497c Study of Proton Exchange Membrane Fuel Cells (Pemfc) Using Detailed Models for Electrode Structure Optimization

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There has been growing interest in the modeling of proton exchange membrane fuel cells (PEMFC) over the last decade. Models proposed during the early years were typically one-dimensional and accounted for steady state mass transport and electrochemical kinetics. Subsequently, both simplified and complex models in terms of dimensionality and physicochemical phenomena have been studied. A common feature in all these models was that the reaction or catalyst layer is not modeled in detail. The reaction layer is treated as an ultra-thin layer, thus neglecting the transport of reactant gases and products. Hence, the catalyst layer is treated as a source/sink boundary condition for transport equations in the gas diffusion layer. Contrary to this assumption, even if gas phase transport is neglected on the consideration of ultra-thin layer, the presence of ionomer in the reaction layer along with carbon and platinum makes transport within the pores of the ionomer important. Moreover, catalyst layer is the region where various limiting mechanisms can occur and thus have a strong influence on the overall performance of the cell.

It is widely accepted that gas-diffusion electrodes (GDEs) used in fuel cells are three-phase electrodes with a complex geometry consisting of conducting solid material for electron transfer, hydrophilic phase for ion transfer and open pores for gas transport. Tantram and Tseung [1] for the first time studied the structure and operation of hydrophobic electrodes under electron micrographs. As GDEs are difficult to characterize, one of the first assumptions that was made to model them was the concept of "flooded agglomerates" by Giner and Hunter [2]. They have considered cylindrical geometry for the agglomerates. Subsequently, many studies conducted by various researchers with the spherical flooded-agglomerate models were presented for both alkaline fuel cells (AFC) and phosphoric acid fuel cells (PAFC). Similarly, researchers have started studying the effects of various phenomena in the catalyst layer of PEM fuel cells based on flooded-agglomerate structure during the last two years [3, 4, 5, 6, 7].

A two-dimensional steady state model for PEMFC cathode with detailed characterization of cathode catalyst layer has been used in this work. Based on the experimental investigations of Middleman [8], the catalyst layer is characterized using spherical flooded-agglomerates. A uniform distribution of spherical agglomerates with an equal number density throughout the catalyst layer is assumed. The steady state model is used to predict the typical i-v characteristic curve of PEM fuel cell for the complete operating regime. Simulation results are presented to show the influence of various operating conditions and electrode structural parameters on the i-v curve.

Based on earlier investigations for a single spherical agglomerate by Rao and Rengaswamy [9], it was found that oxygen is completely consumed at the surface of spherical agglomerate for overpotentials greater than 0.30 V. Hence, Pt nanoparticles in the inner core of a spherical agglomerate are not utilized. As a part of optimization studies, flooded-agglomerates of different geometries and sizes are considered in cathode catalyst layer to study their influence on the transport properties of different species and their effect on the overall performance of the cell. The significance of these results for optimization of electrode structures will be highlighted. We will also discuss the benefits these studies can offer in terms of greatly reducing platinum use and hence reducing the cost of fuel cells.

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