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Water dynamics inside a cathode channel of a polymer electrolyte membrane fuel cell

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ABSTRACT

The present study focuses on the investigation of water dynamics inside a polymer electrolyte membrane fuel cell using two different modelling approaches: Eulerian two-phase mixture and volume of fluid interface tracking models. The Eulerian two-phase mixture model has provided overall information of species distribution inside a fuel cell and identified that the liquid water usually accumulates under the land area. The volume of fluid interface tracking model has then been implemented to investigate the emergence of water droplets from the gas diffusion layer into the cathode channel and the subsequent removal of water from the channel. Further, the effects of the location of water emergence in the cathode channel on the dynamic behavior of liquid water have been investigated. The present study shows that the water emerging into the channel near the side walls greatly reduces the surface water coverage of the channel. In order to control the water path into the channel near side walls, a further discussion has been provided that a gas diffusion layer design based on hydrophilic fibres distributed inside a hydrophobic fibre matrix could provide a precisely controlled water path through the gas diffusion layer.

1. Introduction

A polymer electrolyte membrane (PEM) fuel cell, which has been considered to be a suitable candidate for solving future energy crisis, converts chemical energy into electricity in a cleaner fashion. PEM fuel cells can be employed in many applications including automobiles, combined heat and power unit, stationary and portable power system [1]. Despite having many attractive benefits, the widespread deployment of PEM fuel cell has been hampered by high cost and durability. The high cost of a PEM fuel cell stems from using expensive platinum as catalyst to maintain electrochemical reaction. Much research has been directed to reduce platinum uses [2,3]. Another way to reduce the cost would be to increase the performance of existing design. In this respect, water management is a critical issue in enhancing the PEM fuel cell performance.

A PEM fuel cell operates by combining oxygen and hydrogen and producing water as a byproduct. Moreover, water is also needed to keep the electrolyte membrane hydrated. This is done by hydrating both air and fuel streams. As a result, the cathode gas diffusion layer contains a large amount of water, which eventually flows into the cathode channel and is then carried away with the airstream [4]. In order to improve the performance, the water from the cathode channel should be removed quickly and the water coverage on the gas diffusion layer (GDL) surface should be small. This would allow more oxygen to diffuse through the gas diffusion layer to the reaction sites. A thorough understanding of the process of water removal through the cathode channel is required in order to device a good water management strategy or to develop a new architecture of a PEM fuel cell.

Because of the importance of water management, several studies have been reported that deals with the problem of water management through numerical modelling study by developing of two-phase models that takes into account phase changes in water vapour and liquid water, multi-component species transport and electrochemistry. Natarajan and Nguyen [5] employed a pseudo three-dimensional model to investigate liquid water movement inside the cathode electrode. In the work of Wang et al. [6], and You and Liu [7] both liquid and vapour phase of water flows have been considered, but only inside the cathode gas diffusion layer. In a follow-up paper, You and Liu [8] reported a two-dimensional, two-phase coupled PEM model, which showed that the liquid water also influenced the oxygen transport. Berning and Djilali [9] also developed a three-dimensional, multi-phase, multi-component model considering heat and mass transfer. In their study liquid water transport inside the GDL was numerically modelled by using viscous and capillary effects. This method was also implemented by Mazumder and Cole [10]. Min [11] developed a three-dimensional, two-phase, non-isothermal model based on

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two-fluid model. Meng [12] developed a mixed domain two-fluid PEM fuel cell model, where water transport through the membrane was calculated by solving a conservation equation for the water content in the membrane. Further details in two-phase modelling of PEM fuel cell can be found in the recent review paper by Khan et al. [13].

Though all the two-phase modelling studies mentioned above provided significant contribution to knowledge, these models were unable to predict the dynamic behavior of the emergence of liquid water as droplet, and subsequent droplet growth, coalescing and the formation of slug or water film in the channel. Several papers have appeared recently in literature concerning the dynamic behavior of water droplet movement through the cathode channel [14–26]. Experimental studies have provided visual description of water droplet egress from the GDL and subsequent slug formation in the channel [4,23,24]. However, because of the use of transparent wall for visual access, the experimental technique cannot reproduce the key role played by channel walls in water removal [19]. In this respect, the application of the volume of fluid (VOF) method in the computational fluid dynamics framework has provided many insights into the water dynamics in the cathode channel [14–22]. Cai et al. [14] investigated the effects of surface wettability of GDL on movement of a single droplet and film and concluded that a combination of the hydrophobic GDL with hydrophilic side walls was beneficial for water removal. Zhan et al. [15] also investigated the droplet and film movements through a serpentine channel and provided similar conclusion to Cai et al. [14]. Jiao and Zhou [16] were focused on developing an innovative gas diffusion layer with microchannel linking the catalyst layer with the flow channel. Quan et al. [17] investigated the water dynamics inside a serpentine channel with various initial conditions of water presence in the channel. In a series of papers, Zhu et al. [18–20] investigated the process of water droplet emergence, growth, deformation and detachment. Zhu et al. [18] investigated the dynamics of a single water droplet in the cathode channel by implementing a VOF model. The simulation was carried out on a two-dimensional geometry which was not a realistic presentation of the actual physics. In subsequent papers, Zhu et al. [19,20] modified the computational domain to a three-dimensional geometry. The detail description of water droplet emergence, growth, deformation and detachment of a single droplet has been provided through a parametric study of the effects of surface wettability, air flow velocity, water injection velocity and the size of the pore. Ding et al. [21,22] have provided a more realistic representation of water droplet interaction by setting up water emergence into the channel through a number of pores. Their study shows that water droplets after emerging from pores, merge into larger slugs and then accumulate on the side walls before being driven out of the channel.

Based on the above literature review, it is clear that the water dynamics in a fuel cell has to be understood at multi-levels using models that include the entire detailed physics e.g. multi-phase interface tracking between gas-phase and liquid water-phase, multi-components, mass transfer, electrochemical reaction and water-phase change effects. In the present study, two different modelling approaches have been implemented to provide complete information of water dynamics in a fuel cell. The first modelling approach is based on the Eulerian two-phase concept, which takes into account all parts of PEMFC including the membrane, catalyst layers, GDLs and gas flow channels. In the second modelling approach, the interface of the liquid water and air phase has been tracked through a cathode flow channel by a VOF model.

Water generated in the catalyst layer diffuses through the gas diffusion layer into the flow channel. A GDL is made of randomly distributed fibres and as such water flows through the random flow paths inside the GDL into the channel and it is very difficult to predict which flow path water would take into the channel. In reality, experimental studies [23–26] show that water enters the channel from the GDL preferentially through certain pores and the distance between the pore is quite large. In previous studies, the emergence of water into the channel from the GDL has been modelled by a single pore (inlet) [18–20], multiple pores but very closely packed to each other [21] and two pores across the width [22]. Obviously, the size and the distance between the water emerging pores would have major effects on the surface coverage of a GDL and the water fraction inside the flow channel. The present study seeks to provide a systematic study of water droplet dynamics for different pore distances and pore sizes. The main objective of this study is to identify an optimum pore arrangement that would provide minimum water coverage on the GDL surface.

2. Mathematical model

The numerical simulation procedure in the present study is based on two different modelling approaches. In the first modelling approach, a Eulerian two-phase mixture model, that includes the transport of hydrogen, oxygen, water vapour and liquid water through the flow channels, the GDL, the catalyst layers, the membrane, and the electrochemical reactions and the phase change effects, has been developed. This modelling approach provides information regarding PEM fuel cell performance characteristics and species distribution inside the cell as average values. This method does not provide the crucial information regarding the dynamics of liquid water emergence, growth, coalescence and movement in the channel. Therefore, a second modelling approach based on the multi-phase volume of fluid (VOF) interface tracking between the air and liquid water-phase has been employed to provide further insight into the liquid water transport inside the flow channel and to develop an effective water removal technique.

2.1. Governing equations for the Eulerian two-phase mixture model

The governing equations for the PEM fuel cell model consist of continuity, momentum and species transport equations. These equations represent the transport phenomenon inside the catalyst layers, gas diffusion layers and the flow channels. To represent the electrochemistry and the transport phenomena through the membrane, appropriate source terms are applied at the anode and cathode catalyst layers.

2.1.1. The mass conservation equation (continuity equation)

$$\nabla(\rho \vec{u}) = 0 \tag{1}$$

where ρ is the fluid density and $\vec{u}$ is the velocity vector.

2.1.2. The momentum conservation equation

$$\nabla(\rho \vec{u}\vec{u}) = -\nabla P + \nabla\overrightarrow{\mu\nabla(u)} + S_u \tag{2}$$

where P is the pressure and S_u is the source term.

In the flow channel, S_u is zero. In the gas diffusion layers and the catalyst layers Darcy's law term is added to the momentum equations to represent the momentum related to the porous media. This source term is expressed as:

$$S_u = -\frac{\mu \vec{u}}{K} \tag{3}$$