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Enhanced Performance of Low Temperature PEM Fuel Cells by Introducing Hierarchically Structured Macroporosity to the Cathode Catalyst Layer

Jeffrey A. Marquis, Marc-Olivier Coppens

Isermann Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, 110, 8th Street, Troy, NY 12189 USA, Email: marquj@rpi.edu

1. Introduction

The wide scale implementation of proton exchange membrane (PEM) fuel cell technology is hindered to a large extent by the high cost associated with the platinum catalyst required for the electrochemical oxidation of protons at the cathode. In low-temperature PEM fuel cells, current cathode catalyst layer designs are plagued by inefficient catalyst utilization due to severe diffusion limitations when operating at medium to high current densities [1,2]. These diffusion limitations exist at two distinct levels within the cathode catalyst layer of a PEM fuel cell. Firstly, there are diffusion limitations in the spherical catalyst agglomerates themselves, caused by the low diffusivity of oxygen through the electrolyte. Additionally at high reaction rates, the formation of liquid water in the cathode catalyst layer floods the existing gas pore networks resulting in severe diffusion limitations along the thickness of the catalyst layer.

By introducing a hierarchical network of macropores within the cathode catalyst layer the diffusion limitations caused by liquid water formation can be largely mitigated [3]. These pores allow for continued bulk diffusion of reactants throughout the catalyst layer thus reducing detrimental flooding effects. Furthermore, modifications to the size and composition of the catalyst agglomerates serve to reduce the diffusion limitations caused by the electrolyte. An optimized hierarchical macroporous cathode catalyst layer is developed in this work. The performance of the optimized cathode catalyst layer is compared to conventional strictly nanoporous catalyst layers based on key performance indicators such as power density and catalyst loading.

2. Mathematical Model and Simulation

The PEM fuel cell cathode catalyst layer was modelled using a spherical agglomerate model [4,5]. This model describes the catalyst layer as a continuum of spherical catalyst agglomerates each comprised of platinum, carbon and electrolyte. This work also incorporates a liquid saturation model that accounts for the two-phase transport of liquid water in the membrane, catalyst layer and gas diffusion layer [6]. The catalyst layer macroporosity and the agglomerate composition were optimized to minimize the grams of platinum per kilowatt produced. Optimizations were performed in COMSOL Multiphysics 3.5a in conjunction with MATLAB 2009b.

Figure 1 shows the results of several simulations of numerous agglomerate sizes and catalyst layer thicknesses. Each line represents a catalyst layer comprised of different sized monodisperse agglomerates. A given point on a line represents the results of the

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optimization for that given agglomerate radius and catalyst layer thickness. The optimum macroporosity for each of these simulations was dependent upon the selected agglomerate radius. Values ranged from 50% macroporous for the smallest agglomerates, down to 30% for the largest agglomerate size. Furthermore, we see that the optimum catalyst layer thickness ranges between 10μm and 18μm.

The optimized hierarchical structures show enhanced performance over the conventional strictly nanoporous cathode catalyst layers. As the agglomerate radius decreases the diffusion limitations within the agglomerate are reduced and reaction rates are heightened. As a result, liquid water is formed at a faster rate, which slows down diffusion of oxygen through the thickness of the catalyst layer. The optimized hierarchical structures show an increase in macroporosity as the agglomerate radius decreases to counteract this flooding effect.

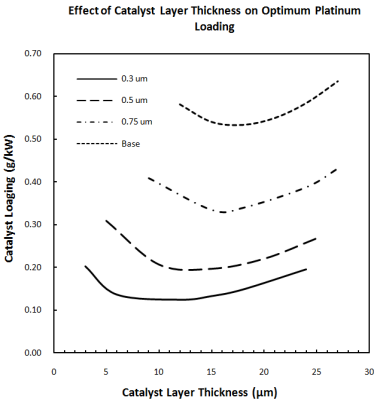

Fig. 1: Comparison of optimized agglomerate compositions at various catalyst layer thicknesses and agglomerate radii. All simulation run at nominal cathode

3. Conclusions

Optimization of a hierarchically structured macroporous cathode catalyst layer in a PEM fuel cell was conducted. The macroporosity as well as the agglomerate size and composition were optimized to minimize the catalyst loading. The introduction of structured macroporosity allows for the continued bulk diffusion of reactant gases through the catalyst layer when operating at high current densities. Optimization of the agglomerate composition results in decreased diffusion limitations within the catalyst agglomerate itself. It has been shown that cathode catalyst layer performance can be enhanced multiple fold by the introduction of hierarchically structured macroporosity.

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