

Simulation of Proton-Exchange-Membrane Fuel Cell Cathode Performance Using an Agglomerate Model
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Much attention is drawn to the development of proton-exchange-membrane fuel cell (PEMFC) for its virtue of high energy density and no pollutant emission in the application of transportation vehicles and residential power generators. Besides many experimental studies to improve the three-phase structure of the gas diffusion electrode (GDE),¹⁻³ theoretical modeling techniques were developed to explore the relationship between cell discharging behavior with the electrode morphology and chemical composition.⁴⁻⁷ Generally, major potential loss of a single PEMFC is caused by cathode since activation resistance of oxygen reduction in cathode is much larger than that of hydrogen oxidation in anode. The electrochemical behavior of cathode is the focus of many theoretical and experimental researches.

An agglomerate model concentrated on the cathode catalyst layer is developed in the present study based on experimentally specified parameters such as platinum and solid polymer electrolyte loadings. Fig. 1a is a schematic of the modeling region. This model is able to account for the effects of gas feed composition, solid polymer electrolyte loading, platinum catalyst loading, gas void fraction, and thickness of the catalyst layer.

It is shown that even in a sufficiently large gas void fraction in the catalyst layer, the diffusion barrier of oxygen in the ionomer phase may impose significant resistance in the cathode performance depending on the relative loadings of Pt and ionomer. For insufficient loading of SPE, cell performance is impeded due to possible reduced active catalytic surface and the inferior ionic conduction in the layer (Fig. 1b). Too high an ionomer loading may cause the mass transfer limitation of oxygen (Fig. 1c). Excessive Pt loading under a specified ionomer loading is also a waste since volume density of active surface area is reduced, and proton migration becomes difficult.

The effect of gas void space, shown in Fig. 2, is a compromise between the higher volume density of active surface at low porosity and the efficient gas transport through the larger pore fraction. A suitably controlled porosity should be an important part of the overall optimization scheme on the making of catalyst layer.

The catalyst layer thickness effect is a consequence of the mass composition and layer void fraction. At a suitable ratio of m_{Pt} to m_n , too thick a layer only increases the materials cost of the cathode without enhancing the discharge rate. A judgment on a proper thickness is needed to optimize the cell performance. Improper ratio of m_{Pt} to m_n causes performance down significantly, and little improvement is expected by managing the porosity or layer thickness.

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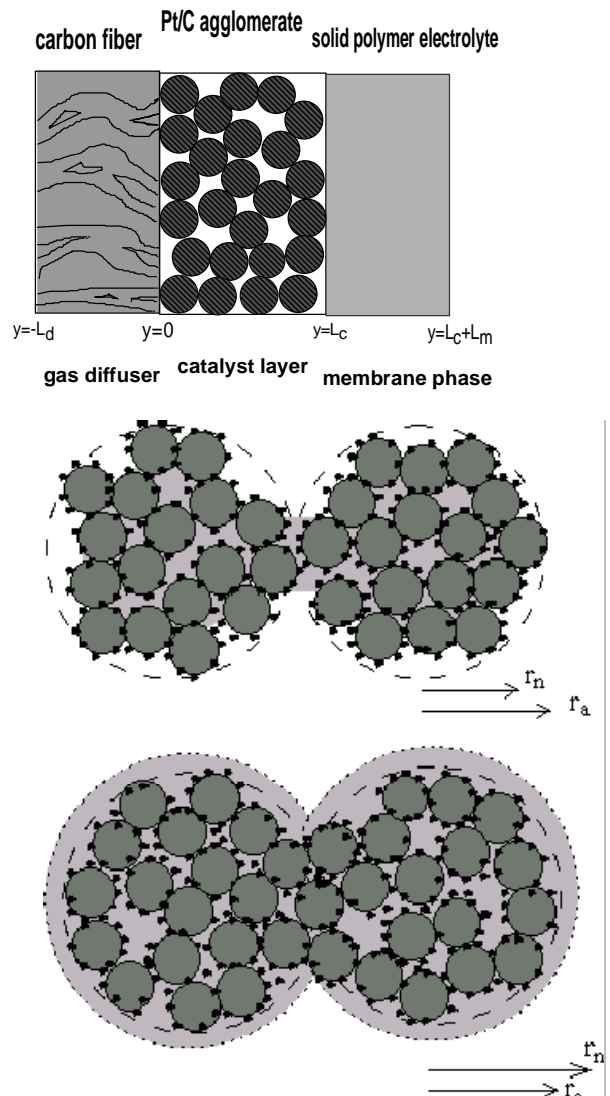


Fig. 1. (a) Schematic of the gas diffuser/catalyst layer/membrane assembly (not to scale). (b) Detailed agglomerate structure for the case when not all catalytic area is covered with ionomer. (c) Detailed agglomerate structure when all the Pt catalytic area is covered with ionomer.

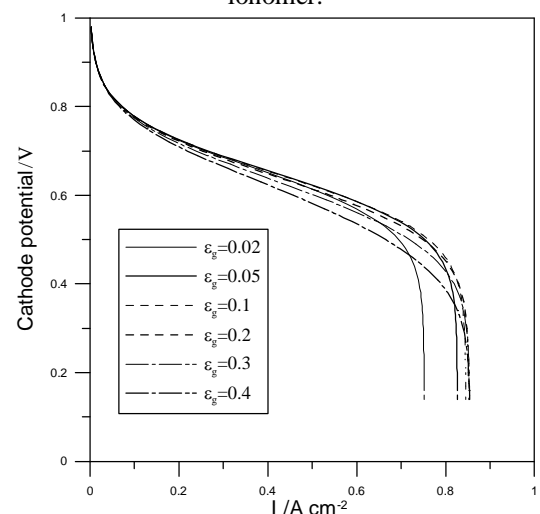


Fig. 2. Effect of gas phase void fraction in catalyst layer on the polarization behavior. Working conditions are adopted from Ref. [3], and mass transfer and kinetic parameters are estimated from the same article.