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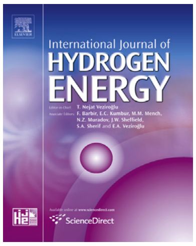

Review Article

A review on microstructure reconstruction of PEM fuel cells porous electrodes for pore scale simulation

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ABSTRACT

PEM fuel cells are currently at the focus of researchers' attention due to their promising potential application in modern vehicles. Fundamental tiny-scale phenomena occurring in the PEM fuel cell porous electrodes can be represented more faithfully by pore scale simulation techniques which entail microstructure reconstruction of porous media such as GDL, MPL and CL rather than conventional simulation methods. In fact, to achieve a realistic and accurate pore geometry is crucial for a trustworthy pore scale simulation, especially when the effect of morphology and structural parameters are to be investigated. In the present article, three classes of the of PEM fuel cells porous media reconstructions which have been performed for pore scale simulation of fluid flow are outlined and reviewed. Stochastic and X-ray tomography reconstruction of carbon paper GDL is well-understood in the literature, even if GDL is compressed or treated by binder/PTFE. However, more efforts are needed to reconstruct the MPL and CL using either stochastic or FIB/SEM methods.

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Introduction

While environmental problems such as air pollution and global warming becomes more and more grave, fuel cell technology offers clean, efficient, safe and reliable power generation to almost any device requiring electrical power. They represent the most versatile energy solution ever invented [1]. Furthermore, fuel cell power systems can be easily combined with energy storage systems such as batteries to provide hybrid power systems with higher reliability and more effective controllability [2–4].

Among different types of fuel cells, proton exchange membrane (PEM) fuel cells are the most promising candidate for future energy demands. A major application of PEM fuel cells is in modern vehicle industry. In more recent decades, some major automotive companies have supported enduring research toward the development of PEM fuel cells for application in fuel cell vehicles (FCVs) [5]. The Toyota Mirai and the Hyundai ix35 were the two FCVs which have been introduced since 2015 for commercial lease and sale in limited quantities. Honda, Mercedes-Benz and Nissan [6] are other manufacturers which decide to sell fuel cell electric vehicles commercially since 2016. The tank-to-wheel efficiency for a FCV in a test procedure such as NEDC (New European Driving Cycle) is more than 45% at low loads and about 36% at average conditions [7]. The corresponding NEDC value of a diesel vehicle is 22% [6].

In recent years, a huge amount of work has been performed in various aspects of fuel cell science and technology ranging from basic electrochemistry to stack design. However, some challenges still exist which must be resolved to extend commercial viability and to remove the big question mark about the future of these FCVs [8]. More specifically, in order to diminish the two main barriers of cost and durability of PEM fuel cells, fundamental research is inevitable [9]. Since the electrodes of these fuel cells are porous media with complicated heterogeneous and anisotropic microstructure [10], fundamental analysis of fluid flow needs pore scale simulation techniques. To identify precisely the microstructure geometry is necessary for high quality pore scale simulation of fluid flow through such porous media, especially when the effect of morphology and structural parameters are to be investigated [11]. Moreover, it can give insight to explore customized porous materials with enhanced properties and performance [12]. Therefore, the microstructure reconstruction which provides the microstructure geometric model (also known as morphological model) plays an important role in PEM fuel cells research and development. In this review article, the reconstructions of GDL, MPL and CL microstructures performed for pore scale simulation via techniques such as lattice Boltzmann method (LBM) [8,13–15] will be surveyed.

Structure of PEM fuel cells

Currently, hydrogen PEM fuel cell development is at the focus of attention by fuel cell systems experts and researchers. Hydrogen PEM fuel cell can be fueled by pure hydrogen or a diluted hydrogen mixture which is produced by a fuel reformation process. In most cases, a noble metal platinum catalyst would be used on the anode and cathode due to the operating temperature range which is from room temperature to ~80 °C. In the hydrogen PEM fuel cell, many technical issues should be taken into account which would complicate performance and control. Besides manufacturing, auxiliary components, cost, and market acceptance issues, the basic technical challenges comprises: (1) water management [16], (2) thermal management [17], (3) durability [18], (4) freeze–thaw cycling [19] and (5) frozen-start capability [20].

The general components of hydrogen PEM fuel cell are shown in Fig. 1. The oxidizer and fuel travel through the cathode and anode flow fields and subsequently disperse through the related porous gas diffusion layers (GDLs) with 200–400 μm thickness and diffuse through the related catalyst layers (CLs) with 5–20 μm thickness. In some PEM fuel cells, micro-porous layer (MPL) is placed between GDL and CL to enhance water management [21–23]. The electrochemical half-reactions at the cathode and anode are shown in Eqs. (1) and (2), respectively [24]:

$$\frac{1}{2}O_2 + 2H^+ + 2\bar{e} \rightarrow H_2O \tag{1}$$

$$H_2 \rightarrow 2H^+ + 2\bar{e} \tag{2}$$

As shown in Fig. 1, a single cell of hydrogen PEM fuel cell consists of the following basic components:

a. *Electrolyte* which consists of a hydrophobic and inert solid polymer in the form of a proton exchange membrane. In order to provide adequate conductivity, it is sulfonated with hydrophilic acid clusters. Dupont has produced the well-known Nafion® material which employs perfluoro sulfonylfluoride ethyl propyl vinyl ether (PSEPVE) [25].

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