A Polymer-Electrolyte Membrane Transport Model

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In order to predict fuel cell behavior better, especially failure mechanisms, a complete model of the fuel cell must be developed. A key reason for this model is to examine explicitly the transport of water throughout all regions of the cell sandwich. One of the most important regions for the operation of a polymer-electrolyte fuel cell is the membrane. The transport through and properties of this ionomer make it a crucial design element. Previous work[1,2] by us developed a physical model of transport that is semi-phenomenological and takes into account the documented water uptake differences due to the membrane being in contact with either saturated water vapor or liquid water (*i.e.* Schroeder's paradox).[3] The model described in this paper is the quantification of the physical model.

The transport model is based on concentrated-solution theory equations. There is some idealization in order to reduce the number of variables, and allow for the model to be easily incorporated into a complete fuel-cell model. All parameters are taken from the wealth of knowledge contained in the literature regarding polymer-electrolyte membranes. The parameters are functions of both water content and temperature. The values and functional forms of the parameters also help to validate the physical model further.

Within the transport model, there are two separate transport mechanisms that occur. The two mechanisms depend on whether the channels with the membrane are expanded or collapsed. When occurring together, the two mechanisms are assumed to operate in parallel, with the fraction of expanded channels acting as a switching function. This function is derived using a simple capillary model framework and isotherm, again with the relevant parameters determined from the literature data.

In order to compare the model to experimental data, several simulations were carried out with a very simple fuel-cell model. The different operating conditions explored included humidity of the feed gases, current density, operating temperature, operating pressure, and membrane thickness and equivalent weight. The complete simulation model had only one fitting parameter, the permeability in the gas diffusion layer, and was fit at only one set of operating conditions. The subsequent conditions were changed, and the net water flux through the membrane calculated. Figure 1 displays these results, which show a good agreement with the experimental data, taken from a variety of sources. Figure 2 displays a comparison of the current-potential profiles as a function of temperature, and again the simulations show good agreement with experiment.

Finally, along with being able to model Schroeder's paradox quantitatively in a transport model, this model also takes into account features that are presently ignored in literature models. For example, the model takes into account the fact that the water content of the membrane in contact with saturated vapor decreases with increasing temperature.[4] In all, the described model yields a complete and concise description of transport in a membrane under various operating conditions.

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References

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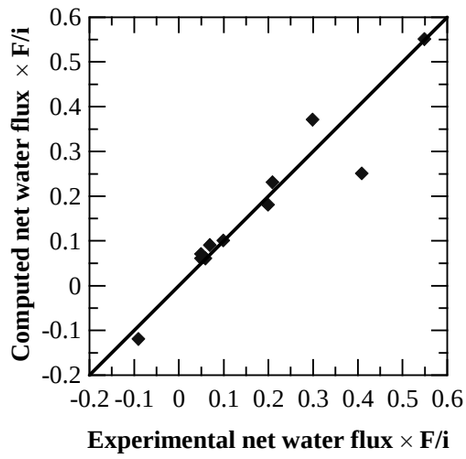

Figure 1 – Correlation graph between simulation and experiment of the dimensionless net water flux through the membrane for a variety of operating conditions. There is only one fitting parameter, which was fit at only one point.

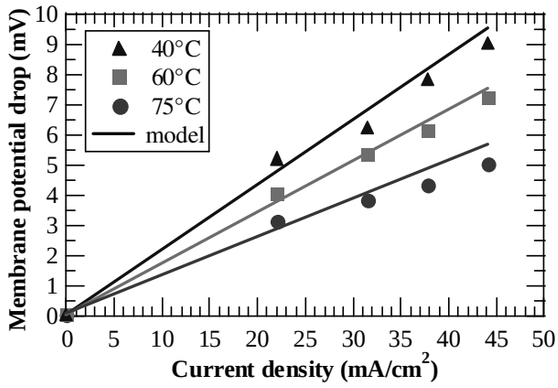

Figure 2 – Comparisons between simulation and experiment of the potential drop in the membrane versus current density at three different temperatures.