Modeling the Effect of Discrete Distributions of Platinum Particles in the PEM Fuel Cell Catalyst Layer

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Abstract

Polymer electrolyte membrane (PEM) fuel cells are one of the most environmentally-friendly energy conversion devices. The catalyst layer (CL) is a critical component of the fuel cell because all of the electrochemical reactions occur within it. The CL requires expensive Platinum (Pt) catalyst to drive the reactions. A model to better understand the effect of Pt particle size and distribution on fuel cell performance will allow one to design and optimize its usage. Bultel et al. [1-4] were the first to model the Pt particles geometrically and accounted for their discrete distribution in the CL. They considered the CL as a set of discrete catalyst nanoparticles that constitute a hexagonal network throughout the CL. Similarly, Yan et al. [5] considered the discrete configuration of Pt particles and proposed a microscopic model to investigate a single catalyst particle consisting of carbon-supported Pt nanoparticles and an ionomer binder. In this study, the work of Yan et al. [5] is extended, and the significance of modeling discrete carbon-supported Pt particles is emphasized by comparing the fuel cell performance results from the discrete particle case to the baseline case which assumes a uniform catalyst coverage (Figure 1). The proposed model is governed by a diffusion equation which is coupled with the nonlinear reaction source term given by the Butler-Volmer equation at the active boundaries. The coupled nonlinear equation system is solved by COMSOL. Performance curves (overpotential vs. current density) for the two cases are studied as a function of catalyst loading in Figure 2 and Figure 3. Higher Pt loading for the particle case is interpreted as an increase in Pt particle size while keeping the number of particles constant. It is apparent that the uniform coverage assumption cannot capture the influence of catalyst loading on performance (Figure 2). This shortcoming is because the diffusion losses for the uniform coverage case arise only at the ionomer film that covers the particle. On the other hand, the discrete particle case provides a more realistic result (Figure 3) and reveals that diffusion limitations at the discrete particle level must be considered for such models. In addition, a parametric study is carried out to understand the effect of inter-Pt particle distance, thickness of the ionomer film, Pt-weight ratio, number of Pt particles, and other geometric variations that are characteristics of the CL microstructure. The study reveals that the particle level diffusion limitations play an important role on the reaction characteristics and should be considered for the fidelity of CL models. Eventually, such microscale models may prove helpful in gaining further insight into the complex phenomena occurring within the CL, and provide guidelines to design novel CL microstructures.

Reference

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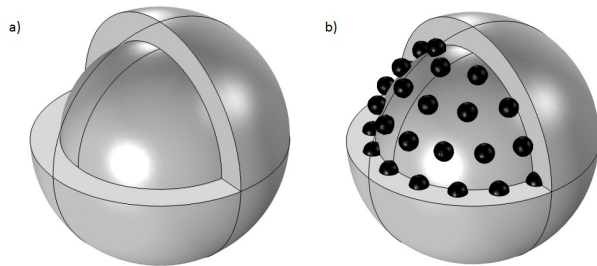
Figures used in the abstract

Figure 1: (a) Carbon support uniformly covered with Pt; (b) Pt particles modeled discretely on carbon support. An ionomer film of prescribed thickness covers both particles.
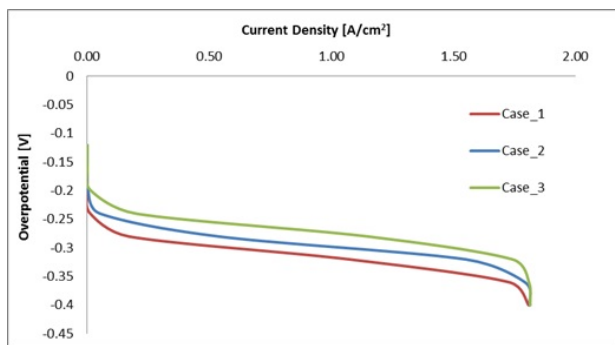

Figure 2: Effect of catalyst loading on performance obtained with the uniform coverage approach.
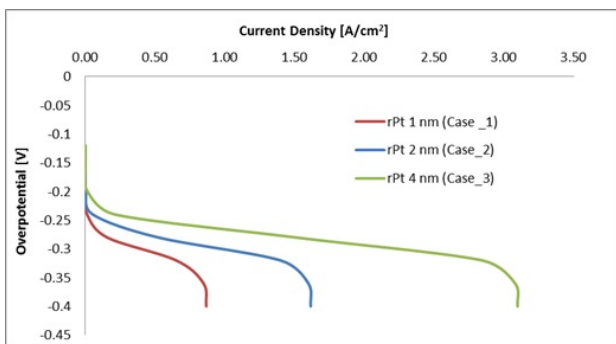
Figure 3: Effect of catalyst loading on performance obtained with the discrete particle approach.