

Modeling the Polymer-Electrolyte Fuel-Cell Catalyst Layer

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It is well known that for optimal performance of polymer-electrolyte fuel cells (PEFCs), the design of the catalyst layers is critical. Even though these layers are the thinnest in a PEFC, they are arguably the most important and least understood. In many respects, making catalyst layers is a black art, where the exact microstructure and its effects are unknown. Through modeling, it is possible to ascertain the important phenomena occurring in the catalyst layers, which leads to improved performance and understanding.

In the catalyst layers, all of the various phases in a PEFC exist. Thus, there is membrane, gas, liquid, and solid (mainly carbon). In addition, there are platinum electrocatalysts where the charge-transfer reactions take place. An accurate model of a catalyst layer requires that all of these phases and their various interactions be modeled rigorously. Furthermore, to understand fully the effect that a catalyst layer has on overall cell performance, at least a one-dimensional sandwich model is required.

Previous work by us involved developing models for transport in a membrane¹ and for two-phase flow in PEFC gas-diffusion layers.² Both models are based on physical principles and observations from a variety of literature sources. In this work, these models are used in the PEFC sandwich model as well as in the appropriate phases in the catalyst layers. Such an approach ensures that the relevant changes in cell performance due to variables and models within the catalyst layer are applied correctly.

There have been various models proposed for the catalyst layers over the last few decades.³ Most are based on examining the effect of mass transport on the reaction rate, and may include such effects as flooding. The two main approaches are porous-electrode theory and the agglomerate model. This work uses a combination of the two models, where two different length scales are used, as shown in Fig. 1. The first length scale involves changes that occur over the length of the porous electrode, L , which mainly include changes in gas-phase concentrations and ionic- and electronic-phase potentials. The second length scale involves changes that occur locally where the reaction occurs.

Because the microstructure of the catalyst layer is unknown, especially in terms of membrane location, two different approaches are examined for the local scale. In the first one, an agglomerate structure is used where the diffusion coefficient of reactant gas in the agglomerate is used as a fitting parameter. This means that an internal effectiveness factor is used to alter the reaction rate where reaction, diffusion, and all phases occur in the agglomerate. In the second approach, the membrane exists only as an external film that covers the reaction sites. In this scheme, the thickness of the membrane layer is used as a fitting parameter, and the concentration of reactant gas at the reaction site is altered correspondingly. By comparing how well both of these approaches agree with and predict experimental data, one learns about the microstructure of the catalyst layer and the appropriate model to use. This information is valuable in the fundamental understanding of catalyst layers.

Using the appropriate model, simulations are run in order to understand various other effects and determine parameters. For example, mass-transfer coefficients are required to describe water moving among the gas, liquid, and membrane phases in the catalyst layer. By matching modeling results with water-balance data, the mass-transfer coefficients are obtained. These provide insight into water management and the membrane structure in the catalyst layer. Further simulations provide answers to such questions as how important is flooding in the catalyst layers relative to the gas-diffusion layers, how can the performance of the catalyst layers be increased through different designs (*i.e.*, changes in property values like porosity), what are the controlling phenomena, tradeoffs, and properties in the catalyst layers, and even what are the effects of microporous layers in PEFCs. By understanding the catalyst layers through theoretical means, one relegates their status from a black art to something more tangible and tractable, eventually leading to PEFC performance gains through better engineering and understanding.

Acknowledgements

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References

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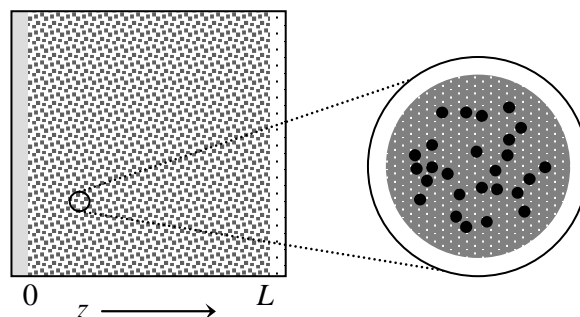


Figure 1 – Schematic showing the two different length scales in the cathode catalyst layer: the porous electrode, and the local reaction sites. The light grey is the membrane, the black is the electrocatalyst, the white is the gas, and the dark grey is the carbon support.