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Modeling and analysis of internal water transfer behavior of PEM fuel cell of large surface area

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ABSTRACT

The PEM fuel cell has been widely used in the area of transportation and power station. The surface area of a fuel cell is enlarged to provide high enough power but the problem of analysis of internal water content behavior follows tightly. Many scholars have investigated the mathematical models of a small fuel cell and validated them through experiment. Besides, the introduction of AC impedance technique helps find relationship between water content and membrane resistance. Based on their research, an approach is put forward in this paper to model and analyze the internal water content behavior in a fuel cell of large surface area. For large surface area, three special cases are studied according to the actual operating states at cathode outlet. The first case applies to a fuel cell with no saturated water vapor at both outlets while in the second and third case, the fuel cell is divided into an electrochemical reaction zone and no reaction zone owing to emerging liquid water. The indicators of model are the water content profile inside membrane and the total membrane resistance. The simulation results show that the net water transfer coefficient has significant influence on the performance of the membrane and the constituents of anode side are easy to be varied. In addition, when the fuel cell is operated in counter-flow mode with emerging liquid water, the only back diffusion of water from cathode to anode helps improve the state of the membrane.

Introduction

The proton exchange membrane fuel cell, as an environmentally friendly electrochemical device, has attracted attention from all over the world. The high efficiency, high power density, low emissions and low operating temperature contribute to its great advantage over the conventional internal combustion engine in the long run [1–3]. Several commercial fuel cell vehicles have been launched in recent

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three years, including MIRAI by Toyota Motor Corp. and Tucson ix35 by Hyundai Motor Group [4,5]. Even so, there is still a long way to go towards mass production and application to transportation area, which is limited by the cost and durability as reported by Department of Energy (DOE) of USA [6]. Therefore, more efforts need to be made to achieve the wide and practical utilization of the fuel cell system.

In terms of the fuel cell system itself, one of the largest obstacle in research is the accurate measurement or estimation of water content of each fuel cell as well as in actual control [7]. As a unique substance, water plays an important role in the performance of the fuel cell [8]. Except the improvement of water content distribution by materials and structures, a great progress is also made in contributing to understanding complex physical and electrochemical processes related to water by enriched mathematical models and large amounts of experiment [9,10].

For instance, Springer puts forward a comprehensive mathematical model of a fuel cell to account for mass transport in flow channels and gas diffusion layers as well as proton conduction in membrane [11]. The processing of water content parameter at the interface of membrane and catalyst layers is the key to an integral model. The local water content and its relation to proton conductivity and back diffusion coefficient are established on the basis of experiment [12]. However, the existence of liquid water in any space when the local water vapor is oversaturated is not discussed in detail about how to deal with it.

Furthermore, Amey proposes a modified interpretation of the water activity presented by Springer and the modification directly affects the membrane water transport between the anode and the cathode in the presence of the liquid water inside the stack [13]. Then based on such modification a zero-dimensional isothermal model is calibrated to predict the flooding and drying conditions in the two electrodes observed at various current levels [14]. After that, they apply this model to study two cases of water management through modification of cathode inlet humidification and anode water removal.

Through analysis it is found that the most complicated part of a fuel cell is the mass transport in the cathode flow channel and gas diffusion layer [15]. This is caused by the by-product water in cathode catalyst layer and the water transferred from anode to cathode resulting from the net influence of kinds of water transport. To better explain phenomena in the cathode, the concept of a multiphase mixture model is presented by Wang [16]. In his model, the liquid water is thought to be totally atomized into micro water droplet and mixed well within the gaseous phase. If so, the governing equation of liquid water transport is in the same form as other gases like oxygen and nitrogen. This model is applied to investigate the composition distribution along the flow channel and inside the gas diffusion layer to evaluate flooding or drying out and a direct indication of the model accuracy is the measurable high frequency impedance [17,18].

When thinking about the demanded computational efforts of a mathematical model, it is usually beyond the capability of common configuration of micro controller unit. Then some researchers pay their attention to experiment in order to search an indicator or even conclude semi-empirical equations. Pei performs experiment on two 274 cm^2 fuel cells and a two-level characteristic of hydrogen pressure drop is observed and analyzed [19]. A conclusion is drawn that the flooding process can be divided into four periods and a water management strategy is proposed to better diagnose and control the fuel cell.

In addition, an available method of monitoring the state-of-health of fuel cell is suggested via AC impedance measurement by Fouquet et al. [20]. To validate this method, the experiment is conducted with full-time measurement of operating conditions and periodical measurement of AC impedance spectroscopy. The time constant of both flooding and drying is at the magnitude of 1000 s when the fuel cell works at constant operating conditions. This proves that the variation of water content is a slow process and a steady-state model may be enough for estimation. As a result of the expensive equipment, this method cannot be put into practice in transportation area. However, with the development of technology, the online measurement of high frequency impedance in vehicles has been realized by Toyota Motor Corporation [21]. The application of high frequency impedance to water content control indicates its effectiveness even without the complete impedance spectroscopy.

More research results show the feasibility of using high frequency impedance to estimate water content. For example, a General Motors' patent presents the correlation between the membrane water content and the high frequency impedance [22]. While studying a purge method of sudden pressure reduction for effective water removal, the internal ohm resistance and the dew point temperature of the exhaust gas in the cathode are measured to verify this method [23].

Though the relation between high frequency impedance can be measured from experiment, it is impossible for us to test each fuel cell to establish such a specific relation. In fact, the high frequency impedance is comprised of contact resistance, electron conduction resistance and proton conduction resistance in membrane but it is dominated by the last one. The measurement of high frequency impedance is an important tool and the combination of this tool with mathematical explanation of the result is more meaningful.

The PEM fuel cell of small surface area has been studied by many scholars but the impact of large surface area on water transfer inside is not clearly elucidated yet, especially from the view of high frequency impedance. Wang experimentally investigates the effects of temperature, flow rate and humidity on impedance spectra of each individual cell and the stack of 280 cm^2 [24,25]. Yan et al. present the AC impedance characteristics of a 2 kW PEM fuel cell stack of 270 cm^2 under different operating conditions and load changes [26]. These experiment results demonstrate the advantage of AC impedance but no more mathematical explanation is given towards better understanding. Some research is focused on segmentation of a large fuel cell to elaborate the effect of operating conditions on the performance as well as the current density distribution [27,28].

Hence, based on literature research, a new approach is proposed in this paper to model the internal water transfer of a fuel cell of large surface area. Meanwhile, the membrane resistance is selected as an indicator of membrane water content and the link between anode and cathode. This paper is organized as follows: Section Fuel Cell Model describes the

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