Numerical investigation of reactant transport, water management, and performance optimization in a planar PEMFC

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Abstract

This work presents a computational fluid dynamics (CFD) model of a proton exchange membrane fuel cell (PEMFC)in three dimensions, with straight flow channels, analyzed in steady-state and non-isothermal conditions. The model, developed using ANSYS Fluent, investigates how relative humidity and flow arrangements (co-flow vs. counter-flow) affect PEMFC performance. It evaluates reactant distribution, power output, and water management across varying humidity levels. Simulation results show that the counter-flow configuration offers more uniform reactant distribution, improved membrane hydration, and reduced water flooding. Optimal power density is achieved at 100% relative humidity. These findings underscore the importance of humidification and flow arrangement in enhancing PEMFC efficiency and operational stability.

Keywords: Proton exchange membrane fuel cell (PEMFC); Computational fluid dynamics (CFD); Flow arrangements; Relative humidity; Power density.

1. Introduction

Due to increasing environmental issues, there has been a significant surge in the demand for clean energy solutions [1]. Hydrogen is anticipated to be pivotal in the transition from fossil fuels to clean and renewable energy sources [2]. In this context, hydrogen fuel cells, especially PEMFC, stand out as a viable alternative owing to their impressive energy conversion efficiency and low hazardous emissions [3]. The advantages have enabled widespread adoption, especially within the automotive sector and for stationary power generation [4].

Many researchers are interested in improving fuel cells, particularly PEMFC. Some focus on system-level optimization [5], while others explore analytical and empirical modeling techniques [6]. In particular, studies have investigated how geometric factors such as cross-sectional [7], flow path [8], and component dimensions [9] affect PEMFC performance. For example, Laoun et al. [10] applied a global sensitivity analysis technique enhanced by the variance method to a theoretical PEMFC model. Similarly, Benmouiza et al. [11] analyzed the contributions of activation, ohmic, and mass transport losses, examining how variables. In the context of flow field design, Brakni et al. [12] developed a three-dimensional, non-isothermal CFD model to optimize channel geometry using configurations with constrictions and enlargements Mohammadi et al. [13]. A three-dimensional, steady-state simulation of planar PEMFC was conducted to identify and establish the optimal dimensions for enhanced performance. Additionally, in another study, Mohammadi et al. [14] investigated the effect of channel cross-section shapes on PEMFC performance using 30 different configurations. These studies collectively emphasize the crucial role of both operating conditions and physical design particularly channel geometry and component dimensions in enhancing the performance and efficiency of PEMFC systems.

This study examines how essential operational parameters, including gas flow arrangement and relative humidity, influence the transport phenomena and performance characteristics of a single straight-channel PEMFC. The aim is to enhance the design of fuel cells by offering a more profound understanding of the intricate internal interactions that influence cell performance. A three-dimensional CFD model is developed and implemented using ANSYS-Fluent to accomplish this objective. The model is considered to be non-isothermal, single-phase, and functioning under steady-state conditions, with the computational domain restricted to a single PEMFC that includes straight gas flow channels.

2. Computational domain and assumption

A three-dimensional, non-isothermal, steady-state model of a single PEM fuel cell with a planar design and straight flow channels has been developed. The geometry of the single planar PEMFC cell is developed utilizing the ANSYS Design Modeler tool. The computational domain consists of nine distinct sub-regions: two gas diffusion layers (GDLs), two catalyst layers (CLs), one electrolyte membrane, two bipolar plates (current collectors), and two reactant flow channels. The combination of these regions delineates the complete configuration of the simulated PEMFC cell. Table 1 presents the dimensions of each component.

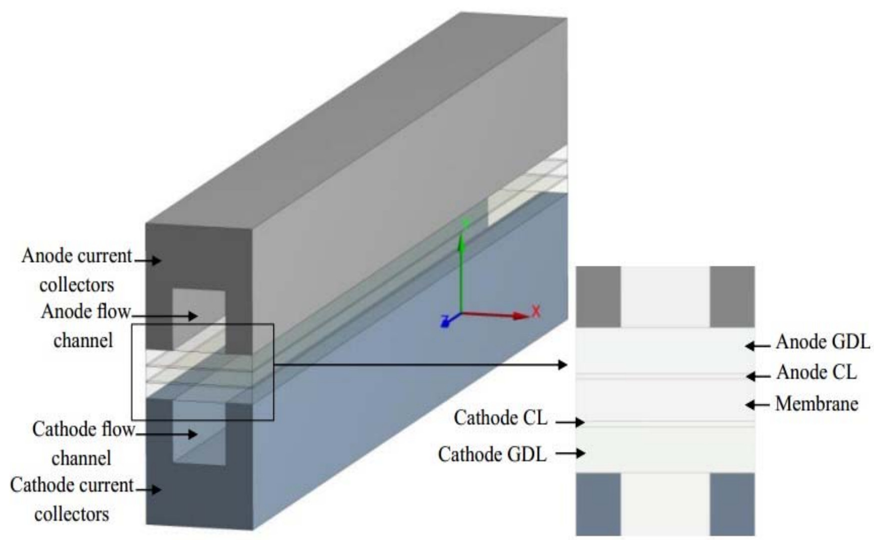

Figure. 2. Structure of the studied PEMFC.

The PEMFC model assumes that the reactant flow is laminar, incompressible, and in a steady-state condition. All gases adhere to the ideal gas law, and porous media are regarded as isotropic. Water phase transitions are overlooked, the membrane is assumed impermeable to reactants, and gravitational effects are excluded to streamline the analysis.

Table 1. Geometric parameters

Parameters	Units	Dimensions
Cell length	mm	100
Channel width/ height	mm	0.8
Membrane thickness	mm	0.1
Catalyst layer thickness	mm	0.048
Gas diffusion layer thickness	mm	0.2

Numerical simulations are performed utilizing the commercial CFD program ANSYS Fluent to examine the influence of flow configurations and inlet relative humidity on the performance, pressure drop, and transport characteristics of the PEMFC. The three-dimensional model integrates the Navier-Stokes, energy, mass conservation, species transport, electrical charge conservation, and Butler-Volmer equations. The governing equations and implementation procedures are thoroughly detailed in the ANSYS PEMFC Add-on Module [14,15].

- Continuity

$$\nabla\left(\rho\varepsilon\vec{u}\right)=0$$

- Momentum conservation

$$\nabla\left(\rho\varepsilon\vec{u}\vec{u}\right)=-\varepsilon\nabla P+\nabla\left(\mu\varepsilon\nabla\vec{u}\right)+\frac{\varepsilon^{2}\mu\vec{u}}{\kappa}$$

- Energy conservation

$$\nabla\left(\rho\varepsilon CpT\,\vec{u}\right)=\nabla\left(k_{eff}\,\nabla T\right)+j\,\eta+\frac{j}{\sigma}+h_{reac}$$

- Species conservation

$$\nabla\left(\rho\varepsilon uY_{i}\right)=\nabla\left(\rho D_{i}^{eff}Y_{i}\right)+S_{c}$$

- Proton and electron transport equation

$$\nabla\left(\sigma_{s}\nabla\phi_{s}\right)+S_{c}=0$$

$$\nabla\left(\sigma_{m}\nabla\phi_{m}\right)+S_{m}=0$$

- Butler–Volmer

$$j_{a}=A_{a}j_{0,a}^{ref}\left(\frac{C_{H_2}}{C_{H_2}^{ref}}\right)^{\gamma_a}\left(e^{\frac{\alpha_a F\eta_a}{RT}}-e^{\frac{-\alpha_c F\eta_a}{RT}}\right)$$

$$j_c = A_c j_{0,c}^{ref} \left(\frac{C_{O_2}}{C_{O_2}^{ref}} \right)^{\gamma_a} \left(-e^{\frac{\alpha_a F \eta_a}{RT}} + e^{\frac{-\alpha_c F \eta_c}{RT}} \right)$$

Boundary conditions

At the inlets of the anodic and cathodic channels, Dirichlet boundary conditions are applied for mass flow rate, temperature, and species concentrations. In all simulation scenarios, the mass flow rates at the channel inlets are kept constant. For other parameters, Neumann boundary conditions are employed. Zero species flux and no-slip boundary conditions are imposed at the fluid/solid interfaces. At the outlets of the channels, a pressure outlet boundary condition is applied, while a zero gradient is assumed in the flow direction (OZ) for the remaining parameters. Additionally, wall boundary conditions are applied at the external surfaces of the PEMFC in the simulations.

3. Results and discissions

After simulating the PEMFC single cell with straight channels in the commercial CFD software ANSYS Fluent, we validated the findings and ensured mesh independence. Our previous work [13,14] examines and details the mesh independence test in great detail, as well as compares numerical and experimental results. The mentioned articles provide the complete facts and in-depth analysis, although this study does include a validation figure.

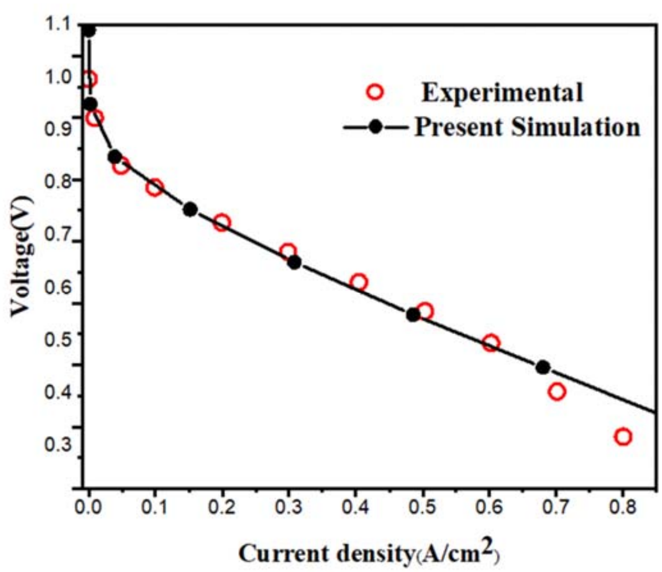

Figure 2. Validation of the present PEMFC simulation.

3.1. Effect of relative humidity on polarization and power density curves in a PEMFC with contre-flow arrangement

Figure 3 displays the polarization and power density curves acquired at three relative humidity levels in a co-flow configuration. The findings demonstrate that the ideal relative humidity for fuel cell efficacy is 100%. The minimal voltages and power densities were recorded at the lowest examined relative humidity of 50%.The performance of the PEMFC at medium and high current densities is significantly influenced by variations in relative humidity. In the investigated PEMFC, voltage and power density exhibit a direct dependence on relative humidity. The improved performance at higher relative humidity is attributed to enhanced proton conductivity and more efficient diffusion of reactants and products, which together optimize the electrochemical processes within the cell.

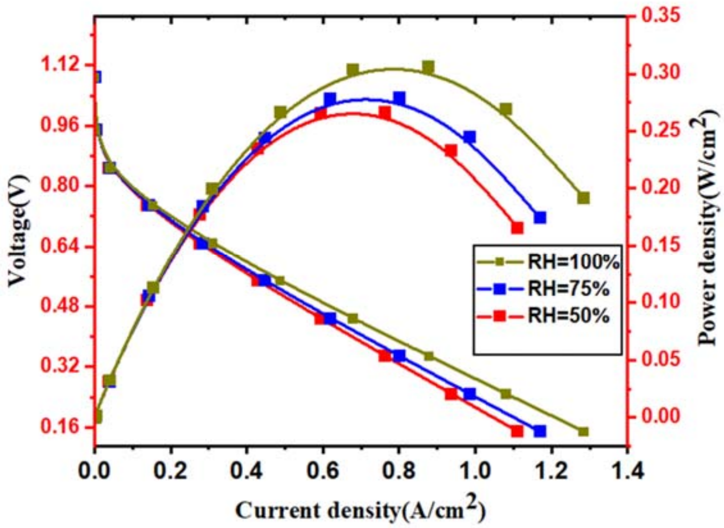

Figure 3. Effect of relative humidity on polarization and power density curves in a co-flow PEMFC.

3.2. Effect of relative humidity on polarization and power density curves in a PEMFC with contre-flow arrangement

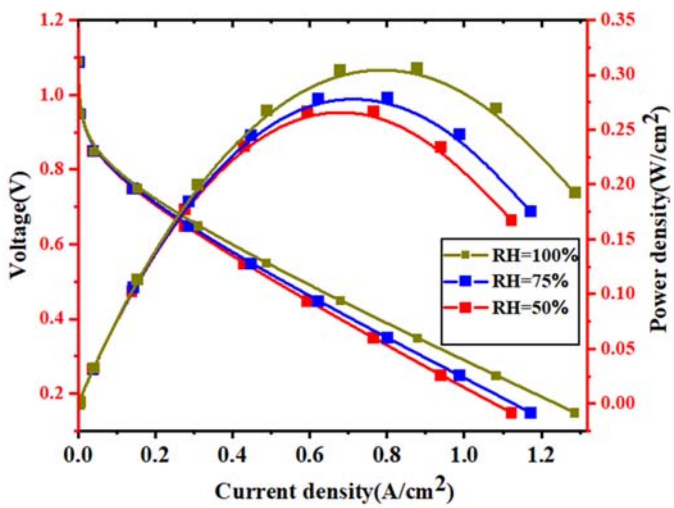

Figure. 4. Effect of relative humidity on polarization and power density curves in a contre-flow PEMFC.

Figure 4 displays the polarization and power density curves acquired at three relative humidity levels in a counter-flow configuration. The findings demonstrate that the ideal relative humidity for fuel cell efficacy is 100%. The minimum voltages and power densities were observed at the lowest measured relative humidity of 50%.The contre-flow arrangement contributes to improved water management within the PEMFC, particularly at higher relative humidity levels, by promoting more uniform distribution of reactants and enhancing the removal of excess water. As a result, the performance of the PEMFC at medium and high current densities is significantly influenced by both the relative humidity and the flow arrangement. In the investigated PEMFC, voltage and power density exhibit a direct dependence on relative humidity. The improved performance at higher humidity levels is attributed to enhanced proton conductivity and more efficient diffusion of reactants and products, which are further supported by the favorable water transport characteristics of the contre-flow arrangement, optimizing the electrochemical processes within the cell.

3.3. Concentration distributions hydrogen, oxygen, and water in PEMFC under co-flow and contre-flow arrangements

Figures 5, 6, and 7 show the distributions of hydrogen, oxygen, and water concentrations within the PEMFC under co-flow and counter-flow arrangements,

respectively, at a relative humidity of 100%.

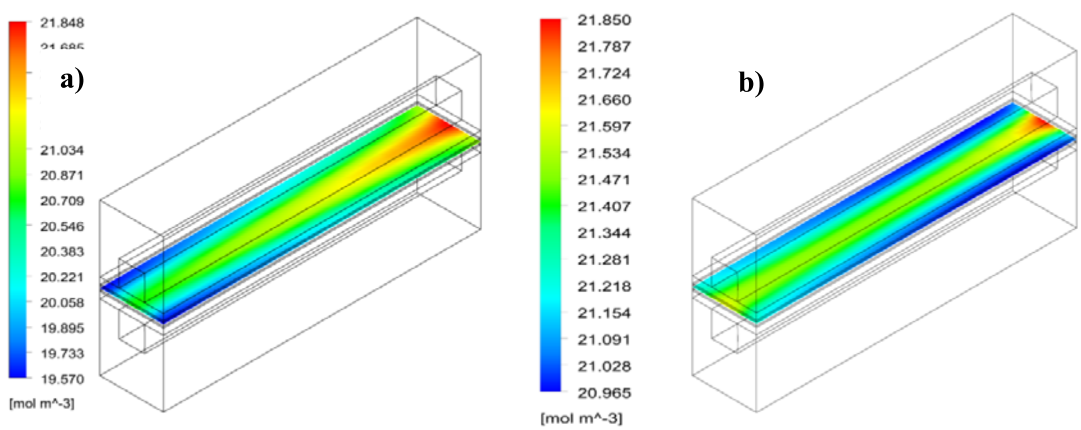

Figure 5. Distribution of hydrogen concentration in PEMFC:

a) co-flow arrangement, b) contre-flow arrangement.

Figure 5 illustrates that the hydrogen concentration diminishes along the flow arrangement in both configurations as a result of consumption through the electrochemical reaction. The co-flow arrangement exhibits a more significant reduction towards the outlet. In contrast, the counter-flow configuration, with its opposing flow directions of the anode and cathode gases, leads to a more uniform distribution of hydrogen throughout the channel length, thereby improving fuel availability in the reaction zone.

Fig. 6. depicts the oxygen concentration profiles within the PEMFC. In the co-flow configuration, oxygen depletion occurs progressively along the channel, resulting in reduced concentrations near the outlet region. The counter-flow arrangement enhances oxygen distribution within the cell, sustaining elevated concentrations in areas where electrochemical reactions remain active, thereby improving cell performance and minimizing concentration losses.

Fig. 7. shows the distributions of water concentrations, which illustrate that the two systems manage water quite differently. Local flooding is more likely in a co-flow arrangement, which can reduce gas movement and cell efficiency since water collects close to the exit. The counter-flow configuration, on the other hand, helps to hydrate the membrane better and remove water more efficiently by spreading it out more evenly across the channel.

The PEMFC's operational stability and longevity are enhanced by this balanced water management, especially in environments with high humidity.

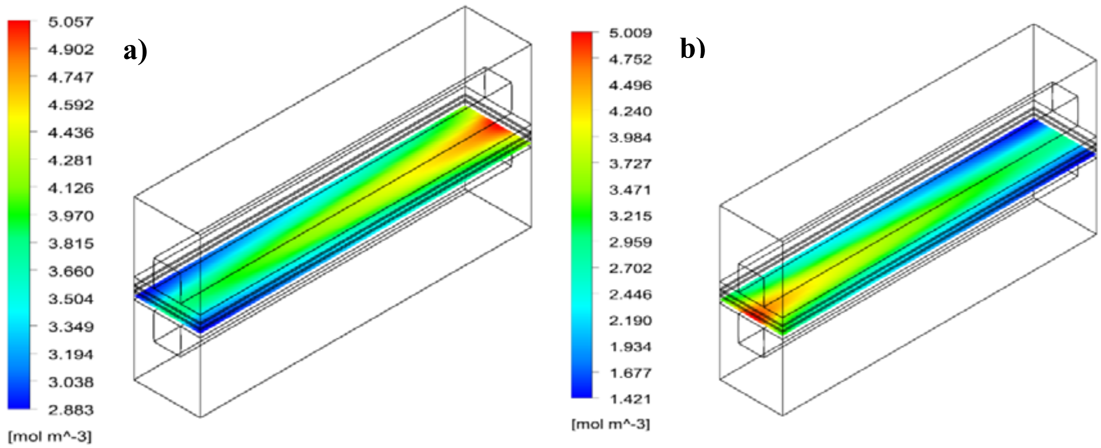

Figure 6. Distribution of oxygen concentration in PEMFC:
a) co-flow arrangement, b) contre-flow arrangement.

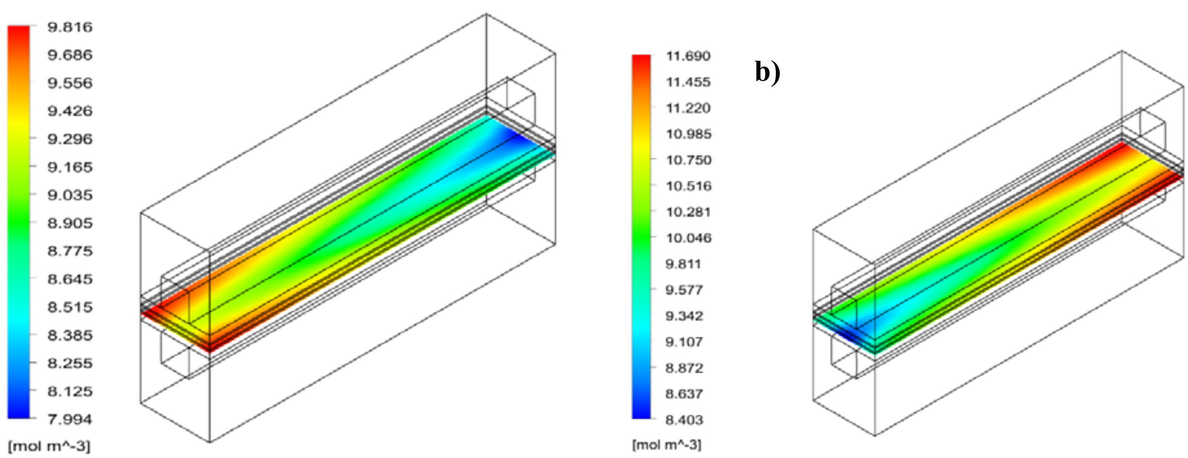

Figure 7. Distribution of water concentration in PEMFC:
a) co-flow arrangement, b) contre-flow arrangement.

These results indicate that the counter-flow arrangement provides enhanced performance for reactant distribution and water management relative to the co-flow configuration, rendering it a more advantageous choice for high-humidity fuel cell operations.

4. **Conclusions**

This study presents a validated 3D CFD model aimed at examining the effects of relative humidity and flow configuration on the performance of PEMFC. The findings indicated that contre-flow arrangements exhibited a marked superiority over co-flow setups, delivering a more uniform distribution of hydrogen and oxygen. Optimal performance was attained at 100% relative humidity, attributed to increased membrane hydration and enhanced proton conductivity. The contre-flow arrangement enhanced water management, mitigating flooding and bolstering operational stability. The improvements resulted in more efficient fuel use and increased power density. The results clearly demonstrate the advantages of contre-flow arrangement in high-humidity PEMFC environments.

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