

Single Catalyst Particle Model of in Cathode Catalyst Layer of PEM Fuel Cells

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1. Introduction

Modeling the operation of PEMFC catalyst layers has been developed greatly over the past decade. Current catalyst layer models can be classified into two groups according to the level these models deal with (i) the macroscopic models which consider the catalyst layer as a whole and (ii) the microscopic models which consider the transport phenomena at the pore level. Many macroscopic models have been developed to describe fuel cell working behavior, such as the flooded agglomerate and homogeneous models [1,2]. The most accepted model is the flooded agglomerate model. According to this model, carbon-supported catalyst particles flood with the electrolyte, and form agglomerates covered with a thin film of electrolyte. The catalyst layer consists of macro-micro porous, interconnected, hydrophobic regions to allow the reactant gas access to the surface of agglomerate regions. Then, the reactant gas diffuses through the film to the catalyst, where the HOR or ORR reactions occur. The flooded agglomerate models are very successful in explaining oxygen diffusion in the hydrophobic pores and electrolyte thin films. However, all these models consider the catalyst layer to be a continuous medium composed of carbon-supported catalyst with recast polymer electrolyte. Therefore, they are not able to identify possible effects resulting from the discrete distribution of catalyst phase in the agglomerates.

Microscopic models developed by Bultel et al. [3] address mass transfer and ion transfer in both the catalyst and supporting materials (carbon particles and Nafion) at particle level. The catalyst and electrolyte are treated as separate, discrete objects. These microscopic models can provide insights to the detailed transfer mechanisms at the pore level and the particle size effects on PEMFC performance. However, Bultel's model cannot predict the platinum particle size effect on the fuel cell performance since their model treated the Pt/carbon particle as a homogeneous mixture of platinum and carbon.

A microscopic approach is proposed herein for predicting the behavior of the active layer from the local mass diffusion at a single catalytic particle level. This model is numerically performed for geometric descriptions of the active layer. The main purpose of this work is to study the effect of catalyst particle size (Pt), platinum loading and electrolyte thickness for the oxygen reduction reaction (ORR) on a cathodic catalyst particle. The modeling results will be used to improve the agglomerate model. Furthermore, the model will be used to optimize the catalyst layer design and preparation.

2. Results and discussion

The modeling results confirm that the platinum particle size, platinum loading and ionomer thickness can each play an important role on local mass and charge transport in the PEM fuel cell catalyst particle agglomerate. The local spherical diffusion, reactant distribution and electrochemical kinetics are strongly influenced by particle size, platinum loading and ionomer thickness.

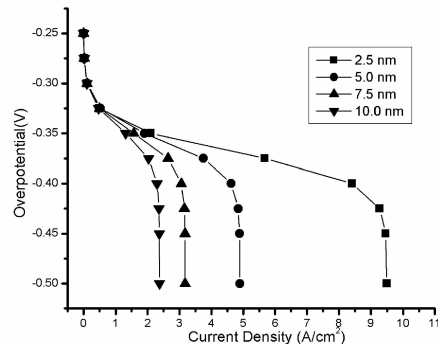


Figure 1. Influence of platinum particle size on PEMFC catalyst specific activity.

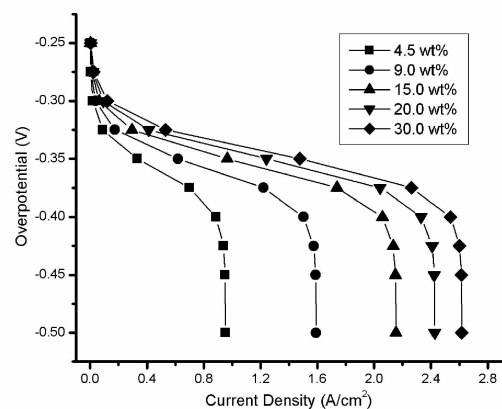


Figure 2. Influence of platinum loadings on PEMFC performance

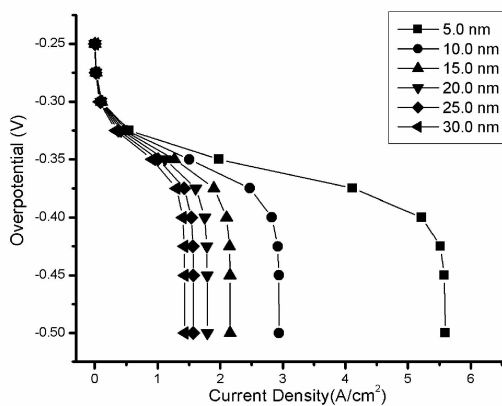


Figure 3. Influence of ionomer thickness on PEMFC performance

Reference

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3. O. Antoine, Y. Bultel, R. Durand, and P. Ozil, *Electrochim. Acta* 43 (1998) 3681.