Numerical study of the effect of the inlet pressure and the height of gas channel on the distribution and consumption of reagents in a fuel cell (PEMFC).

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Abstract

Proton exchange membrane fuel cell (PEMFC) engines can potentially replace the internal combustion engine for transportation because they are clean, quiet, energy efficient, modular, and capable of quick start-up. Since a PEMFC simultaneously involves electrochemical reactions, current distribution, hydrodynamics, multicomponents transport, and heat transfer, a comprehensive mathematical model is needed to gain a fundamental understanding of the interacting electrochemical and transport phenomena and to provide a computer-aided tool for design and optimization of future fuel cell engines. This paper analyses the effects of inlet pressure and channel height on the distribution and consumption of reagents. The gas flow is assumed laminar, unsteady, isothermal and incompressible, flow fields of the anode and cathode sides are modeled as straight channels. The equations of conservation of mass, momentum and species are developed. A program based on the finite volume method was performed to simulate the system of equations governing the phenomenon. The simulation results show that increasing the inlet pressure will improve consumption of reagents and more homogeneous distribution. The effect of channel height on the consumption of reagents is such that, if the height is smaller it is noticed that there is an increased consumption of species and consequently an increase in water production. Channels with smaller heights have shown a higher concentration of oxygen and hydrogen. The effect of height is more important for a higher pressure inlet.

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Key words: fuel cell, PEMFC, hydrogen, channel, reagent, numerical.

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1. Introduction:

The need for a more environmentally friendly and versatile energy conversion device has led to an explosive interest in fuel cell research in the past decade. PEM fuel cells have emerged as one of the most promising types of fuel cells to replace conventional power producing devices such as internal combustion engines and batteries. Fuel cells are, however, still more expensive than most conventional power conversion devices. One way to reduce the cost of fuel cells is to make them more efficient. This requires the optimization of fuel cell performance through effective design and fabrication techniques. The dynamic response of the fuel cell depends strongly on the operating conditions, transport phenomena in the cells, electrochemical reaction kinetics, mechanical design and manufacturing process, etc. Among these, the reactant gas transport in the flow distributor and the gas diffusion layer (GDL) before occurrence of the chemical reaction is one of the crucial points. Many researches have been realized on the flow-field design of the PEMFCs and on their dimensioning in order to improve the distribution and consumption of the reactive and by consequent the performance cell. In the past years, studies related to the above issues have been performed. Wei-Mon Yan et al [1] presents an analysis of a novel serpentine flow field design with reduced outlet channel heights or lengths to improve the efficiency of reactant transport, reactant utilization, and cell performance in PEMFCs. Andrew Rowe and Xianguo Li [2] developed a one-dimensional non-isothermal model of a proton exchange membrane (PEM) fuel cell to investigate the effect of various designed water management and to understand the underlying mechanism. Sungho Lee et al [3] present a parametric study to get the optimal design of the bipolar plate in the PEMFC system for automobiles. D.H. Jeon and his colleagues [4] used a Computational fluid dynamics (CFD) simulations witch performed for four 10 cm^2 serpentine flow-fields with single channel, double channel, cyclic-single channel, and symmetric-single channel patterns to investigate the effect of flow-field design in PEM fuel cell. Karvonen et al. [5] proposed a straight flow channel that has uniform flow distribution by numerical analysis and experimental results. Scholta et al. [6] investigated on the influence of channel size on straight parallel flow-field and reported the specific dimension geometries. Yan et al. [7] developed a two-dimensional model to investigate gas reactant transport at various conditions of flow channel width ratio and GDL porosity. They disclosed that an increase in either $\lambda$ or $\varepsilon$ may lead to a better cell performance. At relatively low overpotential, better uniformity in current density distribution along the width of the cell can be attained. The previous studies mentioned above are all concerned with the flow-field design and the system performance of PEM fuel cells. Many researchers have studied the effect of boundary condition on distribution and concentration of reactant species in a PEMFC. Sukkee Um et al [8] developed a transient, multidimensional model to simulate proton exchange membrane fuel cells. The model accounts simultaneously for electrochemical kinetics, current distribution, hydrodynamics, and multicomponent transport. Bernardi and Verbrugge [9] developed a one-dimensional model to examine the proton transport behaviors in the membrane. Their results indicated that if the membrane is maintained at fully saturated condition, the resistance then becomes significant at the current densities greater than 200mAcm^{-2}. Gurau et al. [10] considered the variations of the concentrations and the partial pressures in the gas channels and developed a two-dimensional model for the entire sandwich of a PEMFC. In the present study, the physical problem involves a two-dimensional cell model of the PEMFC system including the mass and momentum transport of fuel gas in the flow channel and the porous GDL. The effect of the height simple channel with straight geometry and inlet pressure on the gases flows in a fuel cell (PEMFC) is study in this paper.
2. Model Development

2.1. Model Assumptions

A complete fuel cell is an extremely complex system involving fluid dynamic, mass transport phenomena and electrochemical reaction feature. In order to achieve a solution of tow-dimensional model of a complete cell it is necessary to do some reasonable simplifying assumptions. In this model the following assumptions are used:

1. Both the gas mixture and the separated component behave according to the ideal gas model;
2. The fluid flow is unsteady, laminar, and incompressible; all the physical properties of the fluid are taken to be constant;
3. Porous GDL is homogeneous and isotropic with uniform morphological properties;
4. Water in the electrode exists as vapor only;
5. Catalyst layer is considered to be an ultra-thin layer and the fast and complete reaction of oxygen and hydrogen thus occurs only on the surface of the catalyst layer;
6. The fuel cell operates at a constant temperature of 353 K.

2.2. Computational Domain

![Diagram of computational domain](image1)

**Fig. 1.** Selection of computational domain.

![Diagram of computational domain](image2)

**Fig. 2.** Schematic of computational domain.
2.3. Governing Equations

The two-dimensional governing equations for the fuel flow channel and gas diffusion layer in cell of the PEMFC are:

**Continuity equation:**
\[
\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0
\]  
(1)

**Momentum equation:**
\[
\rho \mathcal{E}_a \left( \frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} \right) = -\mathcal{E}_d \frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} \right) - \frac{\omega}{\mathcal{E}_d} \frac{U}{k_d} U
\]  
(2)
\[
\rho \mathcal{E}_a \left( \frac{\partial V}{\partial t} + U \frac{\partial V}{\partial x} + V \frac{\partial V}{\partial y} \right) = -\mathcal{E}_d \frac{\partial p}{\partial y} + \mu \left( \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} \right) - \frac{\omega}{\mathcal{E}_d} \frac{V}{k_d} V
\]  
(3)

**Mass transport:**
\[
\frac{\partial C_k}{\partial t} + U \frac{\partial C_k}{\partial x} + V \frac{\partial C_k}{\partial y} = \frac{1}{\mathcal{E}_k} D_{k,\text{eff}} \left( \frac{\partial^2 C_k}{\partial x^2} + \frac{\partial^2 C_k}{\partial y^2} \right) + S_k
\]  
(4)

Here \( U, V, p \) and \( C_k \) denote the intrinsic fluid velocity vector, pressure, the fluid concentration of chemical species \( k \), and \( D_{k,\text{eff}} \) the effective diffusivity. In addition, the effective diffusivity \( D_{k,\text{eff}} \) is modified by the Bruggman correlation for the effects of porosity in the porous electrode, i.e.
\[
D_{k,\text{eff}} = c_{1.5} D_k
\]  
(5)

The governing equations are normalized by first defining dimensionless independent variables of the form \( u = u/\mu u_{\text{in}}, t^* = (t \mu u_{\text{in}})/H, p^* = p/\mu u_{\text{in}}^2, \mathcal{C}_k = k/H^2, C_{k,\text{ref}} = C_k/\mu C_{k,\text{ref}} \) and the above governing equations are written in the non-dimensional form:

**Continuity equation:**
\[
\frac{\partial U^*}{\partial x^*} + \frac{\partial V^*}{\partial y^*} = 0
\]  
(6)

**Momentum equation:**
\[
\frac{\partial U^*}{\partial t^*} + U^* \frac{\partial U^*}{\partial x^*} + V^* \frac{\partial U^*}{\partial y^*} = \frac{\partial p^*}{\partial x^*} + \frac{1}{Re} \left( \frac{\partial^2 U^*}{\partial x^2} + \frac{\partial^2 U^*}{\partial y^2} \right) - \frac{1}{ReDa} U^*
\]  
(7)
\[
\frac{\partial V^*}{\partial t^*} + U^* \frac{\partial V^*}{\partial x^*} + V^* \frac{\partial V^*}{\partial y^*} = \frac{\partial p^*}{\partial y^*} + \frac{1}{Re} \left( \frac{\partial^2 V^*}{\partial x^2} + \frac{\partial^2 V^*}{\partial y^2} \right) - \frac{1}{ReDa} V^*
\]  
(8)

**Mass transport:**
\[
\frac{\partial C_{k}^*}{\partial t^*} + U^* \frac{\partial C_{k}^*}{\partial x^*} + V^* \frac{\partial C_{k}^*}{\partial y^*} = \frac{1}{ReSc} \left( \frac{\partial^2 C_{k}^*}{\partial x^2} + \frac{\partial^2 C_{k}^*}{\partial y^2} \right) + \frac{1}{\varepsilon \mu u_{\text{in}} C_{k,\text{ref}}} S_k
\]  
(9)

The momentum equations are valid in both the porous gas diffusion layer and the fuel flow channel. They are reduced to the extended Darcy’s law for flow in the porous cathode with a small permeability, and become the Navier–Stokes equations inside the flow channel with the porosity of unity and the permeability of infinite.

\( S_k \): The source term for the species \( K \).

In the cathodic side, the source terms for oxygen and the production of water are respectively given by:
\[
S_{O_2} = -\frac{j_c}{4F} \quad \quad \quad (10) \quad \quad \quad S_{H_2O} = \frac{j_c}{2F} \quad \quad \quad (11)
\]

In the anodic side, the source term for hydrogen is given by:
\[
S_{H_2} = -\frac{j_a}{2F} \quad \quad \quad (12)
\]

The above kinetics expressions are derived from the general Butler-Volmer equation based on the facts that the anode exhibits fast electrokinetics and hence a low surface overpotential to justify a linear kinetic rate equation, and that the cathode has relatively slow kinetics to be adequately described by the Tafel equation.

\[
j_c = a_j^{ref} \left( \frac{C_{O_2}}{C_{ref}} \right)^{\gamma_c} \left( \frac{\eta_c}{\eta_c} + \frac{1}{\frac{\eta_c}{\eta_c}} \right) \quad \quad \quad (13)
\]

\[
j_a = a_j^{ref} \left( \frac{C_{H_2}}{C_{ref}} \right)^{\gamma_a} \left( \frac{\eta_a}{\eta_a} + \frac{1}{\frac{\eta_a}{\eta_a}} \right) \quad \quad \quad (14)
\]

2.4. The initial and boundary conditions

In the computational domain, the initial conditions \((t^* = 0)\) are:
\[
U^* = V^* = C_{O_2}^* = C_{H_2}^* = C_{H_2O}^* = 0; \quad P^* = 1
\]

The boundary conditions are applied to all the external borders of the field of calculation, the condition of Dirichlet is used has the entry of the channels. At the exit of the channels we suppose that the gradients, in the direction of the flow, of velocity, pressure and concentrations of the species are null (condition of Neumann). On the walls of the channels and the ends of MEA, the boundary conditions for the pressure, speeds and the concentrations of the species are also of Neumann type.

The entry Conditions of velocity, concentrations of species, and pressure of admission in the anode and cathode sides are:
\[
U^* = 1; \quad V^* = 0; \quad C_{H_2O}^* = 0.1; \quad P^* = 1
\]

At the cathode, we have:
\[
C_{O_2}^* = 1; \quad C_{H_2}^* = 0
\]

and in the anode, we have:
\[
C_{O_2}^* = 0; \quad C_{H_2}^* = 1
\]

The resolution of the equations of Navier-Stokes presents a difficulty owing to the fact that the field of pressure is not known and there is not equation controlling for the field of pressure \(p\). From the equation of continuity and transport, we can determine the following pressure equation:
\[
\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = \left( \frac{\partial}{\partial x} \left( - \rho \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( - \rho \mu \frac{\partial u}{\partial y} \right) \right) \frac{\Delta t}{\Delta x^2} \quad \quad \quad (15)
\]

The governing equations were discretized using a finite volume method and solved using a computational program. The computational domains are divided into a finite number of control volumes (cells). All variables are stored at the centroid of each cell. Diagram of power is used to express variable values at the control volume surface in terms of the control volume center values.
2.5. Solution Algorithm

The solution begins by specifying a desired current density of the cell to be used for calculating the inlet flow rates at the anode and cathode sides. An initial guess of the activation overpotential is obtained from the desired current density using the Butler-Volmer equation. Then follows by computing the flow fields for velocities U, V and pressure P.

### Table I. Geometric and physical parameters used in this study.

| Symbol | Quantity                        | Value                          |
|--------|---------------------------------|--------------------------------|
| αₐ     | Cathodic transfer coefficient   | 0.5                            |
| αₑ     | Anodic transfer coefficient     | 0.5                            |
| ηₐ     | over-potential on the anode side| 0.3V                           |
| ηₑ     | over-potential on the cathode side| 0.3V                           |
| μ      | fluid dynamic viscosity        | 2x10⁻⁶ Kg/m.s                  |
| kₐ     | permeability of gas diffusion layer| 1.76x10⁻¹¹m²                  |
| kₑ     | permeability of membrane       | 1.58x10⁻¹⁸m²                   |
| ϵₐ     | Backing layer porosity         | 0.4                            |
| ϵₑ     | Membrane water porosity        | 0.28                           |
| Cᵥₑᶠ  | Concentration molaire de référence| 35.55 mol/m³                   |
| H      | Gas Channel weigh              | 1 mm                           |
| L      | Gas channel length             | 10 mm                          |
| Re     | Reynolds Number                | 600                            |
| Sc     | Schmidt Number                 | 0.43                           |

3. Results

3.1. Oxygen Distribution

The detailed distribution of oxygen for two different inlet pressure and height flow channel is shown in Figure 3. In all cases, oxygen concentration decreases gradually from the inflow channel to the outflow channel due to the consumption of oxygen at the catalyst layer. In the GDL, oxygen concentration under the land area is smaller than that under the channel area. The concentration of oxygen at the catalyst layer is balanced by the oxygen that is being consumed and the amount of oxygen that diffuses towards the catalyst layer, driven by the concentration gradient. The oxygen consumption increases clearly with reduction of height flow channel, consequently a reduction in concentration in the catalyst layer. For low height flow channel, the distribution of oxygen in catalyst is homogeneous. The results obtained show that the oxygen uptake is slightly high for P = 3 especially in the outlet.
3.2. Hydrogen Distribution

Fig. 3: Oxygen distribution in the anode for two different inlet pressure and height flow channel.

Fig. 4: Hydrogen distribution in the anode side for two different inlet pressure and height flow channel.
The hydrogen molar fraction distribution in the anode side is shown in Figure 4 for two different inlet pressure and height flow channel gas. In general, the hydrogen concentration decreases from inlet to outlet as it is being consumed. However, the decrease is quite small along the channel and the decrease in molar concentration of the hydrogen under the land areas is equal the oxygen in cathode side due to the same diffusivity of hydrogen and oxygen.

3.3. Water Distribution

The present model does not account for phase change and two-phase flow. This single-phase assumption then allows for super-saturation of water in the gas phase. The water molar fraction distribution in the cell is shown in Figure 5 for two different inlet pressure and heights flow gas channel. The magnitude of water production is higher for large channel than for tight channel.

The concentration of water inside the fuel cell strongly depends on consumption of the reagents; the production of water is higher in the cathodic catalyst layer in which the electrochemical reactions take place. The water produced on the level of catalyst is diffused towards the membrane and the GDL.

According to the results obtained, we denote that the diffusion of water towards the outlet channels for a high inlet pressure is higher.

Fig.5: Water distribution in the anode side for two different inlet pressure and height flow channel.
4. Conclusions:

In the present study, the simulations of flow phenomena in PEM fuel cell with a simple straight geometry of the flow channel gas have been effected. The effects of the flow parameters on the consumption of the reagents are examined in this work. Concentration and the consumption of gases and the distribution of water are obtained. The governing equations of the phenomenon of flow and transport of the species were solved, in all the parts of PEMFC, using the method of finite volumes. The influence of inlet pressure in channel gases and Reynolds number on the distribution and consumption of reagents is study in this paper. The results show that:

- The effect of the inlet pressure in channel gases shows that a weak variation is expressed on the concentration of hydrogen and oxygen.
- The oxygen concentration gradually decreases from admission to exit; this is due to the consumption of oxygen to the catalyst layer. Oxygen concentration near the exit of the cell is lower for the high Reynolds number by providing a low one and this for two pressure values.
- A significant gradient of oxygen consumption between the two ends of the stack is noticed. Oxygen consumption is slightly higher for \( P = 3 \) especially near the exit of the stack.
- In general, the concentration of hydrogen decreases from the admission to exit while it is consumed; it is varied depending on the Reynolds number and the inlet pressure. The hydrogen consumption is twice the oxygen consumption.
- The channels with smaller height showed a highest concentration of oxygen and hydrogen in catalyst layer and GDL.
- There is an increase in the consumption of species if the height is smaller. The influence of the height of the channel becomes important for a high Reynolds number.

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