

PEM fuel cell geometry optimisation using mathematical modeling

**Elena Carcadea¹, Ioan Stefanescu², Roxana E. Ionete³,
Horia Ene⁴, Derek B. Ingham⁵ and Lin Ma⁶**

¹National Institute of Cryogenics & Isotopic Technologies,
240050 Rm.Valcea, Romania, lili@icsi.ro

²National Institute of Cryogenics & Isotopic Technologies,
240050 Rm.Valcea, Romania, istef@icsi.ro

³National Institute of Cryogenics & Isotopic Technologies,
240050 Rm.Valcea, Romania, roxana@icsi.ro

⁴Institute of Mathematics of the Romanian Academy,
014700 Bucharest, Romania, Horia.Ene@imar.ro

⁵University of Leeds, Centre for Computational Fluid Dynamics,
LS2 9JT Leeds, UK, D.B.Ingham@leeds.ac.uk

⁶University of Leeds, Centre for Computational Fluid Dynamics,
LS2 9JT Leeds, UK, L.Ma@leeds.ac.uk

ABSTRACT

There have been extensive efforts devoted to proton exchange membrane (PEM) fuel cell modeling and simulations to study fuel cell performance. Although fuel cells have been successfully demonstrated in both automotive and stationary power applications, there are numerous technical and logistic issues that still have to be solved, such as performance, cost, and system issues. A model based on steady, isothermal, electrochemical, three-dimensional computational fluid dynamics using the FLUENT CFD software package has been developed to predict the fluid flow pattern within a PEMFC. Three types of flow field are investigated with serpentine, parallel or spiral channels in order to determine the best configuration for the fuel cell performance. In this context, the paper presents the results that we have obtained and, as a conclusion of the simulations, we have achieved the best configuration regarding the performance for the fuel cell with serpentine channels. We consider the mathematical and computational modeling as an important alternative for fuel cell optimization and for the exploitation/experimentation in cost reduction.

1. INTRODUCTION

One of the newly emerging technologies in which we are investing considerable human and financial resources is in fuel cell technology. It offers great advantages over the conventional power generation technology in terms of both energy efficiency and reduction in pollutant emissions. However, a success in commercialization of PEM fuel cell technologies will depend on performance, design and manufacture optimizations.

A large amount of work has been published regarding the modeling of the PEMFC. The earliest models were one-dimensional and only account for diffusive mass transport and electrochemical kinetics, such as those published in the early 1990s by Springer [1] and

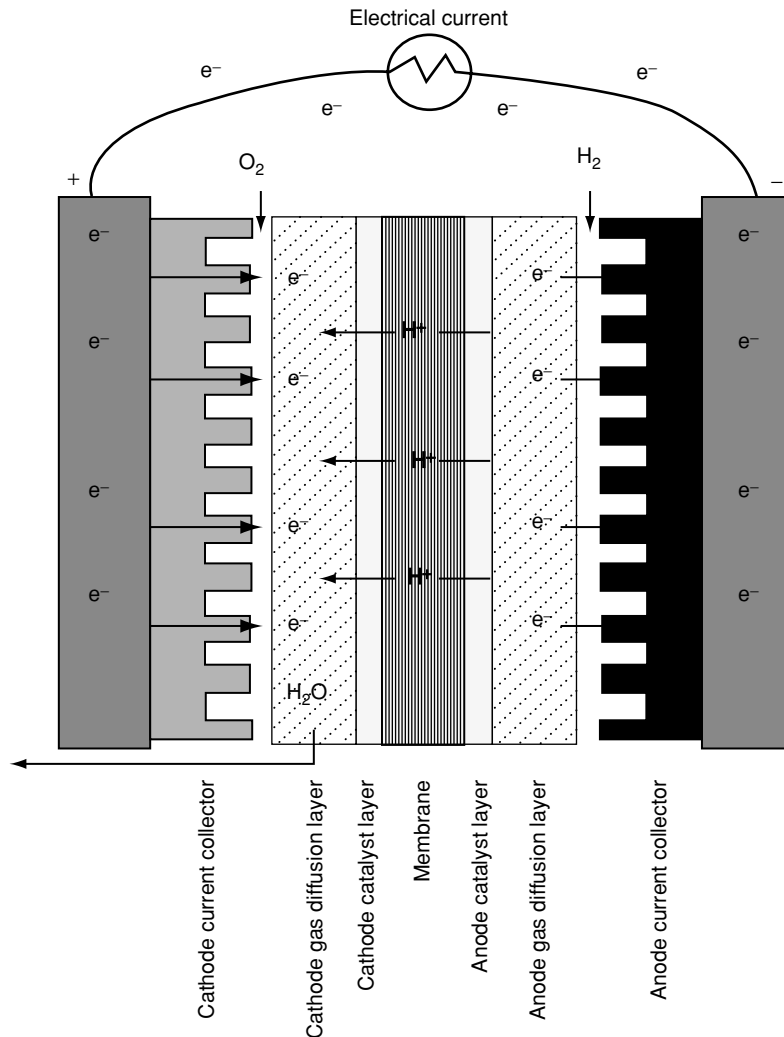


Figure 1 Schematic sketch of a PEM fuel cell.

Bernardi and Verbrugge [2]. Nguyen performed a two-dimensional, steady state, heat transfer and mass transfer model to understand the phenomenon of the water transfer and heat transfer in the membrane [3]. Gurau performed a 2-D computational fluid dynamic (CFD) analysis of a PEMFC [4]. In their work, conservation equations were solved for mass, momentum, energy, species, and electric potential.

A fuel cell is an electrochemical energy conversion device that uses fuel and oxidant to efficiently produce electricity [6]. Like most other electrochemical devices, a PEM fuel cell consists of three parts, namely: an anode, where the fuel that feeds the cell is oxidized; a cathode, where the reduction of oxidant, typically oxygen, takes place; and an electrolyte that acts as a proton conductor and an electronic insulator. Both the anode and the cathode have two different regions, a gas diffusion layer and a catalyst layer. Fuel and oxidant are supplied through the gas channels grooved in the current collector plates placed on two sides of the fuel cell (see figure 1). The electrolyte in a PEM fuel cell system is a polymer membrane,

such as Nafion 112, a suitable and convenient humidification membrane material for fuel cell applications.

The general performance of the fuel cell can be analyzed by the modeling of the transport and the transformation of gas reactants and products and the electrochemical reactions.

In this paper we extend our previous work [5] with particular focus on finding an optimum geometry of the flow field in order to optimize the PEM fuel cell operation based on the geometries that we developed. Thus, the paper presents some of the results that have been obtained in a parametric investigation using CFD techniques performed for a PEMFC with three types of gas distribution channels: serpentine, parallel and spiral. The focus of the paper is on the hydrogen and oxygen consumption, as well as the water and voltage distribution.

Studies of different flow patterns (parallel, spiral, and serpentine) can give us suggestions on how to optimize the flow-field design for a PEMFC stack.

2. FUEL CELL MATHEMATICAL MODELING

Mathematical modeling is used as a tool for optimizing the PEM fuel cell and stack performance. Using a parametric study, a combination of the most efficient design and operating conditions may be found as it can provide detailed information on the various processes that occur within the fuel cell and/or stack investigated. Mathematical and computational modeling also allows the prediction of the behavior of certain parameters that would be almost impossible to obtain experimentally.

A CFD model, based on commercial CFD software packages for fuel cell modeling, can become very complex for two- and three- dimensional studies of the complex physical phenomena that take place inside a PEM fuel cell. A detailed model must include a complete set of equations that take into consideration the fluid flow through the porous anode and cathode, the influence of the multi-component diffusion of the gaseous species, phase change and multiphase flow, the migration of protons through the membrane, the electrical charge transfer, and the heat and mass transfer.

2.1. MODEL DESCRIPTION

In this paper, the performance of the Proton Exchange Membrane fuel cell is studied using a single-phase, steady state, isothermal three-dimensional electrochemical model. Physical and electrochemical phenomena that take place inside a fuel cell are represented by the mathematical model developed and the analysis is based on the solution of the conservation equations of mass, momentum, species and charge transport. A single domain formulation is used in the simulation.

In order to simplify the model, some assumptions are needed and it is important to understand these assumptions in order to appreciate the limitations of the model and to interpret correctly the results. Some of the main assumptions made in the development of the model are as follows:

- The fuel cell operates under a steady state condition.
- The flow in the channels is considered incompressible and laminar.³¹⁴
- The porous electrodes, catalyst layers and membrane are isotropic and homogeneous.
- The water in the fuel cell is in vapor form.
- The temperature of the cell is constant.

Under the above assumptions, the model equations can be written as follows [7]:

$$\nabla \cdot (\epsilon \rho \vec{u}) = S_m \quad (1)$$

$$\nabla \cdot (\varepsilon \rho \vec{u} \vec{u}) = -\varepsilon \nabla p + \nabla \cdot (\varepsilon \mu \nabla \vec{u}) + S_u \quad (2)$$

$$\nabla \cdot (\varepsilon u \vec{Y}_i) = \nabla \cdot (D_i^{eff} \nabla Y_i) + S_i \quad (3)$$

$$\nabla \cdot (\sigma_s^{eff} \nabla \Phi_s) + S_\Phi = 0 \quad (4)$$

where \vec{u} , Y_i and Φ_s denotes the velocity vector, mass fraction of the i species and the phase potential, respectively, ε is the porosity of the material, and ρ and μ are the density and the molecular viscosity of the fluid flow. Further, σ_s^{eff} is the electrical conductivity of the solid elements.

The source term in the mass conservation equation, Eqn. (1), corresponds to the consumption of hydrogen and water vapor in the anode and the consumption of oxygen and production of water vapor in the cathode, are given by:

$$S_m = \begin{cases} S_{H_2} + S_{H_2O} & \text{in anode catalyst layer} \\ S_{O_2} + S_{H_2O} & \text{in cathode catalyst layer} \end{cases} \quad (5)$$

Regarding the momentum equations, Eqn. (2), the source term is different in different regions of the fuel cell. In the gas channels the source term is zero. In the gas diffusion layers and catalyst layers the source term is added based on the Darcy law, representing an extra drag force imposed by the pore walls on the fluid and is given by the formula:

$$S_u = -\frac{\mu}{k} u \quad (6)$$

where k is the permeability of the porous medium (gas diffusion/catalyst layer).

The source term in the species conservation equation, S_i , is zero everywhere except in the catalyst layer where the chemical species i is either consumed or generated in the electrochemical reactions. Therefore, the source terms of the species concentration for hydrogen, oxygen and water from Eqn. (3) are implemented based on electrochemical kinetics as follows [8]:

$$S_{H_2} = -\frac{M_{H_2}}{2F} \cdot j_{anode} \quad (7)$$

$$S_{O_2} = -\frac{M_{O_2}}{4F} \cdot j_{cathode} \quad (8)$$

$$S_{H_2O} = \begin{cases} -M_{H_2O} \cdot \alpha & \text{in anode catalyst layer} \\ M_{H_2O} \cdot \alpha + \frac{M_{H_2O}}{2F} \cdot j_c & \text{in cathode catalyst layer} \end{cases} \quad (9)$$

where M_{H_2} , M_{O_2} , M_{H_2O} are the molecular weight of hydrogen, oxygen and water, respectively, and α is the molar flux of water.

The effective specie diffusivity, D_i^{eff} , is a function of the porosity and the mass diffusion coefficient of the species i , D_i , and is given by the expression:

$$D_i^{eff} = \varepsilon^{1.5} \cdot D_i \quad (10)$$

where:

$$D_i = D_i^0 \left(\frac{p_0}{p} \right)^1 \left(\frac{T}{T_0} \right)^{1.5} \quad (11)$$

$$T_0 = 300 \text{ K}$$

$$p_0 = 101.325 \text{ N/m}^2$$

D_i^0 - mass diffusivity of species i at reference temperature and pressure (T_0 , p_0).

The source term from the charge conservation equation, Eqn. (4), representing the volumetric transfer current, appears only in the catalyst layer of the fuel cell and elsewhere is zero. Thus:

$$S_\phi = \begin{cases} -j_{anode} & \text{in anode catalyst layer} \\ j_{cathode} & \text{in cathode catalyst layer} \end{cases} \quad (12)$$

In these equations, the transfer current densities, j , are given by the Butler-Volmer equation and are the results of the electrochemical reactions that take place on the catalyst surface. The Butler-Volmer equation expresses the relationship between the local current density and the concentration of the reactant species, activation overpotential and temperature in the anode and cathode side, as follows:

$$\text{Anode: } j_{anode} = j_{0,a}^{ref} \left(\frac{c_{H_2}}{c_{H_2}^{ref}} \right)^{1/2} \left[\exp \left(\frac{\alpha_a F}{RT} \eta_{act,a} \right) - \exp \left(-\frac{\alpha_c F}{RT} \eta_{act,a} \right) \right] \quad (13)$$

$$\text{Cathode: } j_{cathode} = j_{0,c}^{ref} \left(\frac{c_{O_2}}{c_{O_2}^{ref}} \right) \left[\exp \left(\frac{\alpha_a F}{RT} \eta_{act,c} \right) - \exp \left(-\frac{\alpha_c F}{RT} \eta_{act,c} \right) \right] \quad (14)$$

where c denotes the reactants concentration, α_a and α_c are transfer coefficients, $\eta_{act,a}$ $\eta_{act,c}$ are the activation over potential from the anode and cathode, and $j_{0,a}^{ref}$ and $j_{0,c}^{ref}$ are the reference exchange current densities from the anode and cathode sides, respectively.

Water management is a critical issue for the performance of a fuel cell. The transport phenomena of water can be described as follows: the water molecules are transported through the polymer electrolyte membrane by the hydrogen protons and this process is called electro-osmotic drag. In addition to the molecular diffusion and electro-osmotic drag, in the cathode catalyst layer water is generated due to the oxygen reduction reaction.

The molar flux of water, α , is based on the electro-osmotic drag coefficient n_d , water content, λ , and water activity, a . All these parameters are given by the expressions [8]:

$$a = \frac{X_{H_2O} p}{p^{sat}} \quad (15)$$

$$\lambda = \begin{cases} 0.043 + 17.18 \cdot a - 39.85a^2 + 36.0a^3 & \text{for } 0 < a \leq 1 \\ 14 + 1.4 \cdot (a - 1) & \text{for } 1 \leq a \leq 3 \end{cases} \quad (16)$$

where the saturation pressure can be computed as follows:

$$\log_{10} p^{sat} = -2.1794 + 0.02953 \cdot (T - 273.15) - 9.1837 \cdot 10^{-5} (T - 273.15)^2 + 1.4454 \cdot 10^{-7} (T - 273.15)^3 \quad (17)$$

$$n_d = 0.0028 \cdot \lambda + 0.05\lambda - 3.5 \cdot 10^{-19} \quad (18)$$

$$\alpha = \frac{n_d \cdot j_k}{F} - D_w \nabla C_w \quad (19)$$

where k is anode or cathode, D_w and C_w are the water diffusion coefficient and water concentration across the membrane.

The expression for the water concentration in Eqn. (18) is given by:

$$C_{wk} = \frac{\rho_{m,dry}}{M_{m,dry}} \lambda_k \quad (20)$$

where $\rho_{m,dry}$ is the dry membrane density, and $M_{m,dry}$ is the membrane equivalent weight.

The water diffusion coefficient in the membrane is obtained from [7,8]:

$$\begin{aligned}
 D_w &= D_\lambda \exp \left[2416 \left(\frac{1}{303} - \frac{1}{T} \right) \right] \\
 D_\lambda &= 10^{-10} & \lambda < 2 \\
 D_\lambda &= 10^{-10} (1 + 2(\lambda - 2)) & 2 \leq \lambda \leq 3 \\
 D_\lambda &= 10^{-10} (3 - 1.67(\lambda - 3)) & 3 \leq \lambda \leq 4.5 \\
 D_\lambda &= 1.25 * 10^{-10} & \lambda \geq 4.5
 \end{aligned} \tag{21}$$

The CFD software Fluent was used for all the numerical calculations performed, using appropriately specified boundary conditions for the fuel cell under investigation. Thus, the solution to the governing partial differential equations is uniquely determined. Typical boundary conditions include the flow rates of the fuel and oxidant (air/oxygen), operational pressure, current density or voltage of the fuel cell, plus the necessary thermal – physical properties of the materials of the cell.

For solving this problem we prescribed at the inlet of both the anode and cathode flow channels values for the mass flow rate, temperature and mass fraction, as we can see from table 2. Regarding the boundary conditions for the outlets, since the reactant gas flow channels are separate and generally have different pressures then pressure boundary conditions are used. The interfaces between the layers are interior faces, and therefore no boundary conditions are prescribed. Dirichlet boundary conditions with constant values are set for the solid phase potential on the lateral sides of the fuel cell and zero flux conditions are applied at the inlet and outlet.

2.2. MATHEMATICAL MODEL IMPLEMENTATION AND ANALYSIS

At present, there are numerous technical barriers that prevent fuel cells from becoming commercially competitive but CFD modeling has been recognized as one of the important tools in the development of new and advanced fuel cell technologies. The mathematical and numerical models offer an alternative solution to experiments and can give us detailed information regarding the geometry used, and the analyzing and optimization of fuel cell operations. Using CFD techniques we can obtain the distribution of important parameters, such as the fluid flow and pressure, or information about the chemical species implied in the reactions, the fuel consumption, the water content and the current density in the fuel cell. These parameters give us detailed information on the efficiency of the fluid flow, the mass transfer, as well as the chemical and electrochemical reactions that takes place in a fuel cell, and as a consequence we can decide on the optimum geometry for obtaining a high performance.

For finding the optimum geometry from the three geometries mentioned above, the Fluent software was chosen in order to analyse the fluid flow dynamics and fuel cell performance. Fluent is a CFD software for the fluid flow and heat transfer modeling of complex geometries, providing flexibility regarding the building of the geometry, the accuracy of the fluid flow, and the grid refinement in important regions, such as the boundary between two layers.

The main objective of this paper is to optimize the fluid flow channel pattern and to improve the performance of a PEM fuel cell system, based on the three patterns mentioned (serpentine, spiral and parallel channels). Simulations were performed using Fluent Fuel Cell 2.1, a specialised module in the fuel cell fluid flow analyses.

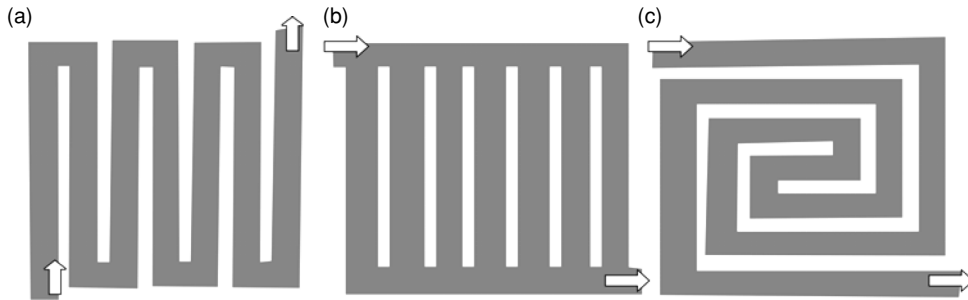


Figure 2 The fluid flow channel geometries: (a) serpentine channel; (b) parallel channel; (c) spiral channel.

3. NUMERICAL SIMULATIONS: RESULTS AND DISCUSSIONS

In solving a problem of fluid dynamics analyses with CFD software there are some steps that have to be followed:

- Define the modeling purposes (what specific results are expected, what accuracy is needed).
- Build the geometry using a pre-processor, such as Gambit or TGrid.
- Choose the model (the problem can be solved in 2D or 3D, where to start and end the numerical domain, what boundary conditions are needed?, etc).
- Choose the physical model for the fluid flow (what type of motion is implied by the flow: laminar or turbulent, steady or unsteady, include heat transfer, etc).
- Determine a solution (can the problem be solved easiest using the initial setting of the software? Can the convergence be accelerated correctly? What memory is needed and how long will it take until a converged solution is obtained?).

Most of these questions have been taken into consideration in developing the model described in section 2 or are discussed further.

3.1. GEOMETRY BUILDING USING THE PRE-PROCESSOR GAMBIT

For the geometry building pre-processors, such as: Gambit, ANSYS, TGRID or other CAD packages, can be used. In this paper, three geometries for the fluid flow channels of a PEM fuel cell were created using the Gambit grid generator in order to establish the optimum fluid flow pattern and to obtain an increased performance, see figure 2.

The dimensions used for the fuel cell geometries built in Gambit are given in the table 1. The values for the fuel cell layers (width, length and height) were established for illustrative purpose only. The parameters in the table refer both to the anode and the cathode of the fuel cell. Also, table 1 presents the electrochemical properties used in the CFD model. It can be noticed that the open cell voltage was set up to 0.95. The maximum reversible potential of a PEMFC running at 80°C is about 1.2 V. However, this is not achievable in practice due to the effect of limited reaction and, in particular, the fuel cross-over. Therefore, the open circuit voltage of a PEMFC is usually less than 1.0V. For the purpose of this study, a typical value of 0.95V was assumed.

A structured uniform grid was used in the computations, having about 1 million cells. In order to investigate the grid independent solution, the grid was refined by adding 50% more cells to the geometry of the fuel cell with serpentine channels. The computations at base case conditions were repeated on this refined grid and the solutions compared. The polarizations curves obtained for the base case and the refined grids are shown in the figure 3. It can be seen that there is very

Tabel 1 Physical dimensions and properties of the fuel cell investigated

Parameter	Value	Unit
Gas channel height	1.5	mm
Gas channel width	2	mm
Bipolar plate thickness	5	mm
Bipolar plate width/ length	22/22	mm
Diffusion layer width (anode/cathode)	0.37	mm
Membrane width	0.07	mm
Catalyst layer width (anode/cathode)	0.12	mm
Porosity of diffusion layer	0.8	-
Porosity of catalyst layer	0.4	-
Permeability for diffusion/catalyst layer	1×10^{-10}	m^2
Open cell voltage	0.95	V

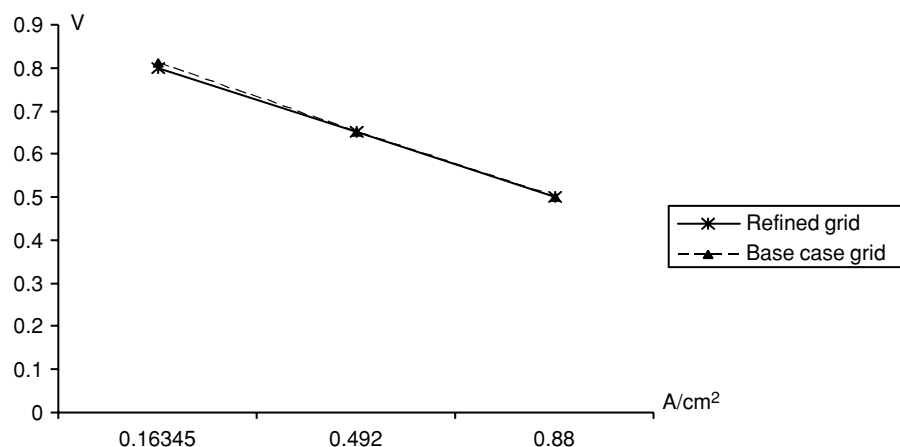


Figure 3 Mesh sensitivity analyses for the fuel cell with serpentine channels.

good agreement between the results obtained using the two grids. This indicates, in terms of the fuel cell performance, that the base case grid provides an adequate resolution. Taking into account the computational effort required by the refined grid (1.5 million cells) and the grid independent solution illustrated in figure 3 we decided to use the base case grid in the calculations.

Table 2 provides the operating conditions used for the simulations and the initial conditions for both anode and cathode (mass flow rate and inlet mass fractions).

3.2. RESULTS AND DISCUSSION

Using a CFD software, such as Fluent, we can display the results obtained in vectorial form, or as a contour or in profile form. Some of the parameters that can be visualized are: velocity, pressure, temperature, species implied in the reaction (mass fraction, molar fraction or concentration) and many other important characteristics such as: material and fluid properties, grid information, the wall flux, etc.

Table 2 Operational parameters

	Parameter	Value	Unit
Initial conditions for anode	Mass flow rate	10^{-7}	kg/s
	Mass fraction for H_2	0.9	-
	Mass fraction for H_2O	0.1	-
Initial conditions for cathode	Mass flow rate	10^{-6}	kg/s
	Mass fraction for O_2	0.22	-
	Mass fraction for H_2O	0.25	-
Operating conditions	Pressure	1	atm
	Potential difference between anode/cathode	0.5	V
	Temperature	353	K

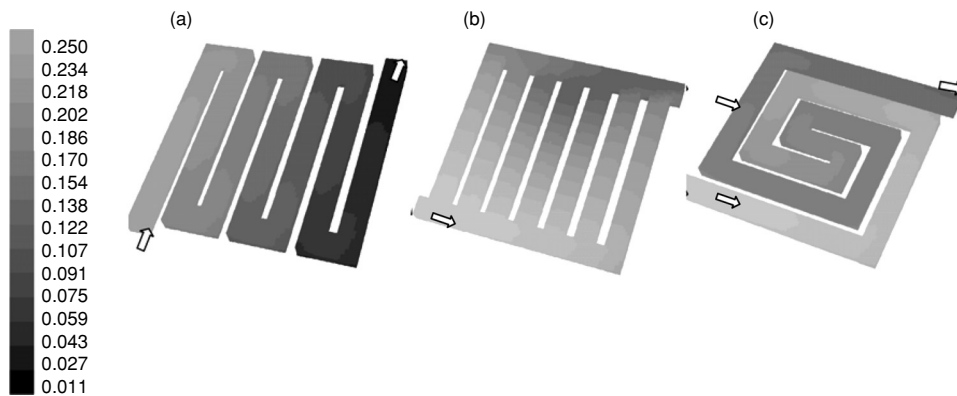


Figure 4 Hydrogen mass fraction distribution in the anode side of a fuel cell with: (a) serpentine channel; (b) parallel channel; (c) spiral channel.

3.2.1. Distribution

The hydrogen mass fraction distribution in the anode gas channels decreases from the inlet, where we set up the initial value to be 0.9, to the outlet where we obtain the values: 0.616 in the serpentine channel, Figure 4(a), 0.679 in the parallel channel, figure 4(b), and 0.703 in the spiral channel, figure 4(c). The mass fraction decreases because the hydrogen is consumed by the reactions that take place inside the fuel cell. It is observed from figure 4 that in the fuel cell with serpentine channels that more hydrogen is consumed.

3.2.2. Oxygen distribution

The oxygen mass fraction distribution in the three channels analyzed has the same trend as that of the hydrogen because the oxygen is consumed by the electrochemical reaction. Thus we have a decrease in the oxygen mass fraction as the flow goes through the channels. For an initial value of 0.25 at the inlet, we obtained different values for the three cases simulated as follows: 0.011 for the serpentine channel, 0.083 for the parallel channel and 0.068 for the spiral channel. Figure 5 shows the oxygen distribution in the cathode side and it is observed that in the serpentine configuration more oxygen is being consumed.

3.2.3. Water management for PEM fuel cells

The water mass fraction distribution in the anode and cathode gas channels is shown in Figures 6 and 7. In general, the water concentration increases from the inlet to the outlet; in

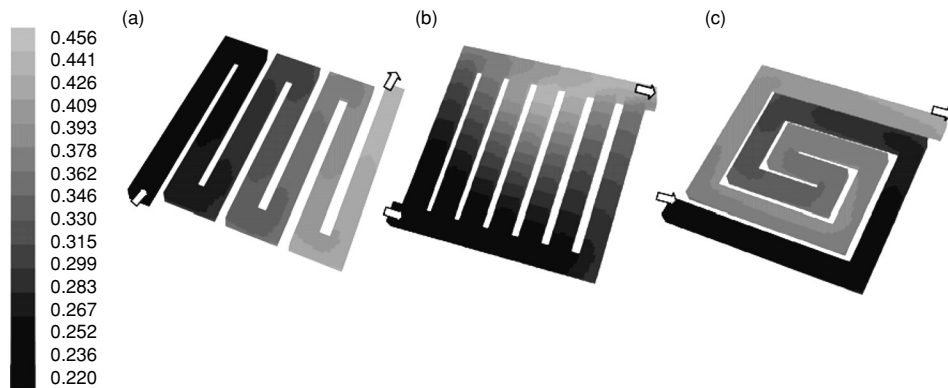


Figure 5 Oxygen mass fraction distribution in the cathode side of a fuel cell with: (a) serpentine channel; (b) parallel channel; (c) spiral channel.

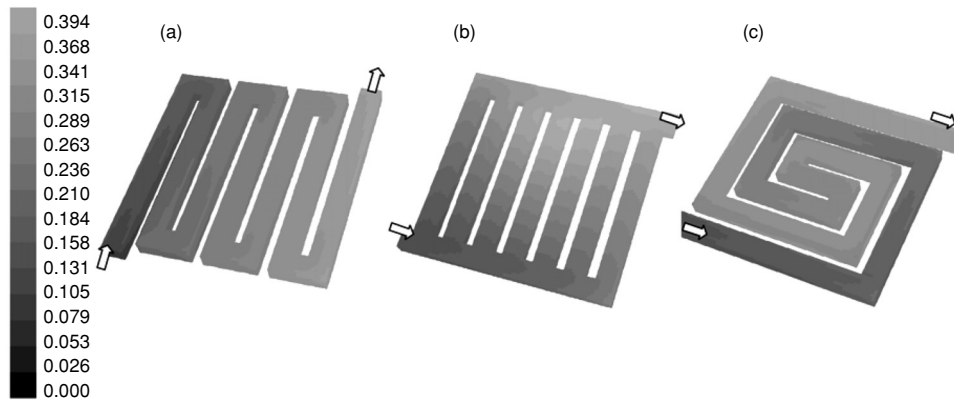


Figure 6 Water mass fraction distribution in the anode side of a fuel cell with: (a) serpentine channel; (b) parallel channel; (c) spiral channel.

the anode side the mass fraction of water increases because of the hydrogen consumption from 0.1 to a maximum value of 0.384 (for serpentine channel configuration) and in the cathode side from 0.22 to a maximum value of 0.456 (for serpentine channel configuration).

The water distribution in the geometries analyzed, both in the anode and the cathode side of the fuel cell, presents an increase in the mass fraction while the flow goes to the outlet. As a consequence of the electrochemical reaction that takes place in the fuel cell cathode, water is produced as a secondary product, and therefore it increases the water flow rates in the cathode of a fuel cell. Figures 6 and 7 present the water mass fraction distributions in the anode and the cathode of the cell.

3.2.4. Voltage distribution

For solving the phase potential equation we can set up the boundary conditions for the external boundaries of the fuel cell based on two possibilities: the voltage, a case in which we consider on the cathode external wall, and a constant value for the voltage, or the current density, a constant flux, on the anode. For these simulations we set up potentiostatic boundary conditions (constant voltage) for both the anode and cathode.

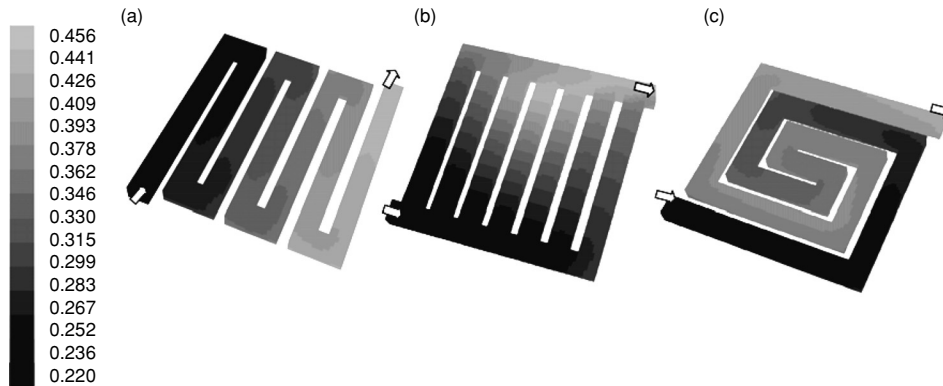


Figure 7 Water mass fraction distribution in the cathode side of a fuel cell with: (a) serpentine channel; (b) parallel channel; (c) spiral channel.

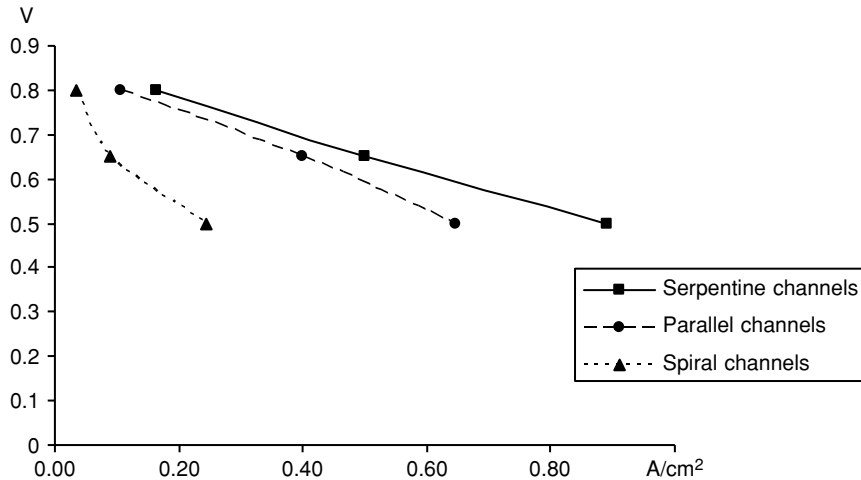


Figure 8 Voltage contours in the cathode diffusion layer (upper plan) and cathode current collector (bottom geometry) for a fuel cell with: (a) serpentine channel; (b) parallel channel; (c) spiral channel.

Figure 8 presents the voltage distributions in the cathode current collector plate and in the cathode diffusion layer. For illustrative purpose, for all three geometries investigated a condition of 0.5V is set on the cathode side boundary. It is seen from Figure 8 that the largest voltage difference in the voltage between the current collector plate and the diffusion layer was in the fuel cell with the serpentine channels. This was what we have expected because the oxygen and hydrogen consumptions were the largest in the serpentine channel configuration which leads to a higher performance.

3.2.5. Polarization curve

The polarization curves for the PEM fuel cells investigated in this paper are shown in figure 9. We have performed 3 simulations with different values of the potential on the external cathode

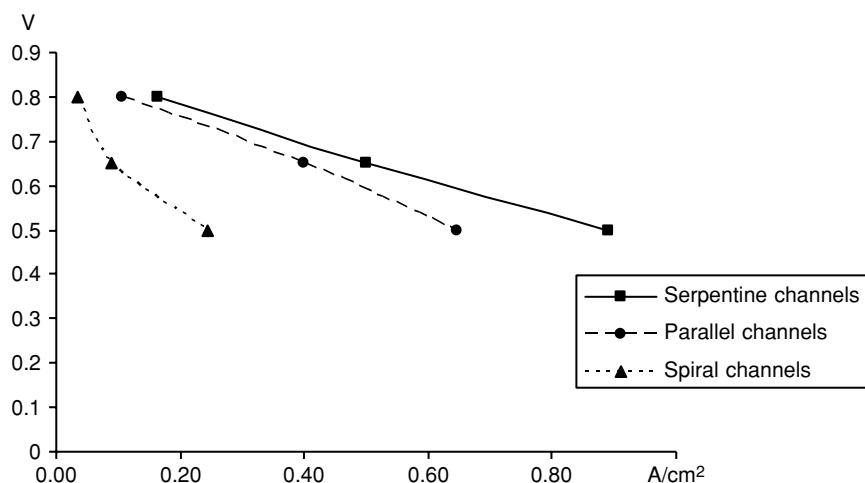


Figure 9 Polarization curve for a fuel cell with: (a) serpentine channel; (b) parallel channel; (c) spiral channel.

wall (0.5V, 0.65V, and 0.8 V) and we have obtained the average current densities as shown in figure 9. It can be noticed that the performance of the fuel cell with serpentine channels, from the electric current generation point of view, is better than for the other two cases investigated.

4. CONCLUSIONS

In general it is appreciated that the CFD modeling of a fuel cell is still facing significant challenges due to the limited understanding of the complex physical and chemical processes that occur within the fuel cell. However, with the further development of the modeling capabilities, the modeling of fuel cells using CFD techniques can be an important alternative to performing numerous costly experiment measurements in providing information that is critical to the fuel cell design and optimization.

A model based on the steady three-dimensional computational flow dynamics using the Fluent CFD software has been developed to predict the fluid flow patterns in the chosen geometries and to determine the best configuration for the gas channel design in order to optimize the performance of a fuel cell. In this context, the paper presents the results that we obtained for the three different geometries mentioned in an attempt to find the best flow field geometry for the Proton Exchange Membrane fuel cell investigated. From the analysis of the hydrogen/oxygen consumption, water production and transport, and the electrical voltage/current generation, it is concluded that among the three geometries studied the best configuration is the serpentine channel design since it gives the highest rate of electrical generation of the three cell designs investigated.

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