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A numerical investigation of the effects of membrane swelling in polymer electrolyte fuel cells

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ABSTRACT

A two-dimensional computational fluid dynamics model of PEM fuel cell is developed by taking into account the electrochemical, mass and heat transfer process occurring in the cathode compartment. Additionally, this model includes the effect of water content in the membrane swelling phenomenon. Several parameters such as gases temperature, inlet velocity and membrane characteristics are too investigated to establish their effect on the PEM fuel cell performance. The membrane water content and the air fraction variation in the gas channel are examined for diverse values of Reynolds number. In particular, the desirable inlet flow for enhancing the performance of the PEM fuel cell is determined by examining membrane water content patterns. The methodology in this study is useful to the control of water management and gas diffusion layer design.

1. Introduction

Fuel cells are electrochemical devices that directly convert the chemical energy from a reaction into electrical energy [1]. During operation, polymer electrolyte membrane fuel cell can meet several defects such as liquid water accumulation in gas diffusion layers (GDL) that obstruct the gas to attain the catalyst sites [2]. Yet, the correct function of a PEMFC is assured just if the membrane water content ranges between reasonably determinate confines. It is therefore necessary to control well the processes occurring in the fuel cell and to make sure that the production of exact water is sufficient for an excellent membrane hydration, without possibility of flooding. The performances of the PEMFC system are additionally linked to many others parameters, touching the operating conditions, which can be studied by a suitable simulation procedure.

Developing numerical simulation tools for the control and optimization of a PEMFC functioning is still a complex assignment. Several mathematical models are available in the literature to study water generation, water transport, and the consequence of membrane water content on the performance of PEMFC. The most representative of such works are those proposed by Ramousse et al. [3] and Baghdadi and Janabi [4].

Based on mass transport processes of reactant gases, a comprehensive One-dimensional model of a PEMFC has been given by Springer et al. [5] to study and optimize fuel cell functioning. However, the one-dimensional models are insufficient to study the velocity field and species distribution along the gas channel. Karimi et al. [6] presented a practical model for describing the phenomenon of water flooding in the PEM fuel cell using semi-empirical equations. They did not take account for the effect of membrane water content and species transport. Prasad and Jayanti [7] proposed a two-dimensional cross-the-channel model to investigate the influence of GDL property and flow-field geometry on the local reaction rate in the PEMFC cathode catalyst layer. But they had ignored the influence of velocity inlet on the membrane water content in the electrolyte. Sahraoui et al. [8] developed a two-dimensional model of electrochemical and transport phenomena in the porous structures of a PEMFC. Their model explains that the membrane water content has to be optimized in order to achieve the highest fuel cell performance.

Shimpalee et al. [9] proposed a three-dimensional model to investigate the performance of a GDL composed of a macroporous and micro porous layer. However, in their model, they assumed a constant porosity of membrane.

Recently, Wang et al. [10] investigated the effect of the channel size on the cell performance with serpentine flow fields using a three-dimensional model. Tseng and Lo [11] investigate the effects of the microstructure characteristics of the gas diffusion layer and micro porous layer, including pore size distribution. But, they did not account for the water content and hence the membrane swelling.

In order to simulate water transport process in a PEM fuel cell, including membrane swelling effects, this study presents a numerical solution to the complete momentum, species concentration and energy equations for dynamic laminar flow resulting from the combined water content effect, thermal and mass diffusion in the cathode side of a PEM fuel cell. Our objective is to develop a

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Nomenclature

A	area (m^2)
C	concentration
C_p	specific heat ($J\ kg^{-1}\ K^{-1}$)
D	mass diffusivity ($m^2\ s^{-1}$)
F	Faraday's number ($C\ mol^{-1}$)
i	current (A)
J	current density ($A\ m^{-2}$)
h	thickness (m)
K	permeability (m^2)
k	thermal conductivity ($W\ m^{-1}\ K^{-1}$)
L	domain height (m)
R	universal gas constant ($J\ mol^{-1}\ K^{-1}$)
Re	Reynolds number
S	source term
Sc	Schmidt number
T	temperature (K)
U	x-direction velocity ($m\ s^{-1}$)
V	y-direction velocity ($m\ s^{-1}$)

Greek

λ	water content
σ	protonic conductivity ($\Omega^{-1}\ m^{-1}$)
ε	porosity
μ	dynamic viscosity (Pa s)
ρ	density ($kg\ m^{-3}$)
η	activation losses (V)

Subscripts

c	catalyst layer
d	gas diffusion layer
eff	effective
gc	gas channel
i	species (O_2, H_2O)
in	inlet
m	membrane
ref	reference

novel approach to investigate the effect of membrane swelling due to the increase of water content and gas diffusion layer flooding on the performance of PEMFC.

2. Mathematical model

A standard PEMFC is composed of a polymer electrolyte membrane sandwiched between two catalyst layers, two gas diffusion layers and two symmetric gas channels. Hydrogen is supplied via the gas channel to the anode and it is diffused through the gas diffusion layer to the membrane electrode assembly (MEA), where reaction takes place [11]. At the cathode the protons are combined with electrons and oxygen to generate electricity, water and heat. Fig. 1 shows a schematic 2D cross section of a PEMFC.

The following assumptions are considered to simplify the model development to investigate the water management transport within the membrane:

- The reaction catalyst layer at the cathode is determined using the Butler Volmer equation.
- Incompressible and laminar flow due to small pressure gradient and Reynolds number.
- Ideal gas mixtures are considered.

Mathematical modeling is an important tool in designing fuel cell systems which describes the significant aspects of the current system and gives an idea of that system in available situation. The present fuel cell numerical model includes the cathode flow channel, gas diffusion layer, catalyst layer and proton exchange membrane. The equations solved in this paper include the conservation of mass, momentum, species and energy equation.

A lot of modeling domains, as gas channel and gas diffusion layer, may be large as opposed to the others. This can create unreasonably large computational problems, which may not be able to be solved. Scaling the equations and dimensions of the geometry can create a more reasonable model size. Dimensional analysis is a method for reducing the number and complexity of experimental parameters that affect the physical phenomena occurring in the cell. In this situation, we can introduce a characteristic length, L, and a characteristic velocity, V_{in}. For flow in a rectangular form, L is the cell height. V_{in}, P_{in}, T_{in}, and $C_{i,in}$, are the input velocity, pressure, temperature and species concentration respectively. In this case, novel dimensionless variables are defined as follows:

$$x^* = \frac{x}{L};\quad y^* = \frac{y}{L};\quad \overrightarrow{V^*} = \frac{\vec{V}}{V_{in}};\quad P^* = \frac{P - P_{in}}{\rho V_{in}^2};\quad T^* = \frac{T}{T_{in}};\quad C_i^* = \frac{C_i}{C_{i,in}} \tag{1}$$

Momentum conservation equation can then be written in the following form:

$$\frac{\partial \overrightarrow{V^*}}{\partial t^*} + \left(\overrightarrow{V^*} \cdot \overrightarrow{grad^*}\right)\overrightarrow{V^*} = -\overrightarrow{grad^*}(P^*) + \frac{1}{Re}\Delta^*(\overrightarrow{V^*}) + S_v\frac{L}{\rho(U_{in})^2} \tag{2}$$

The Reynolds number is a dimensionless number that is used to characterize the flow regime and can be expressed as [12]:

$$Re = \frac{V_{in}\rho L}{\mu} \tag{3}$$

The critical Reynolds number corresponding to the start of turbulence is approximately equal to 2300 [12]. In our study, Reynolds number is less than this value and the flow is then laminar.

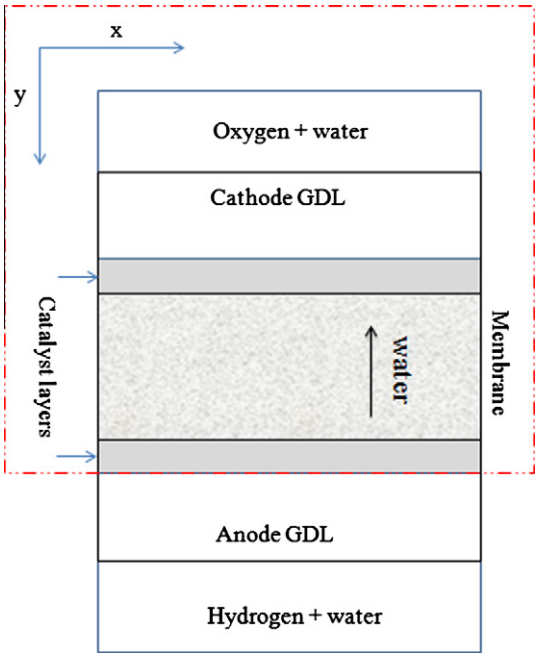

Fig. 1. Schematic diagram of computational domain.