Investigating the Influence of Catalyst Layer Morphology on PEM Fuel Cell Performance by Numerical Simulation

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The performance of a proton exchange membrane (PEM) fuel cell is limited by electrochemical kinetics, proton conductance through the ionomeric material, and mass transport limitations. The electrochemical reaction itself takes place within the porous catalyst layer at the three-phase boundary on the surface of a platinum catalyst. A detailed one-dimensional model was developed to study the material and structural properties of the membrane, catalyst layer, and gas diffusion layer (GDL) of Gore PRIMEA® membrane electrode assemblies (MEAs). The focus of this paper is the application of the model to study the catalyst layer of a PEM fuel cell.

The catalyst layer is a structure of three interpenetrating and continuous networks: a carbon phase for electron transport (which also provides the support for the platinum catalyst), an ionomer phase for proton transport, and porosity for gas and water transport. The design of this complex structure has to consider a balance between electron, proton, and gas transport. To reduce the cost of the PEM fuel cell system it is desirable to minimize the amount of platinum in the catalyst layer. At the same time, it is important to maximize the utilization of the available platinum in the cell to optimize the fuel cell performance. Therefore, it is necessary to understand the influence of the morphological structure of the catalyst layer and how it influences the transport processes and electrochemical reaction.

Since it is challenging to experimentally measure concentrations and transport processes inside a running fuel cell, numerical modeling was chosen to provide a detailed insight into the fuel cell. The Gore Electrode Model (GEM) is a one-dimensional description of all essential processes in the PEM fuel cell. The model consists of five different domains: anode GDL, anode catalyst layer, membrane, cathode catalyst layer, and cathode GDL. Transport processes that are considered in the model are proton transport in the catalyst layers and membrane, electron and gas transport in the catalyst layers and GDL, and water transport in all five domains (see Fig. 1). The electrochemical reactions on anode and cathode are described by Butler-Volmer kinetics, which utilize the difference between protonic and electronic potential as the main driving force.

The model was validated against a set of experimental data of catalyst layers with varying structural properties. The model calculations represent the experimental data very well. The numerical results can now be used to analyze potential and concentration profiles as well as the distribution of the fluxes and reaction rates throughout the MEA.

Several examples will be presented to demonstrate the usefulness of the model. The catalyst utilization indicated by the local reaction rates throughout the thickness of the catalyst layer is compared for different electrode structures. It will be shown that it is possible to reduce the amount of platinum in the MEA considerably without a dramatic loss in performance.

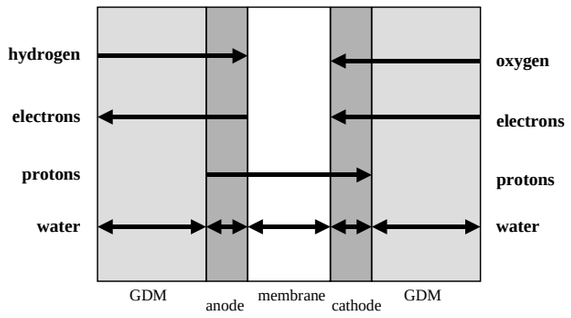

Figure 1: Transport Processes considered by the model.