1-D model of a solid oxide fuel cell incorporating the charge transfer and mass transport limitations

Introduction

A 1-D model of a solid oxide fuel cell (SOFC) considering transport and charge transfer limitations. The code samples provided by Dr. DeCaluwe are heavily used here to expedite the modeling process. A quite ambitious topic is chosen and considered to be analyzed at first, in which the impact of pressure on the performance of a reversible solid oxide cell is attempted to be assessed. Nevertheless, a simple SOFC model is considered here and only the effect of different operating temperatures are studied. SOFCs are mid to high temperature fuel cells that have relatively higher power densities compared to other types of fuel cells including protonic exchange fuel cells. Even though higher operating temperature is seen as an advantage to the SOFCs, where a bottoming cycle can be incorporated to increase the overall efficiency. Nonetheless, higher operating temperature is also translated as higher capital costs including material costs and manufacturing costs. The main application of SOFCs is in stationary power generation systems, due to their higher efficiency and longer startup time that deters their use in mobile applications.

Model formulation

The overall reaction taking place in a SOFC follows as:

$$H_2 + \frac{1}{2} O_2 \rightarrow H_2O$$

The Overall reaction breaks down to the following anode side and cathode side reactions with an oxygen ion conductor electrolyte in between, respectively:

$$H_2 + O^{2-} \rightarrow H_2O + 2e^-$$
$$O_2 + 4e^- \rightarrow 2O^{2-}$$

The charge transfer is modeled via Butler-Volmer equation that connects the chemical reactions on the surface to the thermodynamic potentials.

$$i = i_0 \left[exp\left(\frac{\beta_{fwd} F \eta}{RT}\right) - exp\left(-\frac{\beta_{rev} F \eta}{RT}\right) \right]$$

Where β_{fwd} and β_{rev} are both considered zero and η is defined as the difference between the thermodynamic potential of the electrode subtracted by the double layer potential in that electrode. At a given external current, the double layer current of an electrode can be obtained by an equation that dictates the charge neutrality. For example, at the anode:

$$i_{ext} - i_{Far,an} - i_{dl,an} = 0$$

Where i_{ext} is an assigned quantity and $i_{Far,an}$ can be determined via Butler-Volmer equation. Besides, the double layer current that is represented by the far-right term in the equation above, can be obtained via the double layer charge capacity, as follows:

$$C_{dl,an} = \frac{Q_{dl,an}}{\Delta \varphi_{dl,an}}$$

Where $Q_{dl,an}$ is the charge transferred and $\Delta\varphi_{dl,an}$ is the potential difference between the overpotential and the thermodynamic potential of the electrode (anode in this case). The required equation to solve the double layer potential can be attained by rearranging the above-mentioned equation and taking the derivative with respect to time:

$$\frac{\partial \Delta\varphi_{dl,an}}{\partial t} = \frac{i_{dl,an}}{C_{dl,an}}$$

For the sake of simplicity of the calculations, the anode half-cell potential is set to zero as a reference potential and the anode and cathode double layer potentials are stored in a solution vector to be determined. Once they are calculated, the anode and cathode layers' potentials can be obtained which then gives the cell potential at a given external current. The mass transfer limitations are not illustrated here but they are implemented into the model.

Results and discussions

All the files to solve the system of equations that solve the charge transfer and the mass transport equations in an orderly manner. The input parameters are stored in the input file, then they are initialized by another file that classifies the parameters. They all are called by a function that solves for the double layer potentials. A polarization curve is made at a temperature of 800 K, that can be seen in Fig. 1. There are several flaws with regard to the following figure, including the lack of use of the parameters that are in reasonable range with the operating conditions of a SOFC. The parameters are not altered since an ample amount of time is not devoted for the project. Nevertheless, I believe I now understand the fundamentals and have a working model that can be modified later so that it represents a reasonable SOFC model. However, the trends that are represented here perfectly aligns with the electrochemical fundamentals. The cell potential reduces as the current density increases exponentially. This can be justified due to the conflicting effects of equilibrium potential and the electrochemical reactions that moves in an opposite direction. The exponential effect comes from the exponential function buried into the Faradaic current calculation via Butler-Volmer equation.

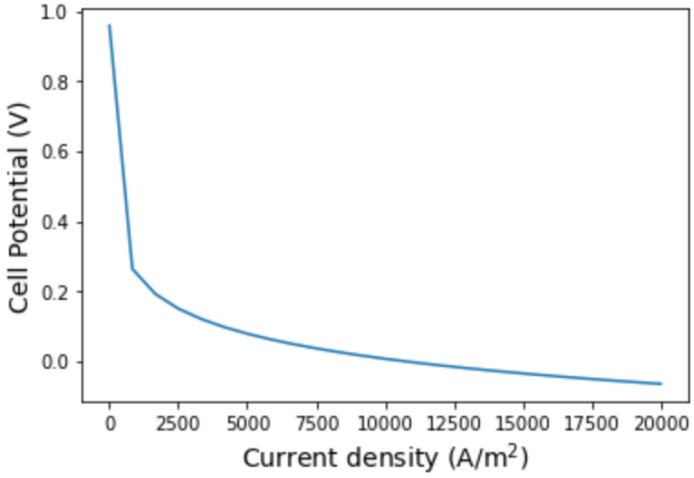

Figure 1: Polarization curve for the SOFC model at 800 K

The polarization curve then is plotted via defining a new function that calls the polarization function and changes the operating temperature each time. The polarization curves at different temperatures can be seen in Fig. 2. The cell voltage goes down as the temperature rises, due to the increasing effect of the double layer potential at each electrode. Although the equilibrium potential is not adjusted with respect to the temperature change which causes abnormalities in the figure.

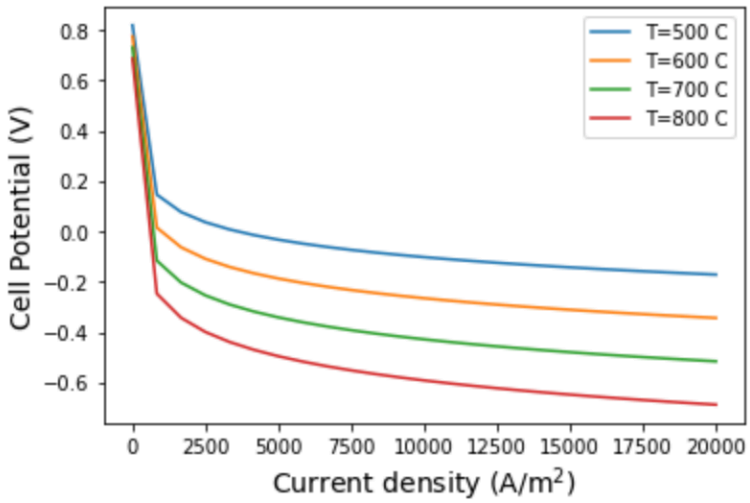

Figure 2: Polarization curve of SOFC at different operating temperatures

Conclusion

A perfectly working model is developed to model a solid oxide fuel cell that incorporates both charge transfer and mass transport limitations. Even though the developed model does not necessarily address the questions developed previously, nevertheless it can be adjusted easily to match a SOFC model. The reason for that is that the model is attempted to be developed using the PEMFC model developed by Dr. DeCaluwe, so the parameters and fuel cell geometry and material characteristics should match the correlated values of a SOFC. However, the model shows quite properly shows the trends, including the polarization curve and the effect of the temperature on the polarization curve. This model is going to be used as a reference later on for further development of an appropriate SOFC model.