MEGN 570 - Electrochemical Systems Engineering

Project: Transient model of an electrochemical device

Due at Scheduled Time for Final Exam (TBD)

For your semester-long project, you are to construct a limited-dimensional (one or quasi two-dimensional) numerical model of an electrochemical system/device of your choosing. You will use this model to explore some fundamental aspect of the device performance - in essence, performing a parametric study to optimize some aspect of the device design. Your 'device' of interest could be a model system (lab-scale), a consumer device, or an industrial-scale system.

The model should include the following elements: (*i*) conservation of mass, (*ii*) conservation of energy, (*iii*) conservation of species, and constitutive models for (*i*v) mass transport, (*v*) chemical reactions (including at least one charge-transfer reaction), and (*vi*) species thermodynamics. Your model may omit, at most, one of the three conservation equations and the associated constitutive model, but must justify why such effects do not influence system performance. The models should be transient in nature, and I would recommend simplifying the geometry and/or physics involved so that you can model system as one-dimensional. Note that you can integrate your transient equations out to long time spans to model steady-state behavior, or model transient phenomena.

The system you choose should have some basic relevance to current scientific/industrial efforts. When identifying your system, you will be asked to provide 1 citation from the literature to demonstrate why the application is important, or preferably why the parameter you choose is important. If there is experimental data that inspires the basic question you are trying to answer, or data that you can attempt to fit with your model, this would certainly help guide your efforts.

However, please keep in mind that this project will be within one semester, and pick a project that is appropriately challenging, but still realistic: Constructing a basic system model and varying some parameter to study its effect on device performance will be a significant achievement, and give you the tools necessary to construct more complex and/or realistic models, going forward. Some example topics are specified further below. HW assignments throughout the semester will guide your efforts, and matlab files with a basic structure and some suggested function calls will provide further assistance.

Still, if you are feeling ambitious, I will consider up to 20% extra credit on this project for results that I feel approach "publication-worthy" status (see below for further clarification). Projects that are directly related and contribute to your graduate research are encouraged, so long as they do not rely overtly on models that you have constructed prior to this course. Please consult me if you would like to discuss possible exceptions to this last point.

As a very basic example, consider your instructor's first publication (DeCaluwe, Zhu, Kee, and Jackson, *J. Electrochem. Soc.*, 2008). This was a 1-D transient solid oxide fuel cell (SOFC) model to explore the impact of anode microstructure on device performance. The basic architecture is shown in Figure 1.

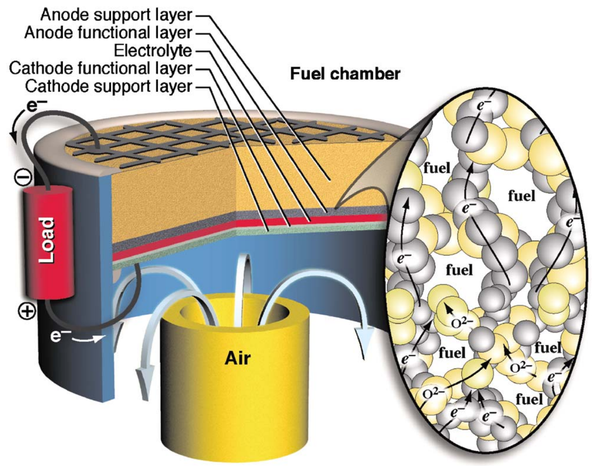

Figure 1: Layout of 1-D SOFC cell. The balloon illustrates ion and electron current paths near the interface between the anode support layer and anode functional layers.

Initial simulations varied the anode porosity and tortuosity to determine their effects on SOFC performance, as shown in Figure 2. This is the level of modeling intended for this project - a simple study to determine the effects of some parameter (or set of parameters) on device performance, durability, or system integration.

The model was then run to match experimental data for SOFCs with varying porosities. It is commonly assumed that porosity and tortuosity will vary together, but co-variation of these parameters within realistic ranges did not lead to suitable fits. Only by also varying the "utilization thickness" (δ, the anode thickness over which electrochemical reactions took place) were suitable fits obtained. This led to the realization that trans-

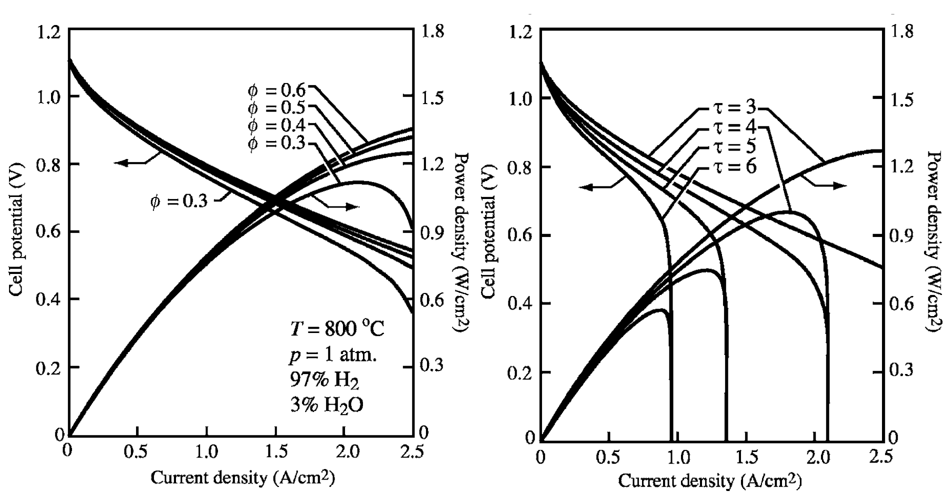

Figure 2: Parametric variation of porosity ϕ (right panel) and tortuosity τ (left panel) to study the effects on SOFC performance.

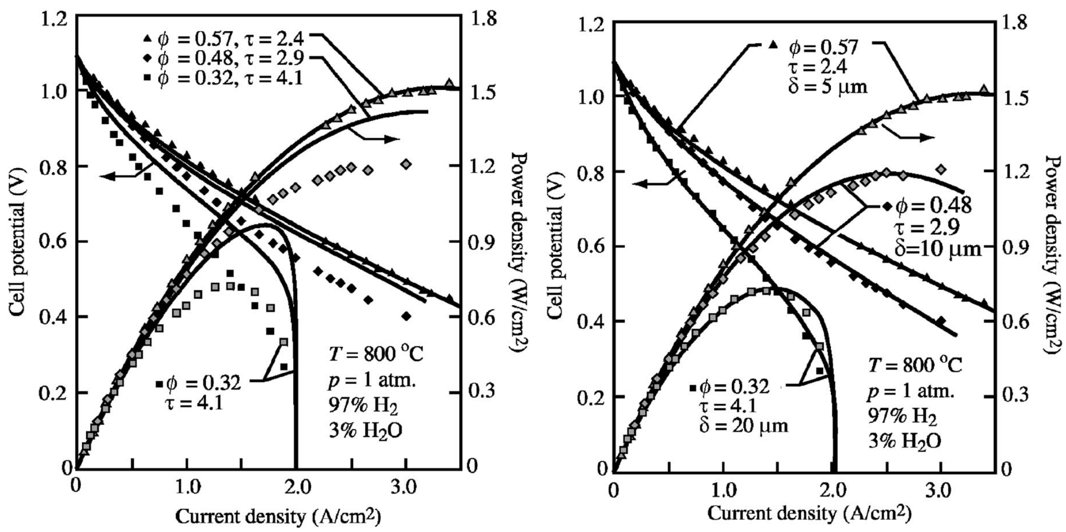

Figure 3: Simulated polarization and power density curves (a) with covarying porosity and tortuosity and (b) with covarying porosity, tortuosity, and utilization thickness δ. Simulations are fit to experimental data from Zhao and Virkar, *J. Pow. Sour.*, 2005. Results demonstrate that transport limitations result in the expansion of the utilization thickness, to increase the total reaction rates.

port limitations imposed by lower porosity led to slower reaction rates in the active layer of the anode, which led to an increased δ value to maintain the total current density. This increased δ, in turn, increased the ionic resistance. So transport limitations showed up in the performance curves as higher ionic resistances - a non-intuitive result. These results are summarized in Figure 3. This level of analysis would constitute the full 20% extra credit.

At the end of the semester, you turn in a write-up of your study, which should be written in the form of a journal paper, and include sections for (*i*) Introduction/motivation, (*ii*) Model formulation, (*iii*) Results, (*iv*) discussion, and (*v*) conclusions. You should present plots of device performance as a function of your parametric variation, plus relevant plots of fundamental properties (species concentrations, density, current density, etc.), as relevant, to elucidate the fundamental phenomena that explain the performance variations.

Sample topics are listed below. You are free to use any of these, but are still required to provide a citation to demonstrate the relevance of the topic. Also, these topics are still rather open-ended - you will need to narrow the focus, over the course of the semester.

- The effect of operating temperature on fuel cell performance.
- The effect of catalyst loading on glucose sensor signal strength.
- The effect of SEI thickness on Li-ion Battery performance.
- The effect of current density on thermal management in PEM fuel cells
- The role of electrode microstructure in Li-ion Battery discharge rates.