with its fresh reactants, can produce a significantly higher current density (at a given voltage) than the downstream portions with depleted reactants.

Fortunately your button cell is, in essence, a differential element along the length of the channel cell. As such, if you string button cells together, keep track of the gases they are exposed to in the channels, and insist that they all produce current at the same output voltage, then the sum of their efforts will be the output of the cell (the cumulative current and power).

Begin by writing a function that wraps around your button cell code such that it returns the current density (and anything else you need) produced by the button (now a differential element) at a specified voltage. This should sound familiar since it is similar to what you had to do to implement the *h-P* flash using the *Flash_zTP* function. Once that is functioning, string elements together, add the channels, and you are off to the races.

Track the following quantities as a function of position along the channel: current density, cumulative current up to that point in the cell, gas composition in each channel, and the heat flux required to maintain the cell at isothermal conditions. (Note that this heat flux will have to be managed to avoid local inhomogeneities that can lead to either loss of performance or excessive thermal stress. Note too that these can be coupled effectively with the endothermic steam-methane reforming reaction in order to implement complete or partial internal reforming of natural gas in the cell. I had hoped that we could get to that—it is a logical next step—but we are out of time, so we will have to let it go.)

The deliverables for this part will include plots of the overall electrical potential vs. current (not current density this time, total current), power vs. current, and fuel utilization vs. current for a few yet-to-be-specified flow conditions. I will also ask you to supply plots showing how the quantities you track along the channel vary with position for a few flow conditions and/or output potentials.

The Write-Up

Again only the figures are required. As always, please provide a brief statement of how much time was spent and the most/least useful aspects of the assignment.

The Deliverables (for Project 9 only)

(1) Plot the following vs. current density (kA/m^2) all on one plot (busy!):

- Electric Potential (V)
- Power Density (kW/m^2)
- H_2 mole fraction at the anode
- H_2O mole fraction at the anode
- O_2 mole fraction at the cathode

Plot the losses of electrochemical potential (eV/rxn) vs. current density (A/m^2) on one plot:

- Combined GDL Loss
- Ohmic Loss
- Anode Activation Loss
- Cathode Activation Loss

Plot how the losses above reduce the electrochemical potential of the button cell on a electrochemical potential (eV/rxn) vs. current density (kA/m^2) plot. There are five lines:

- Overall Affinity (straight line)
- Four more lines after each additional loss is included (one by one, cumulative).

(The last line of this plot should take into account all of the losses, and have the same shape as your electrical potential curve from the first plot in this problem.)

(2) Plot the following vs. temperature ($^{\circ}\text{C}$) from 600-1300 $^{\circ}\text{C}$ on one plot, normalized by each quantity's value at 1000 $^{\circ}\text{C}$:

- Overall Reaction Affinity
- O_2/N_2 Diffusivity
- $\text{H}_2/\text{H}_2\text{O}$ Diffusivity
- Ionic Conductivity of YSZ
- Cathode Exchange Current Density

(3) For temperatures between 700 and 1100 $^{\circ}\text{C}$ in steps of 100 $^{\circ}\text{C}$:

Plot electrical potential (V) and power density (kW/m^2) vs. current density (kA/m^2)

Make a second version of this plot showing the first-law efficiency (LHV basis) and power density vs. current density (just to emphasize the effect on efficiency).