Electrochemical Systems Engineering, Homework 2: Charge Transfer Modeling and Project Initialization

Due Monday, February 24, 2026

This homework will be submitted as a series of two GitHub Pull requests:

1. A pull request to the 'Projects' repository with your updated project

2. A pull request to the 'Assignments' repository with:

   - A completed version of '`sofc_model_template.py`' that executes the simulations below, and

   - A pdf that includes the two requested figures and associated discussion.

1 Project Initialization

Start your project model by creating a code that, at a minimum, does the following:

- Creates a solution vector SV containing at least one electric potential in your system. Other variables are fine to include if you wish, but start with variables needed to define your double layer potential for at least one system interface.

- Creates a residual function that defines $\frac{dSV}{dt}$ and integrates over some set time span.

You do not have to use my variable names (i.e. there are plenty of good variable names for your state other than SV. Many online examples will simply use y). Also, your residual function can, for now, just return zeros. We will soon add additional calculations in future updates, so if you want to add some of the charge-transfer details, such as in the SOFC model below, that would not be a bad idea, either. In general, you can use the SOFC code as a template, if you are having trouble getting started.

1.1 Submission requirements:

1. Email Dr. DeCaluwe with your GitHub handle so he can invite you to the 'MEGN-570' organization.

2. Submit a *well-documented* code to the 'MEGN-570/Projects' repo via a GitHub pull request.

2 SOFC Model: Charge Transfer Modeling

We will model charge transfer in an SOFC operating at 700°C. Implement conservation of charge and model the double layer at each anode as a capacitor, such that

$$\frac{d\Delta\Phi_{\text{dl}}}{dt} = -\frac{i_{\text{dl}}}{C_{\text{dl}}}, \tag{1}$$

where the double layer potential is $\Delta\phi_{\text{dl}} = \phi_{\text{ed}} - \phi_{\text{elyte}}$, the electrode phase potential minus the adjacent electrolyte phase potential, and the double layer current i_{dl} comes from the assumption of charge neutrality:

$$i_{\text{dl}} = \pm i_{\text{ext}} - i_{\text{Far}}, \tag{2}$$

where the sign on the external current i_{ext} depends on the electrode (positive i_{ext} delivers positive charge to the anode, and removes it from the cathode), and i_{Far} represents Faradaic current due to charge transfer. We will model this last term using Butler-Volmer kinetics:

$$i_{\text{Far}} = i_{\circ} \left[\exp\left(-\frac{\beta n_{\text{elec}} F \eta}{\overline{R}T} \right) - \exp\left(\frac{(1-\beta) n_{\text{elec}} F \eta}{\overline{R}T} \right) \right]. \tag{3}$$

For i_{dl}, and i_{Far}, positive current represents the flow of positive charge to the bulk electrode phase. As noted above, positive i_{ext} represents the flow of positive charge in the external circuit from the cathode to the anode (i.e. the device produces electrical work if the current is positive).

Using the 'sofc_model_template.py' code, create a model that stores sufficient information to resolve the double layer potential difference at each electrode interface, as well as the drop in electric potential across the electrolyte.

We will use a fairly simple electrochemical model, for now, assuming constant exchange current density $i_{\circ}$ and constant reversible potential U for each electrode interface, as given below. Some suggestions / hints, for your coding:

- Pay careful attention to units and signs.

- It is likely that not all of the template is in its final form. You may have to play with the integrator (solve_ivp) options, for instance.

- Ask questions by posting discussions to Canvas.

2.1 Submission requirements

Build a model that predicts and plots the following potentials as a function of time:

- The electrolyte potential at the anode interfade $\phi_{\mathrm{elyte, an}}$

- The electrolyte potential at the cathode interfade $\phi_{\mathrm{elyte, ca}}$

- The cathode potential ϕ_{ca}.

(we assume that the anode potential $\phi_{\mathrm{an}} = 0$). Run the model and save figures for two conditions:

 i Open circuit, $i_{\mathrm{ext}} = 0$

 ii For $i_{\mathrm{ext}} = 0.5$ A/cm^2.

For each plot, explain the shape of the three electric potential traces. What explains their shape? To guide you, your plots should look like this (minus some formatting changes – yours will have a legend and no subfigure formatting):
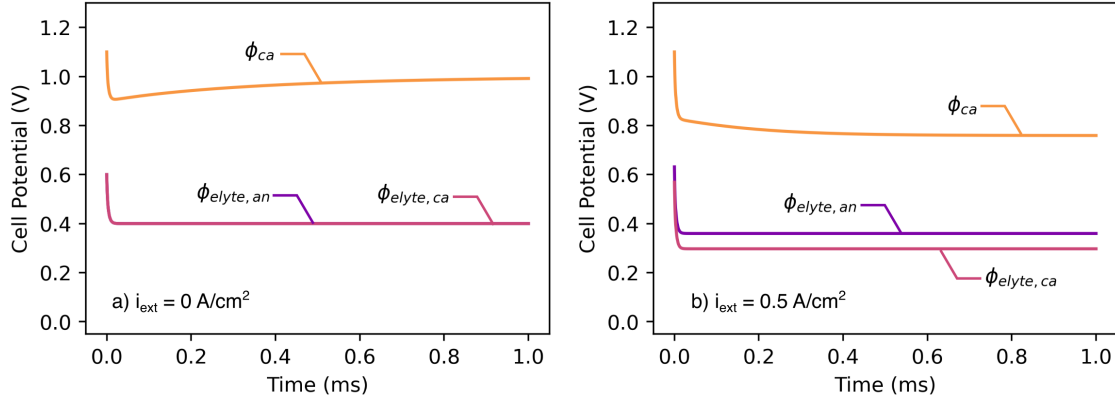
2.2 Anode Details

At the anode O^{2-} in the electrolyte reacts with 2 hydrogen atoms adsorbed on a Ni surface ($H_{Ni(s)}$) to form adsorbed water ($H_2O_{Ni(s)}$) and electrons in the Ni (e^-_{Ni}).

$$O^{2-}_{elyte(s)} + 2\,H_{Ni(s)} \leftrightarrows []_{elyte(s)} + H_2O_{Ni(s)} + []_{Ni(s)} + 2\,e^-_{Ni}$$
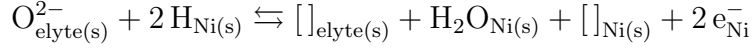
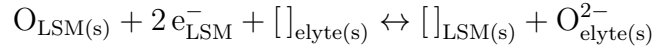where $[]_{elyte}$ is a surface vacancy on the ceramic electrolyte surface, where the oxide formerly resided, and $[]_{Ni(s)}$ is a vacancy on the Ni surface. The parameters for this reaction are as follows:

Parameter	Description	Value	Units
U_{an}	Equilibrium potential difference	-0.4	V
$i_{o,\,an}$	Exchange current density	5×10^{-2}	$A\,cm^{-2}$
$C_{dl,\,an}$	Double layer capacitance	5×10^{-6}	$F\,cm^{-2}$

Table 1: Anode charge transfer parameters. All area-specific units are per total SOFC geometric area

2.3 Cathode Details

At the cathode, an Oxygen atom adsorbed on an lanthanum strontium manganite (LSM) perovskite surface reacts with two electrons to form O^{2-} in the electrolyte:

$$O_{LSM(s)} + 2\,e^-_{LSM} + []_{elyte(s)} \leftrightarrow []_{LSM(s)} + O^{2-}_{elyte(s)}$$

where $[]_{elyte}$ is a surface vacancy on the ceramic electrolyte surface, and $[]_{LSM(s)}$ is a vacancy on the LSM surface. The parameters for this reaction are as follows:

Parameter	Description	Value	Units
U_{ca}	Equilibrium potential difference	0.6	V
$i_{o,\,ca}$	Exchange current density	1×10^{-2}	$A\,cm^{-2}$
$C_{dl,\,ca}$	Double layer capacitance	1×10^{-4}	$F\,cm^{-2}$

Table 2: Cathode charge transfer parameters. All area-specific units are per total SOFC geometric area