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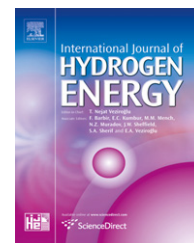**ScienceDirect**

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Analysis of liquid water transport in cathode catalyst layer of PEM fuel cells

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ABSTRACT

The performance of a polymer electrolyte membrane (PEM) fuel cell is significantly affected by liquid water generated at the cathode catalyst layer (CCL) potentially causing water flooding of cathode; while the ionic conductivity of PEM is directly proportional to its water content. Therefore, it is essential to maintain a delicate water balance, which requires a good understanding of the liquid water transport in the PEM fuel cells. In this study, a one-dimensional analytical solution of liquid water transport across the CCL is derived from the fundamental transport equations to investigate the water transport in the CCL of a PEM fuel cell. The effect of CCL wettability on liquid water transport and the effect of excessive liquid water, which is also known as "flooding", on reactant transport and cell performance have also been investigated. It has been observed that the wetting characteristic of a CCL plays significant role on the liquid water transport and cell performance. Further, the liquid water saturation in a hydrophilic CCL can be significantly reduced by increasing the surface wettability or lowering the contact angle. Based on a dimensionless time constant analysis, it has been shown that the liquid water production from the phase change process is negligible compared to the production from the electrochemical process.

1. Introduction

Over the last decade, polymer electrolyte membrane (PEM) fuel cells have drawn immense attention as high-efficiency and low-emission power sources, particularly for portable and automotive applications [1]. However, the performance and cost of the PEM fuel cells need to be improved significantly in order to be viable for commercial applications. Among the several key factors that are hindering the PEM fuel cells to be competitive with portable and automotive applications, water management is most crucial [2–9]. The ionic conductivity of PEM is significantly dependent on the membrane hydration. Inadequate membrane hydration results in high electrical resistance as well as the formation of dry and hot spots leading to membrane failure. Conversely, the excessive amount of liquid water in the cathode catalyst layer (CCL), produced from the electrochemical reaction and due to electro-osmotic drag effect, could block the access of reactant gas to the reaction site and lower cell performance. Hence, liquid water is one of the key factors responsible for degradation of electrolyte membrane as well as performance reduction.

Water transport in the CCL of a PEM fuel cell involves several transport and physical processes: (a) electro-osmotic transport of water from the membrane to the CCL, (b) back-diffusion of water from the CCL to the membrane, (c) condensation and evaporation of water, and (d) removal of

liquid water to the gas flow channel through the gas diffusion layer (GDL). The electro-osmotic transport occurs due to the proton transport. Proton migrations drag water along with it from the anode side to the cathode side that can eventually reduce the membrane hydration and block the active reaction site in the CCL. Conversely, the back-diffusion represents the water transport back to the membrane due to the concentration gradient. Since water is produced at the CCL and protons are dragging liquid water from the anode side, the liquid water concentration in the cathode side increases significantly compared to the anode side during the operation of fuel cells. This concentration difference causes diffusion of water from the CCL to the membrane. Further, if the reactant gases are fully humidified, water vapors in the gas mixture tend to condense. Conversely, if the gases are partially hydrated, liquid water will start to saturate the gas mixture through the evaporation process. Furthermore, the liquid water can be removed from the cathode GDL by the flow of reactant gas in the gas flow channel that can eventually dry out the electrode, hence the membrane, if the rate of water removal is too fast. Clearly, the entire water transport process in a PEM fuel cell is a complex phenomenon, hence it is essential to make a delicate water balance for better and optimum fuel cell performance, and prevent material degradation.

There are numerous theoretical and numerical studies related to liquid water transport available in literature [2–4,10–15], however, most of them addressed the liquid water transport in the membrane or the GDL of a PEM fuel cell. These studies also addressed the water flooding in the GDL and gas flow channel, and none of the previous studies specifically addressed the liquid water transport in the CCL of a PEM fuel cell. Further, these studies were based on the assumption that most of the liquid water produced at the GDL/CCL interface or the catalyst layer is very thin. While the highest reaction rate occurs at the membrane/CCL interface [16] and the CCL thickness needs to be higher than 10 μm to obtain optimum performance from a PEM fuel cell [17]. Therefore, the approximation of a thin CCL or considering the CCL as an interface seems to be insufficient to explore the overall liquid

water transport in a PEM fuel cell. Substantial amount of experimental studies have also been conducted for the flooding in PEM fuel cells to understand the fundamental water transport processes [5–9,18–20]. Further, Pasaogullari and Wang [21] developed an analytical model of liquid water transport in the GDL of a PEM fuel cell. Although water flooding in the CCL likely occurs prior to that in the flow channel and GDL because of water is produced in the CCL from the electrochemical reaction and is expelled from the CCL to the flow channel through the GDL, the studies related to the CCL flooding are still elusive.

The objective of this study is to investigate liquid water transport in the CCL of a PEM fuel cell. In-situ measurement of water flooding in the CCL is very difficult. Even if possible, for instance, by using NMR Microscopy [22] and Neutron Radiography [18,23], it can only yield a qualitative picture of liquid water distribution in a PEM fuel cell. Therefore, our objective is to provide a simple, easy to implement and quick estimate of liquid water transport in the CCL of a PEM fuel cell. The liquid water transport process has been dealt with analytically, including electro-osmotic transport, back-diffusion, condensation and evaporation of water, and removal of liquid water through GDL. A simplified formulation has been developed from the conservation of mass and momentum equations and the one-dimensional (1D) analytical solutions of liquid water profile have been derived for both hydrophilic and hydrophobic CCLs. Then the effect of catalyst layer wettability and effect of CCL flooding on the performance of a PEM fuel cell have been investigated.

2. The physical problem

In the present study, a typical PEM fuel cell is considered that consists of a cathode and an anode electrode with a proton-conducting membrane as the electrolyte that separates the anode side and the cathode side. Fig. 1 shows a schematic of a PEM fuel cell with key components (left figure) and a cathode catalyst layer with the coordinate system (right
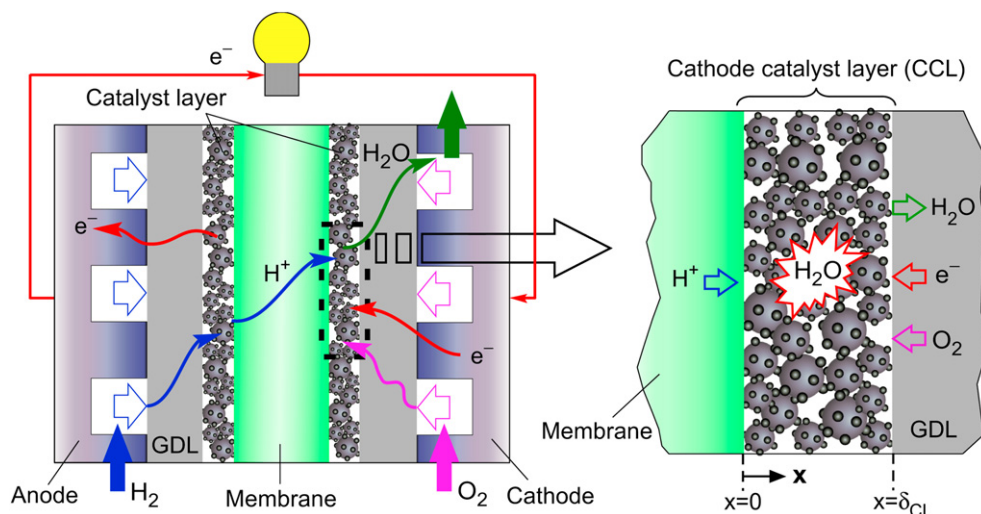

Fig. 1 – The schematic of a PEM fuel cell with key components (left) and a cathode catalyst layer with the coordinate system (right).