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Exergetic Simulation and Performance Analysis of the Effect of Flow Patterns in PEMFCs

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Abstract

In this study, 6 different novel flow channels of the "proton exchange membrane" (PEM) type fuel cells were designed and modeled, while evaluations were conducted on three-dimensional channels of various designs using COMSOL Multiphysics simulation software. Proposed fuel cell designs and flow channel geometries were compared to existing exergetically-efficient fuel cell designs in terms of total exergy efficiency in a 3D manner as a novel tool for fuel cell investigations. Exergy efficiency analyses were conducted on the membrane surfaces of the proposed designs in addition to the anode and cathode side exergy analyses, and exergetic efficiencies of the alternatives. It is found that Design 6 is the best flow channel design with relatively high values and homogeny in exergy efficiency. The multi-inlet/outlet style while sustaining the reaction long enough for the reactant depletion leads to high-efficiency levels as seen from the results with average efficiency of 24%.

Keywords: *Fuel cell; pem; comsol multiphysics; modeling and simulation; flow plates; exergy.*

1. Introduction

Fuel cells have both portable and embedded applications and are becoming increasingly significant alternative energy production systems. In parallel with the developments in nano-technology, PEM fuel cells have drawn the attention of researchers throughout the world with a growing momentum, mostly due to their ability to use various fuels like hydrogen, methanol and formic acid. As evidenced by scientific and industrial efforts focused on them, the number of fuel cells and related applications are increasing, perhaps affected by aforementioned advances in nanotechnology.

Inspection of the literature reveals a substantial amount of research on fuel cell systems. These studies mostly focus on catalyst and membrane improvements, performance analyses for various cell systems, exergy-energy analyses, and storage of the hydrogen fuel.

Henriques et al. [1] has used COMSOL software to observe potential improvements in a mobile PEM fuel cell by altering cathode channel geometry. Another study inspected and compared thee different geometric collector designs in a Proton Exchange Membrane fuel cell (PEMFC) while keeping fluid dynamics in mind. The geometries inspected were serpentine, parallel and square layouts [2]. Hamilton and Pollet designed flow channels for a fuel cell in a planar space by transforming 3D mathematical space into a 2D model, running simulations in this environment [3]. Ly et al. [4] developed a mathematical model that was used to gather detailed results for a mechanical fuel cell's parallel flow channels. In the study of Mehta and Cooper [5], two versions of a flow channel plate for PEM fuel cell was inspected under high voltage and current in terms of reactants' spread over catalyst surface. Another study has inspected three variations of a flow plate (straight, serpentine and mixed) and simulated spread properties, discussing the results [6], [7].

Falcao et al. [8] studied the 1D and 3D numerical simulations in PEM Fuel cells using simple serpentine flow field seeking optimum conditions for operating the fuel cell. It is seen that 3D results have great importance for fuel cell studied before managing the laboratory experiments. There are also various studies [9]–[11]about the modelling, simulation and validation of the fuel cells as each seeks to understand the complex behavior of the fuel cell behavior.

More recent studies about the effect of bipolar plate and flow field design of the fuel cells on performance is also investigated numerically [12] the effect of temperature, pressure and humidity is taken into account for calculation of material consumption and power generation and stack efficiency. Besides in another study [13] common existing designs of flow plates of fuel cells and suggests modifications to some of them to help reduce the pressure drop in the flow channels are investgated. It is seen that modifications of fuel cell designs in existence using a system similar to the diesel injection system design approach reduced the pressure drop in the fuel cell as shown by the simulation results.

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Differing from the literature and previous studies, this study inspects six types of novel flow channel designs by modeling and simulating them with COMSOL Multiphysics software, and compares them in terms of exergy and performance analyses. Implementation of the exergy analysis to the CFD environment and applying these to a 3D fuel cell design is the main contribution of this study with the main objective of emphasizing the effect of flow patterns in PEMFCs and to propose a design that is efficient in fuel cell operation.

2. Fuel Cell

A fuel cell is a system that generates electrical energy as a result of an electrochemical reaction between an oxidant and a suitable fuel. After the fuel cell reaction -which can be described as the reverse of electrolysis reaction- electricity is produced in the form of direct current (DC). Basically, a fuel cell is composed of the electrolyte, and electrodes which are in contact with a surface of the electrolyte each; the anode on one side and the cathode on the other.

2.1 PEM (Proton Exchange Membrane) Fuel Cell

The cost of energy keeps increasing, perhaps tied to the ever increasing energy demand. The standards set by civil requirements in developed countries also affect the trends in developing countries, which lead the world towards new, innovative and green energy sources. In terms of thermal cycles, fuel cell systems are capable of producing electrical energy from the chemical energy stored within the fuel with efficiencies of up to 80%. Due to the nature of PEM fuel cells, the only waste produced is usable water and heat, which makes PEM's quite compatible with nature.

2.2 Fuel Cell Performance

Fuel cell performance is generally seen as the sum of performances of the cell's components. These performances are tightly coupled to the reaction's occurrence on the catalyst, generation of current by a collection of electrons, transfer of hydrogen ions through the membrane, water production as a result of the combustion reaction, and finally, electrical resistances of intracellular components.

This is a complex process composed of many chemical thermodynamic processes. As is the case in many thermal systems, operating conditions have strong influences on these processes. The main operating conditions, which affect fuel cell performance that are temperature, pressure, membrane thickness, humidity and current density.

A uniform reaction with constant speed along the catalyst surface depends on the optimal distribution of temperature, humidity, and concentration. Such a distribution can only be achieved by an optimum distribution of content over the flow plates. As a frontier study in this respect, simulation and modeling of alternative flow plate geometries were inspected with an exergetic perspective, in search for the most effective distribution pattern. As a result, a homogeneous distribution of the performance-affecting criteria of the fuel cell -like the temperature, concentration, and humidity- has been achieved over the cell surface and the results were examined and interpreted.

3. Material and Method

3.1 Simulation with COMSOL Multiphysics

As the first stage of the study, the proposed fuel cells and their flow channels were designed using COMSOL Multiphysics program. This software has an integrated multi-physics infrastructure for various engineering endeavors. It includes various equipment in the simulation environment already modeled [14]. The software also gives quick results as the physical interfaces of many theoretical processes are pre-modeled within it. It has a wide coverage of applications from to the fluid flow problems to the transport of heat, and from structural mechanics to electromagnetic analyses [7], [15]

All the proposed designs in this study were based on this model [16] designed of a single rod. The anode and cathode flow channels, gas diffusion layers (GDL's), the membrane and the porous electrodes are the primary constituents of a fuel cell model.

A total of six alternate fuel cell designs were analyzed exergetically in these simulations, and the results were discussed. The modeling of the fuel cell includes modeling of electrochemical currents, mass transfer, and momentum transfer.

The electrochemical current modeling is done by using reacting flow in porous media and current distribution interfaces in COMSOL. The models based on Ohms law and solving for these considering the cell GDLs, and in the porous electrodes, and in the electrolyte membrane. These are dependent on the concentration of the species and ionic and electronic potentials.

The current density of the anode of the fuel cell is calculated depending on the following formula locally that is basically based on Butler-Volmer expression

$$H_2 \rightarrow 2H^+ + 2e^- \tag{1}$$

$$i_a = i_{0,a}\left(\frac{c_{H_2}}{c_{H_{2,ref}}}\right)^{0.5}\left(\frac{\alpha_{a,a}+\alpha_{c,a}}{RT}\right)F\eta_a \tag{2}$$

where i is current density (A/cm^2); i_0 is exchanged current density at anode (A/cm^2); R is the universal gas constant (J/kmol-K); n is the number of electrons involved; F is the Faraday's constant (C/mole); α_A and α_C are the empirically determined electron transfer coefficient of the reaction at the electrodes at the anode and cathode, c_{H2} is the local hydrogen concentration and $c_{H2,ref}$ a hydrogen reference concentration

Cathode reaction is as follows in a PEM fuel cell

$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \tag{3}$$

for the oxygen reduction reaction, the following current density equation is used that is a version of Tafel-equation which is derived to implement the effect of concentration.

$$i_c = -i_{0,a}\left(\frac{c_{O_2}}{c_{O_{2,ref}}}\right)\exp\left(-\frac{\alpha_{c,c}}{RT}\right)Fn_c \tag{4}$$

where i is current density (A/cm^2); i_0 is exchanged current density at the anode (A/cm^2); c_{O_2} and $c_{O_{2,ref}}$ are the Oxygen concentration local and reference, respectively, R is the universal gas constant (J/kmol-K); n is the number electrons involved; F is the Faraday's constant (C/mole); α_C is the empirically determined electron transfer coefficient of the reaction at the cathode, respectively.

Comsol Multiphysics software has interfaces dedicated to the solution of mass transfer phenomena, called "Transport of Concentrated Species". These interfaces use the Maxwell-Stefan equations which are used in calculations of GDL, and flow channels and electrodes alike. These equations are mathematical representations of the diffusion phenomena, and the diffusion flow of the species depends on all (n-1) independent affective factors in a mixture of n species, where no net mole transfer takes place. The Maxwell-Stefan equations help simulate multi-component mass transfers by defining them as a whole. The data for species' mass fractions are set at inlet points, while the rest of the concentration data are dynamically calculated by the program [17].

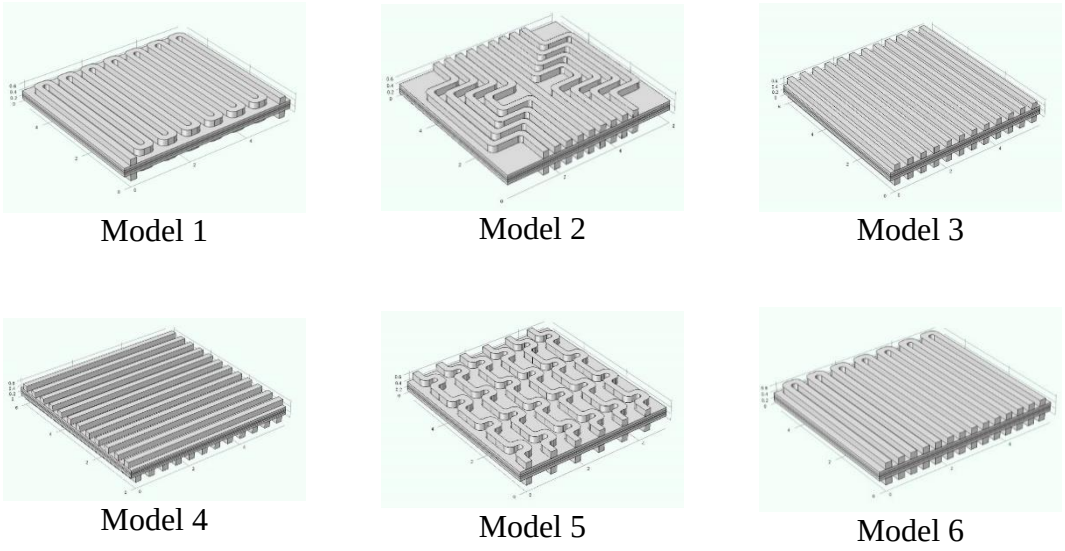

Figure 1 3D Geometry of proposed geometries

On the other hand, Brinkman equations are used for electrodes and porous GDL's, while the Navier-Stokes equations are employed in momentum transfer calculations, and to determine the relationship between the temperature, pressure, velocity, density, and viscosity of the flow [18]. The Brinkman equations describe fast flows in porous media with kinetic potential related to fluid velocity, pressure, and gravitational potential.

These equations are used for the solution of the CFD model of PEMFC with specific flow field design. As the exergy analysis and the efficiency is a result of the chemical, electrochemical, and physical results of the ongoing phenomena's through the fuel cell, the solution of this complex model is very crucial for sake of the analysis.

Some general assumptions are made regarding the cell geometry;

- Boundaries at the anode side are assumed as to have zero electronic potential,
- The boundaries at the cathode side are assumed to be at the cell potential.
- Remaining boundaries are assumed as electrically isolated and have zero flux for mass transfer

The model is verified with the previous PEMFC studies [19]–[21] using same configurations and data. It is seen that overall potential and exergy efficiency lies within a 5% of difference with the previous studies that depends on the experimental results.

4. Proposed Flow Channel Geometries for PEMFC

Figure 1 displays geometrical views of six proposed fuel cell designs in 3D. The geometries are developed regarding the currently used geometries and the geometries that are thought to be good candidates of having a high and homogeneous distributed fuel cell exergetic efficiency.

The 3D Mesh (Meshwork) for the geometries are developed using physics oriented mesh algorithm of the COMSOL with fine meshes in order to have better results structure. Figure 2 displays the meshwork for the Model 6 geometric design.

Figure 2 3D Mesh view of the 7 Inlet-Outlet Fuel Cell Design

The solution based on this meshwork took approximately 8 to 12 hours for each model with the RenderBox Pro workstation (Dual Intel Xeon Processor E5-2620, 32 GB DDR4-1333MHz). Corner refinement and additional boundary layers are used as complementary tools for solving the model with 1.510.434 Tetrahedral , 53.919 pyramid, 474.059 prism, 296.911 triangular elements smallest element size is 0,0034 cm while mean element size is 0,63 cm.

4.1 Exergy Analysis

Compared to thermodynamics' first law which focuses on the quantity of the energy in a system, exergy analyses utilize the second law to also inspect the energy's quality [22], [23]. This makes it a very good tool to compare energy systems with similar sizes in terms of actual work they can produce.

Since the quality of the energy is also evaluated along with quantity, exergy analysis is useful in figuring out the real work-related value of a given system, which in turn helps to locate the sources of inefficiencies, energy losses, and thermo-dynamic inadequacies within it.

Considering all these, exergy analysis becomes an unavoidable method if accurate and consistent evaluations and calculations are strived for in determining a system's true potential [24], [25].

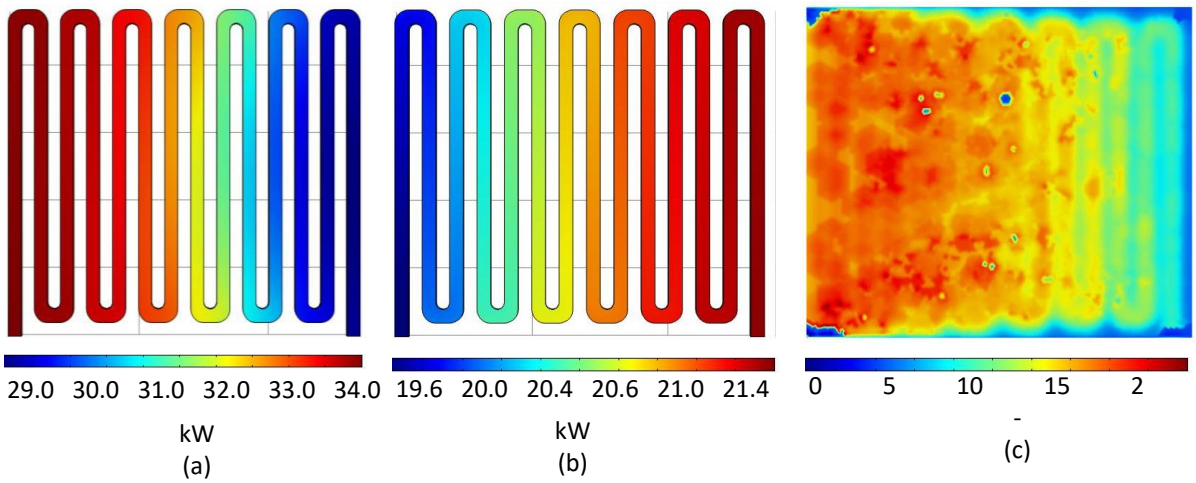

Figure 3 Hydrogen (a) , Oxygen Exergies (b) [kW] and Exergy Efficiency (c) [-] for Design 1

Fuel cell voltage and power, and the current feed will also be added to the aforementioned equations in order to analyze the exergy within the system of the fuel cell, with the equation given below. This equation is implemented in the COMSOL software and solved for each node in the mesh of the fuel cell flow-field design. The necessary properties and data are gathered directly by the COMSOL itself regarding the solution of the momentum, mass and energy balances.

$$I_{FC} = \sum \dot{E}x_{mass,i} - \dot{E}x_{mass,o} - \dot{E}_{xheat} - \dot{E}x_{work} \quad (5)$$

where I refers Exergy Destruction (Irreversibilities), mass denotes the exergy transferred through flowing mass inlet (i) and outlet (o), heat and work used for the flowing heat and work from the system boundaries [26].

System efficiency is calculated based on the energy and exergy analyzes and is achieved with the below equations:

$$\eta_{sys,en} = \frac{\dot{W}_{net}}{HHV_{H_2} \cdot F_{H_2,in}} \quad (6)$$

$$\eta_{sys,ex} = \frac{\dot{W}_{net}}{\dot{E}x_{in}} \quad (7)$$

The derived exergy equations are implemented in the COMSOL and the 3D flow of the exergy and exergy efficiency in the fuel cell is simulated. As the necessary equations are implemented to the COMSOL program regarding the method, these calculations are repeated and converged in each physical point in the system, and the results are then interpreted.

5. Exergy Analysis Results on Proposed Fuel Cell Designs and Discussion

The results of the analyses on the 6 proposed flow plate designs in this study will be given below. Hydrogen and Oxygen exergies will be indicated on the x-y axes, while exergy efficiency values based on current density will be indicated with graphs.

Active membrane surface area was kept the same between all the proposed designs, and channels were designed with the same total area and dispersed on the plate surface as homogeneously as possible. Voltages were also kept fixed (0.5V – 0.7V)

In order to have consistently accurate comparisons between alternative geometries, channel width and height was fixed, resulting in the same amount of pressure loss per unit distance traveled in all models.

5.1 Exergy Analysis Results for Design 1

In this classic one inlet-one outlet flow channel model, the x-y axis for the hydrogen within the fuel cell anode side is given in Figure 3-a. It is evident that towards the +x direction, hydrogen exergy dissipates rather steadily, due to consistent reduction of hydrogen over the channel as it travels on the anode side.

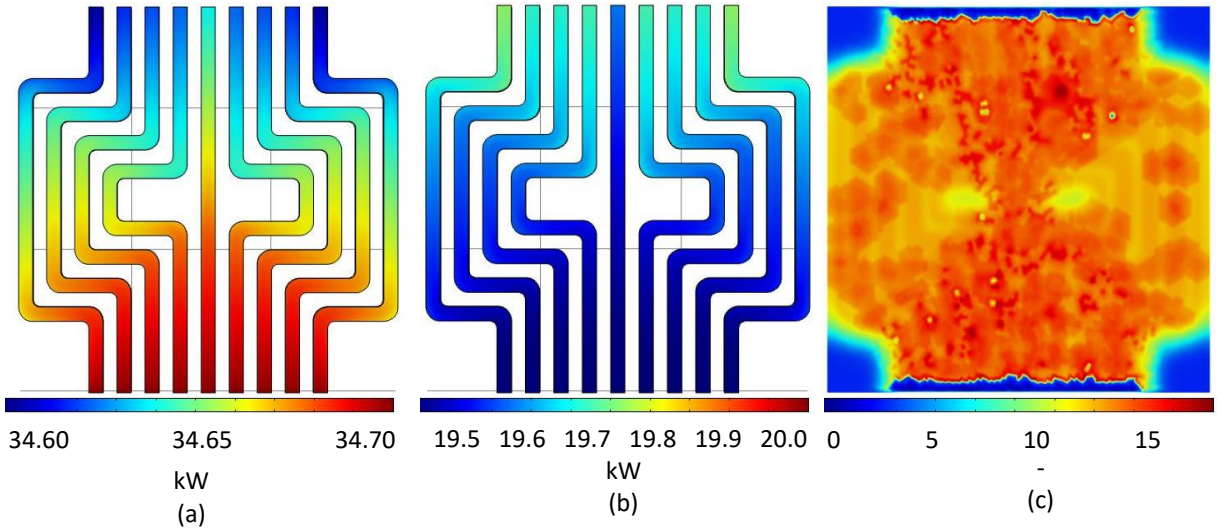

Figure 4 Hydrogen (a) , Oxygen Exergies (b) [kW] and Exergy Efficiency (c) [-] for Design 2

As can be seen in Figure 3-b, oxygen exergy in the cathode side drops steadily as it moves in the channel, similar to the hydrogen in the anode side given in Figure 3. As the amount of water produced in the cathode side, the effect of oxygen increases.

Figure 3-c displays the exergy efficiency of the system. The position based exergy efficiencies are calculated using the data of the CFD system regarding the definition of the exergy efficiency. As evident in the figure, the efficiency is high in the entrance area of the plate where reaction speed and current density is high, while efficiency is comparatively low in the other areas. This is caused by the build-up in the entrance area, which also causes more strain on the membrane. High concentration levels at the inlet of the fuel cell lead to high reaction rates and efficiencies but as the concentration levels drop through the flow of the reaction

effluents the situation reverses and the homogeneity is lost. The aim of testing alternative flow patterns is to achieve the homogenous high-efficiency table in the whole surface.

5.2 Exergy Analysis Results for Design 2

The aim of this model is to improve the entrance conditions throughout the surface by introducing more than one inlet and sustaining the homogeneity. x-y axes for the hydrogen within the proposed fuel cell's anode side shown in Figure 5-a. Considering the sudden drop of hydrogen amount towards the middle in y direction, hydrogen exergy could be evaluated to be decreasing rapidly due to the reaction and various inefficiencies.

Oxygen exergy for this design can be seen in Figure 8. Oxygen exergy is relatively lower compared to hydrogen exergy given in Figure 5-b due to the water production. As it can be seen, the oxygen and hydrogen exergy values generally change in the opposite direction as expected due to the reaction stoichiometry.

Figure 4-c displays the total exergy efficiency derived from hydrogen and oxygen exergies, indicating the exergy efficiency of the system. As evident in the figure, there is a significant build-up towards the middle. Membrane activity is rather high up to this point, but drops suddenly henceforth, plummeting the efficiency. Furthermore, the unused space in the corners of the design adversely affects the overall efficiency. Therefore, it is safe to state that Design 2 has lower exergy efficiency compared to Design 1.

5.3 Exergy Analysis Results for Design 3

The hydrogen exergy x-y values for Design 3 are displayed in Figure 5-a, while the oxygen exergy values are given in Figure 6-b. As can be seen in these figures, gasses fed to the system have a homogeneous distribution on the surface. This is a good indication in terms of operating costs.

Total exergy efficiency for Design 3 is displayed in Figure 5-c. The fuel and the oxygen clearly disperse homogenously on the plate, creating a positive impact on the efficiency and thus decreasing the running costs for the system.

5.4 Exergy Analysis Results for Design 4

Hydrogen exergy values for Design 4 are displayed in Figure 6-a, while the oxygen exergy values are given in Figure 6-b. As can be seen in these figures, the performances are quite similar to that of Design 3. Total exergy efficiency for Design 4 fuel cell is given in Figure 6-c. When exergy efficiencies values over the active surface are evaluated, the homogenous distribution is clearly evident again, like in the Design 3, but the overall average exergy is only slightly higher than that of Design 3, due to the positive effect of the perpendicular flow of the reaction effluents. This indicates that the change in geometric direction of the hydrogen flow did not have a considerable effect on the efficiency.

5.5 Exergy Analysis Results for Design 5

The hydrogen exergy values for Design 5 are displayed in Figure 7-a, while the oxygen exergy values are given in Figure 7-b. As evident in these figures, there is a fall in concentration for both the hydrogen on the cathode side and oxygen on anode side in towards the middle regions. This situation affects exergy efficiency of the design adversely.

The total exergy efficiency for this design is displayed in Figure 7-c. Due to having more unused space compared to other flow plate designs, Design 5 suffers a lowered exergy efficiency. This situation arises due to the wavy geometrical design of the plate. It causes a lower flow density with the unused space and lower homogeneity of the distribution.

5.6 Exergy Analysis Results for Design 6

A U-shaped multi-inlet/outlet design scheme is used in Design 6 with the experience gained from previous designs. The aim here is to sustain a sufficient retention time for the reactants in the fuel cell beside having a high-profile concentration through the surface. The hydrogen exergy values for Design 6 are displayed in Figure 8-a, while the oxygen exergy values are given in Figure 8-b. As seen, the gasses are dispersed along the whole channel quite smoothly.

Total exergy efficiency for the system proposed in Design 6 is displayed in Figure 9-c. The high efficiency is clearly visible, and it's due to the uniform distribution of both the air and the fuel over the membrane. Even though there seem to be some spots where the efficiency seems to have gone down slightly, overall efficiency is still higher than all the other designs. The local drops in the efficiency seem to be due to calculation errors or local concentration drops and could be investigated using smaller mesh size in proceeding studies.

6. Conclusion

In this study, six alternative versions of flow channel plate designs were proposed. All of them were modeled in COMSOL Multiphysics software and analyzed under simulation. Exergy changes on the hydrogen and the oxygen flows and total exergy efficiency were evaluated regarding the 3D results of these fuel cells.

It can be seen that the flow channel design has considerable effects on the performance of the fuel cell. The homogenous distribution of the reactant effluent and removal of the excess and exhaust materials directly affect the system performance based on the reaction rates. On the other hand, the thermal and water management is also affected directly by the design and retention times in the fuel cell. This is why another aim is to increase the retention time of the flow in the fuel cell for the sake of hydrogen depletion and to use the fuel effectively, as the unreacted hydrogen is also a loss from the exergy efficiency point of view. Following these tracks lead to an optimum design for flow patterns. As a result of this study, it is seen that the multiple inlet designs had somewhat of an advantage in distributing the fuel over the plate uniformly, enabling them to reach higher efficiency levels. Cross-channel designs have a positive effect in case of short channeled designs, while have negative effects in case of long channel designs.

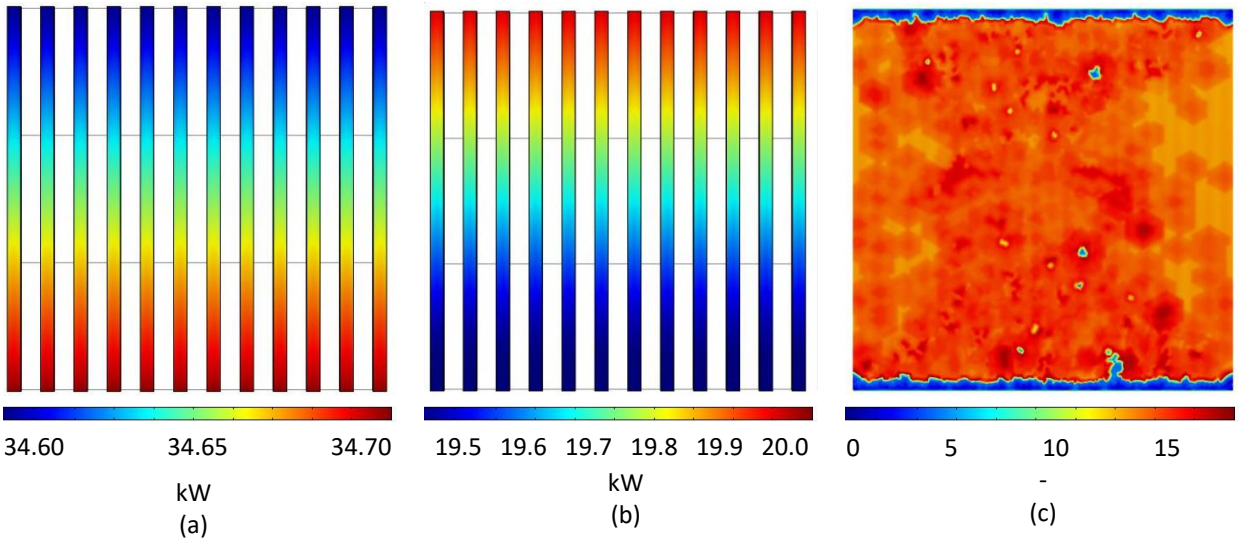

Figure 5 Hydrogen (a) , Oxygen Exergies (b) [kW] and Exergy Efficiency (c) [-] for Design 3

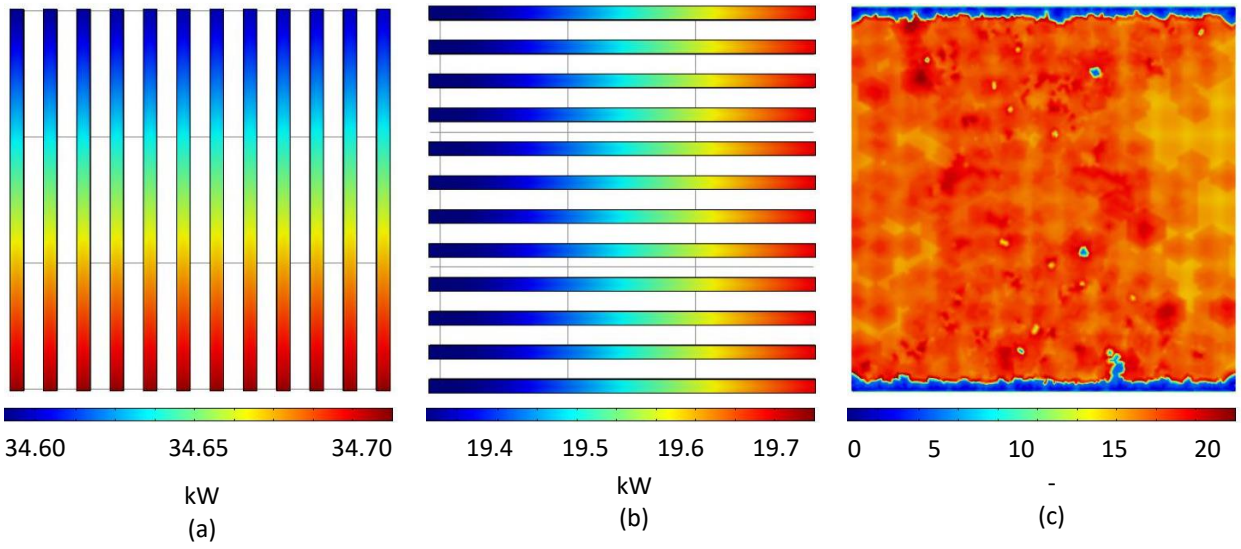

Figure 6 Hydrogen (a) , Oxygen Exergies (b) [kW] and Exergy Efficiency (c) [-] for Design 4

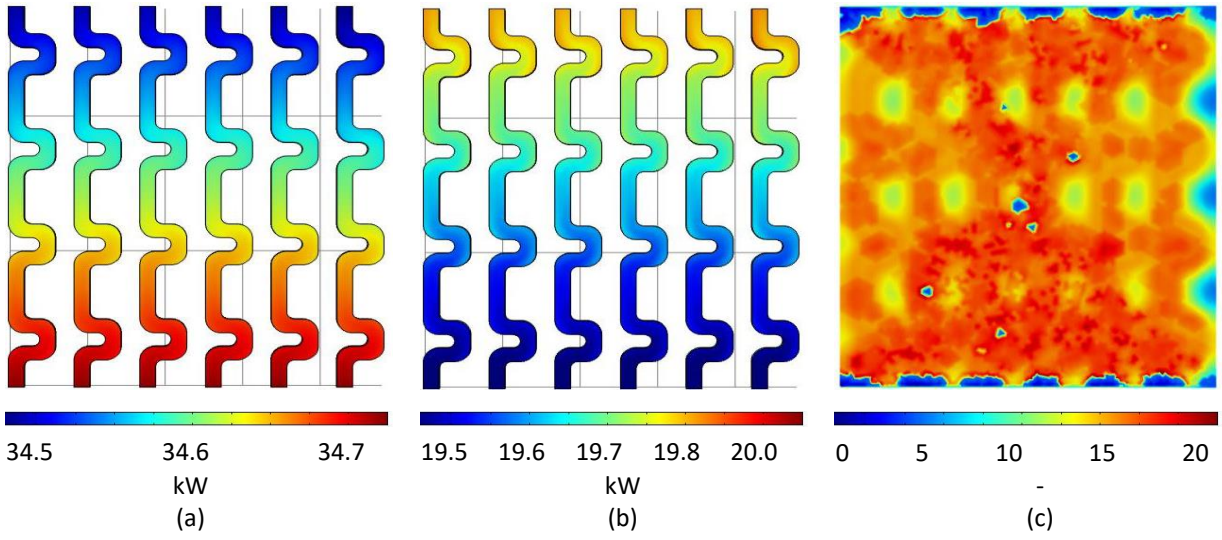

Figure 7 Hydrogen (a) , Oxygen Exergies (b) [kW] and Exergy Efficiency (c) [-] for Design 5

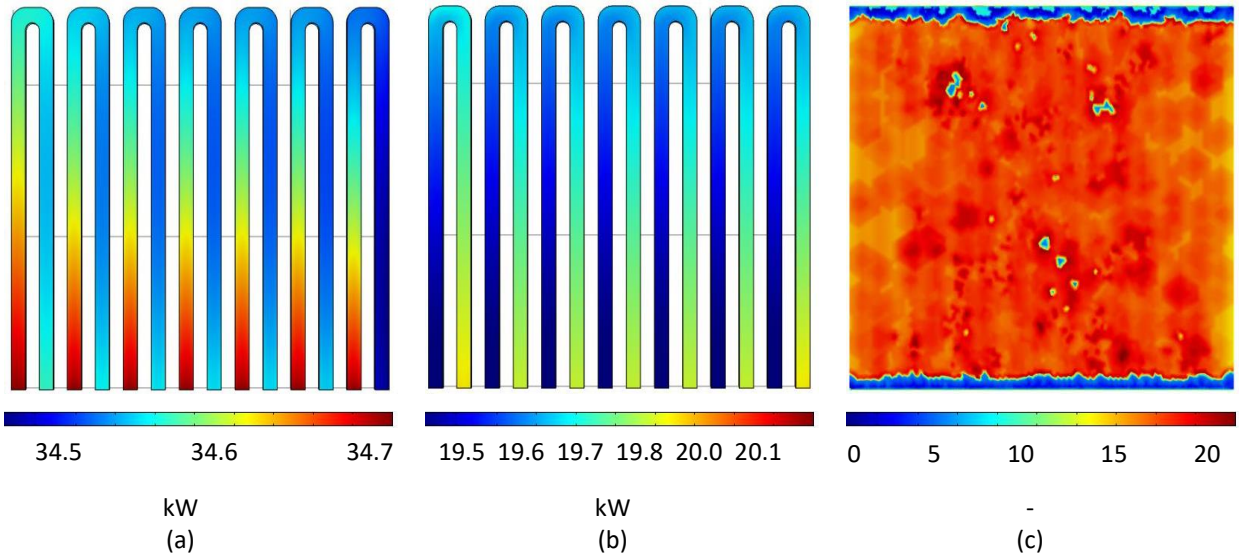

Figure 8 Hydrogen (a) , Oxygen Exergies (b) [kW] and Exergy Efficiency (c) [-] for Design 6

Design six is chosen to be the best flow channel design in the scope of this study due to relatively high values and homogeny in exergy efficiency. The multi-inlet/outlet style while sustaining the reaction long enough for the reactant depletion leads to high-efficiency levels as seen from the results.

When the fuel cell surface area is utilized homogenously, the fast and evenly distributed reaction of hydrogen and air inside the system along the plate. This prevents any over-worn spots that could cause physical damage to the plate. Modeling and simulating various flow plate designs reduce the otherwise expensive actual tests and reduce the time needed for the best results. They are henceforth valuable tools for researchers working on fuel cell design. In addition to this study, more comprehensive optimization studies may be implemented in the future regarding the numerical modeling of the system for the sake of reaching the optimum flow structure for fuel cells.

Acknowledgment

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