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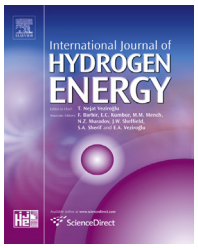

Two dimensional modelling of water uptake in proton exchange membrane fuel cell

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ABSTRACT

With the focus on water uptake by proton exchange membrane, a two-phase, non isothermal, transient and two-dimensional model of fuel cell is developed. Further, in order to obtain the equilibrium concentration of water in the membrane, two different approaches of water-uptake by the membrane are considered; though each takes into account the Schroeder's paradox as well as individual contributions of water vapour and liquid water. Furthermore, in both the approaches, rate of water uptake is proportional to the difference between equilibrium concentration and actual concentration of water in membrane. Model results show good agreement with the experimental results. A comparative analysis of the two approaches has been presented for various results, such as liquid saturation, net drag coefficient, temperature, water content in membrane, etc. Obtained results revealed significant difference between predicted current densities, water content of membrane and temperatures for the two approaches. These differences may be reflecting the need to correctly understand water uptake by membrane and its importance for accurate modelling of fuel cell. Response in transient state of fuel cell is also studied when a step change to cell voltage is applied. Likewise, studies on rate of sorption and desorption of water by membrane explain the increase or decrease of the water content of membrane.

Introduction

Proton exchange membrane (PEM) fuel cells have already made in-roads in assisting to our daily life. They are being used for portable applications (such as mobile phones, laptops etc.), power source in transportation (such as hybrid cars, buses etc.) and stationary applications such as backup power source. However, still there are umpteen problems that need to be addressed and solved before commercialization of fuel cells on wider scale. Among these, one of the crucial problems is water management which needs to be correctly understood and solved.

Several computational models of PEM fuel cells have been developed. Pioneering amongst those are 1-dimensional (1-D) and single phase systems developed by Springer at al [1], Nguyen et al. [2], Bernardi et al. [3] etc. The relations for electro osmotic drag coefficient, protonic conductivity of membrane and diffusivity of water (in membrane) suggested by Springer et al. [1] are still widely used in many modelling works and have set the framework for development of many 1-D, 2-D and 3-D models; for example [4], a 2-D, single phase model of

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cathode side with interdigitated flow field [5], a three layer 2-D model [6] simulation, full 3-D simulation [7] etc.

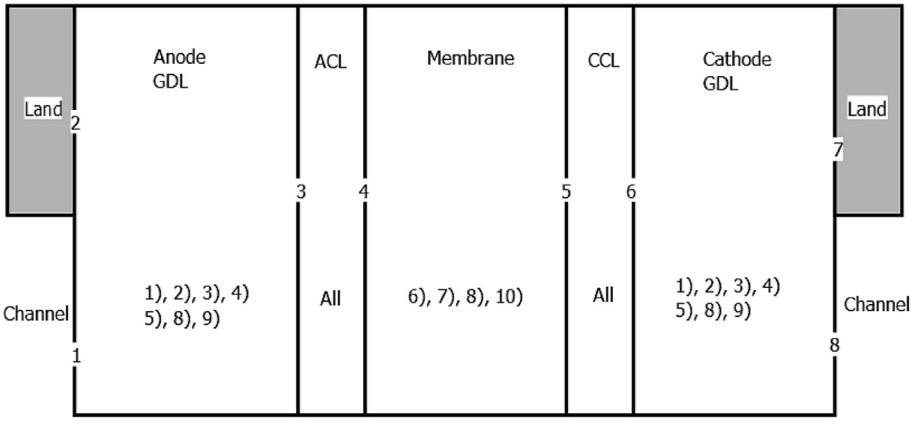
It is understandable that single phase models are unable to capture the phenomena of flooding in fuel cell, necessitating the advent of two phase models. Nguyen et al. [8] developed a two phase model of cathode with interdigitated flow field. In this model, liquid water transport occurs due to capillary pressure gradient and due to shear force exerted by gas flow. Similar model of cathode side with conventional flow fields has also been developed [9] and has been extended to include transport in membrane [10]. Several other two dimensional and three dimensional models [11–15] have used similar approach.

In most of the two phase models, individual contributions of water vapour and liquid water to water uptake by membrane has been neglected. Following text highlights few such examples. In some works [8,9], flux due to water vapour at membrane-gas diffusion layer (GDL) interface is set equal to zero, thus total water flux across membrane becomes equal to liquid water flux. In contrast some researchers [11,15] have utilized the effective water transport equation as proposed by Kulikovsky [16] who has used it in catalyst layers (CL). This equation takes into account the flux of water vapour and water in membrane phase only, thereby neglecting the contribution of liquid water. Similarly, few others [12,13,17] have modelled water uptake by including a source term in the water vapour conservation equation thus neglecting liquid water phase.

A different approach which has been widely used to model the two phase phenomenon in fuel cell is Multiphase Mixture theory. Several two and three dimensional models [18–21]. have utilized this approach where, instead of solving conservation equations for each phase of water, single equation is solved for water mixture. Therefore, when a source term (which accounts for water uptake by membrane) is included in the water balance equation, contributions of both water vapour and liquid water are taken into account. However, still these models neglect contribution of liquid water and indirectly Schroeder's Paradox (i.e., different uptake of a liquid solvent and its vapour) [22].

A useful insight regarding water transport across membrane has been provided by Wu et al. [23]. Here the approach is to model non equilibrium rate of water uptake by membrane; thus, rate of uptake is proportional to the difference between equilibrium concentration of water in membrane and actual concentration of water in membrane. Similar approaches of water uptake are also reported [24,25]. Accordingly, contributions of both water vapour and liquid water get accounted. Still these models may be considered to be neglecting Schroeder's paradox as these consider the water content of membrane to be a function of only water vapour activity. The present work, therefore, has been undertaken to understand and address such discrepancy in modelling water uptake by PEM with the following adopted methodology:

- Two phase, non isothermal modelling
- Considering two different approaches for water uptake by membrane; both accounting Schroeder's paradox as well as individual contributions of water vapour as well as liquid water
- Considering agglomerate approach to model local rate of reaction in catalyst layers
- Studies on response of fuel cell under transient state when step change is applied to cell voltage



$$1)\ \frac{\partial(\epsilon^{eff}\rho_g)}{\partial t}+\nabla.(\rho_g u_g)=S_m \qquad 6)\ \frac{d(\epsilon_m C_w)}{dt}+\nabla.N_w=S_d$$

$$2)\ u_g=-\frac{KK_{rg}}{\mu_g}\nabla p \qquad 7)\ N_w=\frac{n_d I}{F}M_{H_2O}-D_w\nabla C_w$$

$$3)\ \frac{\partial(\epsilon^{eff}C_i)}{\partial t}+u_g.\nabla C_i+\nabla.(-D_i^{eff}\nabla C_i)=S_i \qquad 8)\ (\rho c_p)_{eq}\frac{\partial T}{\partial t}+\rho_f c_{p,f}u.\nabla T=\nabla.k_{eq}\nabla T+S_T$$

$$4)\ \frac{\partial(\epsilon s\rho_l)}{\partial t}+\nabla.(\epsilon s\rho_l v_l)=S_l \qquad 9)\ \nabla.(-\sigma_s^{eff}\nabla\phi_s)=-S_\phi$$

$$5)\ v_l=-D_c\nabla s+\frac{K_{rl}}{K_{rg}}\frac{\mu_g}{\mu_l}u_g \qquad 10)\ \nabla.(-\sigma_m^{eff}\nabla\phi_m)=S_\phi$$

Fig. 1 – Computational domain along with boundary labels with governing equations to be solved in each domain.