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Research Article

Optimization Oxygen and Hydrogen Input Velocities by Golden Section Method with 3D Multifluid Model in COMSOL for PEMFCs

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ABSTRACT

A three dimensional (3D), gas-liquid multi-phase flow and transport model in COMSOL Multiphysics has been developed to simulate flow and transport phenomena in a proton exchange membrane fuel cell (PEMFC) with several operational parameters. The effects of changes in oxygen and hydrogen input velocities on concentration change at electrodes, current density in polymeric membrane and cell performance have been investigated in PEMFC. The simulations, made in COMSOL for numerical method, were presented with an emphasis on the physical and fundamental insight afforded by distributions of velocity vector, local current density, overpotential, oxygen and water concentrations. Using Golden Section Method, optimization of the change in the speed vector was made based on the numerical models for velocity values. Results showed that computational and numerical methods are in great harmony. The polarization curve, which is used as a measure of efficiency in cell performance, were supportive with results. The data show that the power density obtained for the optimum model is higher, with such a model performance of 92.87%. Compared to the currently used PEMFC, while hydrogen saving achieved between 4.2% and 7.1%, electrical efficiency increase were between 1% and 2.4%.

Keywords: *Fuel cell, CFD analysis, water management, golden section method, Comsol Multiphysics, optimization*

PEMYH için COMSOL'da Üç Boyutlu Çoklu Akış Modeliyle Altın Oran Yöntemi ile Oksijen ve Hidrojen Giriş Hızlarının Optimizasyonu

ÖZ

Üç boyutlu (3D), gaz-sıvı çok fazlı bir akış ve taşıma modeli, birkaç farklı operasyonel parametre ile bir proton değişim membranlı yakıt hücresinde (PEMFC) akış ve taşıma olaylarını simüle etmek için COMSOL Multiphysics'te geliştirilmiştir. Oksijen ve hidrojen giriş hızlarındaki değişikliklerin elektrotlardaki konsantrasyon değişikliği, polimerik membrandaki akım yoğunluğu ve hücre performansı üzerindeki etkileri PEMFC'de incelenmiştir. Sayısal yöntem için COMSOL'da yapılan simülasyonlar, hız vektörü, yerel akım yoğunluğu, aşırı potansiyel, oksijen ve su konsantrasyonlarının dağılımlarının sağladığı fiziksel ve temel anlayışa vurgu yapılarak sunulmuştur. Altın Oran Yöntemi kullanılarak, hız vektöründeki değişimin optimizasyonu hız değerleri için sayısal modellere dayalı olarak yapılmıştır. Sonuçlar, hesaplamalı ve sayısal yöntemlerin büyük bir uyum içinde olduğunu göstermiştir. Hücre performansında verimliliğin bir ölçüsü olarak kullanılan polarizasyon eğrisi, sonuçları destekleyici niteliktedir. Veriler, optimum model için elde edilen güç yoğunluğunun % 92,87 gibi bir model

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başarımı ile daha yüksek olduğunu göstermektedir. Mevcut kullanılan PEMFC ile karşılaştırıldığında % 4,2 ile % 7,1 arasında hidrojen tasarrufu sağlanırken, elektrik verimliliği artışı %1 ile %2,4 arasında olmuştur.

Anahtar Kelimeler: *Yakıt hücresi, HAD analizi, su yönetimi, altın oran metodu, Comsol Multifizik, optimizasyon*

I. INTRODUCTION

There is a significant need to understand of internal processes (reactions, mass transport, heat transport) in a PEMFC [1]. Considering PEMFC durability, design and optimization, one of the key challenges and crucial aspect is water management [2, 3]. Therefore, water management, that is responsible to both water flooding at electrodes and remaining dry of the membrane, has been extensively investigated as experimentally and numerically to control the especially liquid water transport characteristics in PEMFC for the last years [4, 5]. Management of the high amount of water is quite crucial when performed at high current densities, excessive water passes through the membrane and as a result of water generation at the cathode causes in water flooding and thus increasing on concentration losses. Otherwise, quite little water is insufficient and causes dehydration of the membrane at anode side when operating at low current densities [6, 7]. The water management categorized into three subsections such as water management in a membrane, water management in gas diffusion layers, and water management in reactant flow channels. Different numerical models have preferred for lots of the two-phase flows' studies in the perspective of water management [8]. For the last decades, computational fluid dynamics (CFD) based models have been mostly preferred due to their success in providing specific solution of process components such as concentration, pressure distributions, temperature gradients, electrical potentials and current density in the each parts of the unit cell [9, 10]. Although the beginning applications of CFD for PEMFCs performed with two dimensional models [11, 12]. The improvement of more appropriate models, which is considering fluid, thermal and electrochemical transportation management, 3D geometries (consist of flow and cooling channels, and two-phase transportation), have improved due to existence of CFD and developed transport models in recent times. A physical model approach formulated and numerically given a place into multi-dimensional CFD framework to describe free liquid water transportation through the polymer membrane managed by liquid pressure difference [13]. A single-phase 3D PEMFC model developed and examined the impacts of liquid water flooding on cell performance parameters [14]. A two phase CFD Volume of Fluid (CFD) method utilized for simulating water droplet movement and slug formation in PEMFC mini channels. They concluded that too much water in mini channels resourced from the collision and coalescence of droplets could easily cause slugs in PEMFCs [15]. For liquid water management, a basic 3D unsteady model designed and concentrated with detailed thermo-electrochemistry, multispecies and two-phase effects with the interface tracking by using the method was applied on the CFD software package fluent. The impacts of liquid water on fuel cell with serpentine channels were examined [16].

In this study, by providing water management with simulation and modeling processes, it was planned to avoid flooding in order to prevent the corrosion caused by water on the membrane surface and obtain the extension of the cell life. It was also aimed to use a little amount of oxygen and hydrogen. According to these targets, 3D, multi-phase flow and transport model has been developed to investigate oxygen and hydrogen velocities on concentration (hydrogen at anode, oxygen at cathode, water at anode and cathode) and the cell performance investigated under various operating conditions considering water management. In here, an investigation from the perspective of stoichiometry and flow transfer were made. Operations were performed for cell and mass, energy and momentum balances were applied. In this study, PEMFC has been simulated with COMSOL programme and CFD has been examined. Previously, the effects of concepts such as stoichiometry and flow transfer on cell performance were investigated. While most of them examine the flow rate only at the anode or cathode only, few of these researches have studied and compared the performance effects for both electrodes. In studies conducted, it was observed that the effects on relative humidity, diffusion, temperature, pressure or performance of cell geometry on the electrodes are reflected in the results. The performance of PEMFC evaluated (anode and cathode) at a stoichiometric flow rate in their study about two dimensional PEMFC. When they increase the flow rate to a higher amount, the increase in the current density has slightly changed, and after a while, the effect of the increase in the flow rate on the current density has become almost negligible [17]. The flow occurring along the flow channels were examined in their study. According to their findings, oxygen use and cell tension increased, and the current density on the stalk structure decreased. As a result, it was observed that the cell warms up and the losses increase. This study shows that the losses in the cell change in direct proportion to the current density [18]. The effects of excess air volume investigated on the cathode and current density along the channel for a two-dimensional PEMFC in their study [19]. Water management on a two dimensional and multi flow PEMFC was examined. They concluded that partial water floods occurring inside the cell decreased efficiency and had a negative impact on concentration and stable work. It was determined that the change in concentration caused a decrease in current density and blockages on GDL. They observed that downstream causes more flooding in PEMFCs, and this negative effect is higher in PEMFCs operating at high current densities. This article emphasizes that, like us, "water distribution, mass distribution and temperature control" must be analyzed together. We tried to offer solution by using velocity change as the base to perform this process in our study [20]. An experimental and numerical model developed to control water management in PEMFC. They repeated the flow on their parallel-serpentine with various variables. In their studies, they reported that liquid water floods had a negative effect on the cell and that these effects occurred in a similar way in the parallel-serpentine [21]. This article advocates the following view, similar to our study: “If the water is excessive, water control becomes difficult, if the water is low, the temperature control becomes difficult”. An intermediate cell operation condition should be provided for the control of these parameters. This is only possible with an optimization in the current conditions. Our study is about the study of the flow in PEMFC shows great compatibility with the mentioned publications above. Conversely, different from all the articles, an optimization study was carried out to obtain the maximum power value for hydrogen and oxygen input velocities in this study. In addition, simulations using COMSOL were confirmed by the Golden Section Method [21]. The most important difference from the studies in the literature is the use of the Golden Section Method. Our study is about the study of the flow in PEMFC shows great compatibility with the current publications. Our study contributes to the literature by investigating the stoichiometry and flow transfer on cell performance and confirming the simulations by Golden Section Method. As mentioned below, despite there are limited researches which studied and compared the performance effects for both electrodes, there are many studies on examining the flow rate only at the anode or cathode only. This article investigated the changes on performances of both electrodes.

II. MODEL DESCRIPTION

A. MODEL FEATURES AND ASSUMPTIONS

The 3D computational domain and mesh of PEMFC for this article were presented in Figure 1, which comprised of channels, gas diffusion layers for cathode and anode (GDLs), cathode and anode parts, anode catalyst layer (ACL), cathode catalyst layer (CCL) and membrane. The structural properties as well as material characteristics were given in Table 1. The mathematical model has been created based on the assumptions as written below, without having lose any significant effect in the cell performance:

1. Isothermal condition- any temperature variation was not considered in the simulations. The anode, cathode and membrane are the same temperature (62 °C).
2. The voltage between the two electrodes is 0.4 Volt.
3. The GDL is modeled as homogenous porous media without taking into consideration detailed pore structure. Therefore, liquid water passages from the porous areas in the GDL layer were omitted.
4. Nafion was used as polymer membrane and platinum was utilized as catalyst. Nafion® membrane was only permeable to proton and dissolved water.

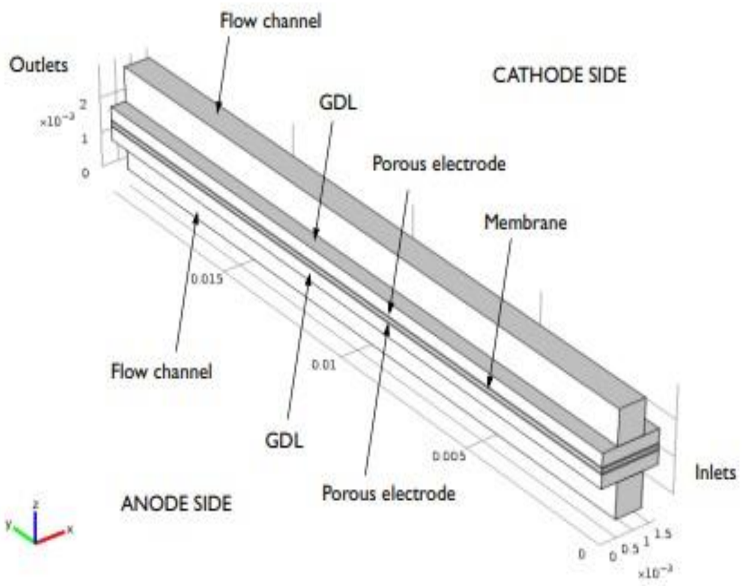

Figure 1. *Computational domain and mesh of the studied PEMFC [22].*

5. Liquid water could exist in both the electrodes, containing catalyst layers, GDLs and channels. This study examined the hydrogen and oxygen input velocities effects on PEMFC in the perspective of stoichiometry. PEMFC, which worked at optimum conditions, was formed at the end of the performed analysis. The algorithm belongs to obtained model is given in Figure 2.

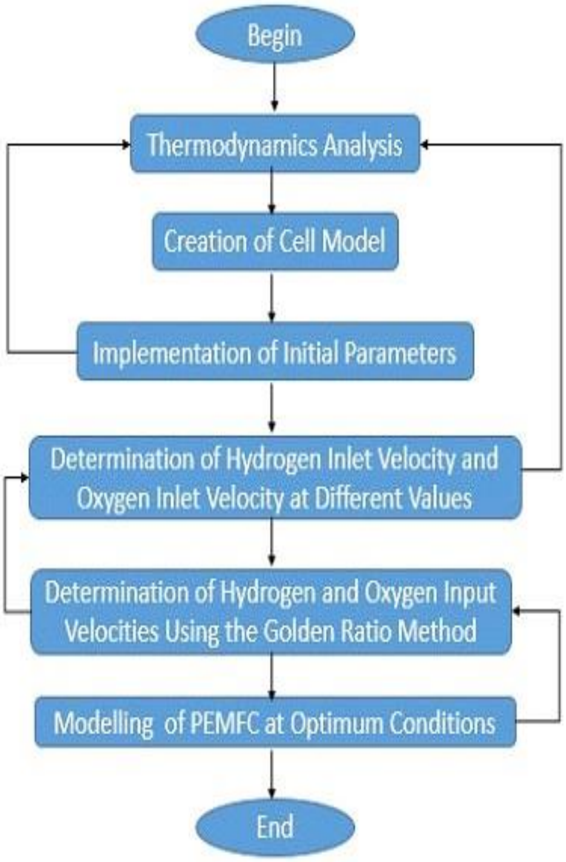

Figure 2. *Flow diagram of the solution algorithm.*

Table 1. *Structural parameters and material properties of the PEMFCs.*

References	Parameters	Symbol	Unit	Value
[23, 24]	Channel height	H_{ch}	m	0.001
[23, 24]	Channel width	W_{ch}	m	$0.7874e^{-3}$
[23, 24]	Cell length	L	m	0.02
[23, 24]	Rib width	W_{rib}	m	$0.90932e^{-3}$
[23, 24]	GDL width	W_{GDL}	m	$380e^{-6}$
[25, 26]	Porous electrode thickness	t_{elec}	m	$50e^{-6}$
[25, 26]	Membrane thickness	t_{memb}	m	$100e^{-6}$
[24]	GDL porosity	ε_{GDL}	-	0.4
[24]	GDL permeability	kp_{GDL}	m^2	$1.18e^{-11}$
[24, 27]	GDL electric conductivity	S_{GDL}	$S.m^{-1}$	222
[26, 27]	Inlet H_2 mass fraction	$w_{H_2\ in}$	-	0.743
[26, 27]	Inlet H_2O mass fraction	$w_{H_2O\ in}$	-	0.023
[26, 27]	Inlet O_2 mass fraction	$w_{O_2\ in}$	-	0.0228
[13, 24]	Anode inlet flow velocity	$U_{in-anode}$	$m.s^{-1}$	0.2
[13, 26]	Cathode inlet flow velocity	$U_{in-cathode}$	$m.s^{-1}$	0.5
[24, 27]	Anode viscosity	μ_{anode}	Pa.s	$1.19e^{-5}$
[24, 27]	Cathode viscosity	$\mu_{cathode}$	Pa.s	$2.46e^{-5}$
[28, 29]	Hydrogen molar mass	m_{H_2}	$kg.mol^{-1}$	0.002
[28, 29]	Water molar mass	m_{H_2O}	$kg.mol^{-1}$	0.018
[28, 29]	Oxygen molar mass	m_{O_2}	$kg.mol^{-1}$	0.032
[27, 28]	H_2 - H_2O Binary diffusion coefficient	$D_{H_2-H_2O}$	$m^2.s^{-1}$	$1.0662e^{-4}$
[27, 28]	O_2 - H_2O Binary diffusion coefficient	$D_{O_2-H_2O}$	$m^2.s^{-1}$	$3.2674e^{-5}$
[23, 24]	Cell temperature	T	K	335.15
[23, 24]	Reference pressure	P_{ref}	Pa	101325
[26, 29]	Cell voltage	V_{cell}	V	0.4
[29]	Oxygen Reference Concentration	$C_{O_2\ ref}$	$mol.m^{-3}$	40.88
[29]	Hydrogen Reference Concentration	$C_{H_2\ ref}$	$mol.m^{-3}$	40.88
[27, 28]	Electrolyte phase volume fraction	$\in_l$	-	0.3
[27, 28]	Permeability (porous electrode)	κp_{cl}	m^2	$2.36e^{-12}$
[27, 28]	Membrane conductivity	σ_m	$S.m^{-1}$	9.825

B. MODELING METHOD AND PROCEDURE

In the simulation of PEMFC, different simulations such Modeling Method and Procedures Membrane Electrode Interface, CL and GDLs were performed for cell sections. Expressions such as:

- Regional mass concentrations for hydrogen, oxygen and water
- Tension intensity occurring locally
- Voltage occurs in anode-membrane and cathode-membrane interface.
- Current density on the membrane surface were analyzed according to parameter of velocity.

Polarization curve is formed by examining the responses of PEMFC for multi-phase flow systems by creating different geometries for three dimensions. Thermal management is also provided due to carrying out the water management. In this study, COMSOL programme was utilized in CFD analysis for PEMFC. For modelling PEMFC; chemical matter conduction module, electrochemistry module, fluids module, heat transfer modules, batteries and fuel cell modules were used among from 13 different modules of COMSOL designed for ease of analysis in different engineering fields. While simulation of PEMFC with COMSOL approach steps; system simplification, geometry, equation, boundary conditions, initial value, mesh creation, solution method were followed as simulation steps to be followed.

C. SECONDARY CURRENT DISTRIBUTION

Secondary current distribution was used to model current density and cell voltage that occur as a result of electrochemical reaction. If any current does not flow through the cell, the voltage is max capacity in here. When a load is connected onto the cell, the current begins to transfer and the cell voltage begins to drop. This changing situation between current and voltage gives the power characteristic polarization curve in the cell.

The electrodes developed for PEMFC are metallic conductors. For the essential equation in this case, utilizing OHM Law is sufficient. Conversely, the electrons released due to reactions occurred inside the cell make this law insufficient. For this reason, the equations formed considering the change in the cell are shown as below [29]. Current density changes in membrane (Nernst-Planck Equation);

$$\nabla \times -(\sigma_I \times \nabla_{\Phi I}) = Q_I \tag{1}$$

where Q_I is equilibrium potential in ionic region, σ_I ($S.m^{-1}$) shows the electrical conductivity in ionic media, ΦI (Volt) is ionic potential.

Faradic currents that occur reverse to normal of surface were neglected;

$$-n \times i_s = 0 \tag{2}$$

In this equation, -n points the direction of surface normal, i_s (Ampere) shows the current caused by electrodic potential.

$$\nabla \times i_I = Q_I + i_{v,total}, \quad i_I = (\sigma_{I,eff} \times \nabla_{\Phi I}) \tag{3}$$

where i_I is current sourced from ionic potential, Q_I points the equilibrium potential in ionic region, $\sigma_{I,eff}$ shows the electrical conductivity that is effectively used in ionic media, ΦI is ionic potential, $i_{v,total}$ ($A.m^{-2}$) is total current density in cell.

$$\nabla \times i_s = Q_s - i_{v,total}, \qquad i_s = -\sigma_s \times \nabla_{\Phi s} \tag{4}$$

In here, i_s is current based on electrodic potential, Q_s points the equilibrium potential in electrodic region, $i_{v,total}$ ($A.m^{-2}$) is total current density in cell, σ_s ($S.m^{-1}$) is electrical conductivity in electrodic media, Φs shows the electrodic potential.

$$i_{v,total} = \sum m \times i_{v,m} \tag{5}$$

where $i_{v,total}$ ($A.m^{-2}$) is total current density in cell and $\sum m \times i_{v,m}$ ($A.m^{-2}$) is the total current density amount on membrane. The sum of the change in current density at the anode electrode and the change in current density at the cathode electrode is equal to the total charge change between the two electrodes.

$$\eta = \Phi_s - \Phi_i - E_{eq} \tag{6}$$

In here, η is over potential (V), E_{eq} points the equilibrium potential (V).

The efficiency of the electrochemical reaction is limited to electrical conductivity and never occurs at 100% efficiency. This formula is among the important equivalents and was written because of the entropy change.

D. MASS TRANSPORTATION AT ELECTRODES

Mass transportation at electrodes is used in PEMFC where hydrogen is oxidized and forms water. The resulting water is generally present in different phases depending on the cell temperature and pressure Liquid-Gaseous water requires a advantageous analysis and the calculation of the moisture content. Diffusion, conduction and convection effects are observed thanks to physics. In this study, assuming that the mole fraction in the cell is not changed, it is separately applied for Anode GDL and Cathode GDL.

The effects of liquid and gaseous water in PEMFCs on polymer membranes and electrodes were observed. It was determined that the thickness of the electrode and the thickness of the polymer membrane substantially effected the cell efficiency of the study with the PEMFC. The most important factor in the fuel cell was found to be membrane humidity. Liquid water, which was formed inside the cell, caused pressure on the membrane surface, reduces and destroys the efficiency of polymer membrane.

Various studies have been carried out on a large number of components in order to achieve realistic results in simulation. Different types of boundary conditions have been indicated in simulations which is examining PEMFC operation. This is the section where the top and bottom points were determined for PEMFC. Upper limit value changed according to PEMFC efficiency.

In order to obtain results in PEMFC, the initial value must be entered into the programme. Initial value is the first value given in the boundary conditions to control COMSOL. Another step used in modeling is the mesh creation process. With the use of mesh, the fuel cell is divided into so different parts and the results of the main part are examined by combining separate results for the solution. Golden Section Method was used for the shapes and densities of these grids. In the modeling of the PEMFC, the simulation was solved for the structured and unstructured mesh. The structured mesh was preferred as appropriate mesh in here. The mesh of the polymer membrane was preferred in a finer manner, while a coarse mesh was preferred for the anode electrode. In general, a fuel cell has two electrodes (anode, cathode) and one electrolyte. In addition, advanced fuel cells consist of CL, GDL, bipolar plates and support layers. PEMFC was modeled using Finite Element Method and Finite Volume Method in this study. According to this method, a large number of mesh were formed in the cell and divided into small pieces. Structured mesh was used in 3D modeling of PEMFC. The mesh points for the mesh vary according to the structure and parts of the PEMFC. The mesh points formed in this case are more numerous on the surface of the polymer electrolyte membrane, although less frequently in the channel. The last part of the simulation is the solution method which shows how close we are to real systems. In order to make the simulation performed in COMSOL give parallel values to the experimental results, it should be compared with suitable mathematical methods and validation process should be performed. All acceptances were applied to cell after equations are introduced to programme. When all operations are true, the result could be waited. If there is a wrong in operations, solution could not substantiate and the reason of error is stated.

III. RESULTS AND DISCUSSION

The PEMFC was examined theoretically and required numerical model was performed. The model was evaluated using COMSOL and then modelling of a 3D, multiphase PEMFC as a simulation was basically performed. Three simulations: (I) changing only the hydrogen input velocity, (II) changing only the oxygen input rate, (III) simultaneous change of hydrogen and oxygen input velocities were run on the created model. As a result of the simulations performed; hydrogen concentration in anode, oxygen concentration in cathode, water concentration in anode, water concentration in cathode, current density on polymeric membrane were examined. Each simulation was repeated at different velocity values. A PEMFC operating under optimum conditions was obtained based on the performed simulations. For simulation, experimental parameters in the literature were considered. Changeable and unchanging expressions were determined on the parameters. Current Density–Polarization Curve was formed by evaluating simulation results for 0.4 V while it was studied at constant temperature and atmospheric pressure. General expressions as physical and geometrical parameters utilized in this study are shown in Table 1. In the initial parameters, the hydrogen inlet velocity was accepted as 0.2 $m.s^{-1}$ while the oxygen inlet velocity was accepted as 0.5 $m.s^{-1}$ Simulations were repetitively run for 62 °C temperature, 1 atm pressure and 0.4 V. The simulation results for the initial parameters are shown in Figure 3 and Figure 4a. For the initial parameters.

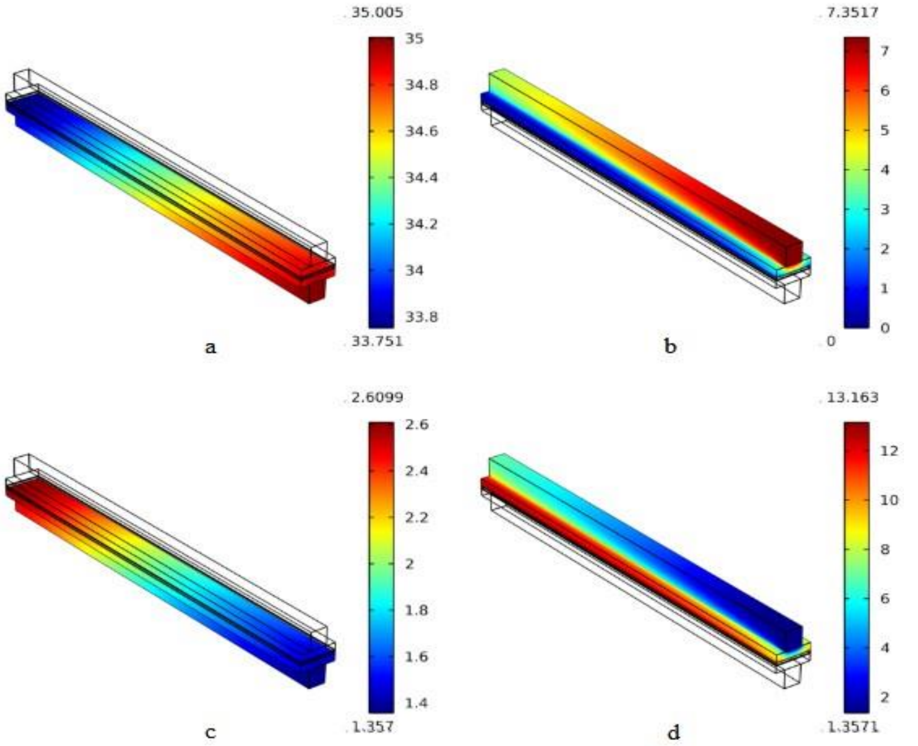

Figure 3. *Investigation of changes in PEMFC by application of initial parameters: a) Hydrogen concentration at anode, b) Oxygen concentration at cathode, c) water concentration at anode, d) Water concentration at cathode.*

Hydrogen inlet velocity was 0.2 $m.s^{-1}$ and oxygen inlet velocity was 0.5 $m.s^{-1}$ hydrogen concentration in anode electrode was between 33.751 and 35.005 $mol.m^{-3}$ oxygen concentration in cathode electrode was between 0 and 7.3517 $mol.m^{-3}$, water concentration in anode electrode was between 1.357 and 2.6099 $mol.m^{-3}$, water concentration in cathode electrode was between 1.3571 and 13.163 $mol.m^{-3}$, current density in the polymeric membrane was between 8336-17328 $A.m^{-2}$.

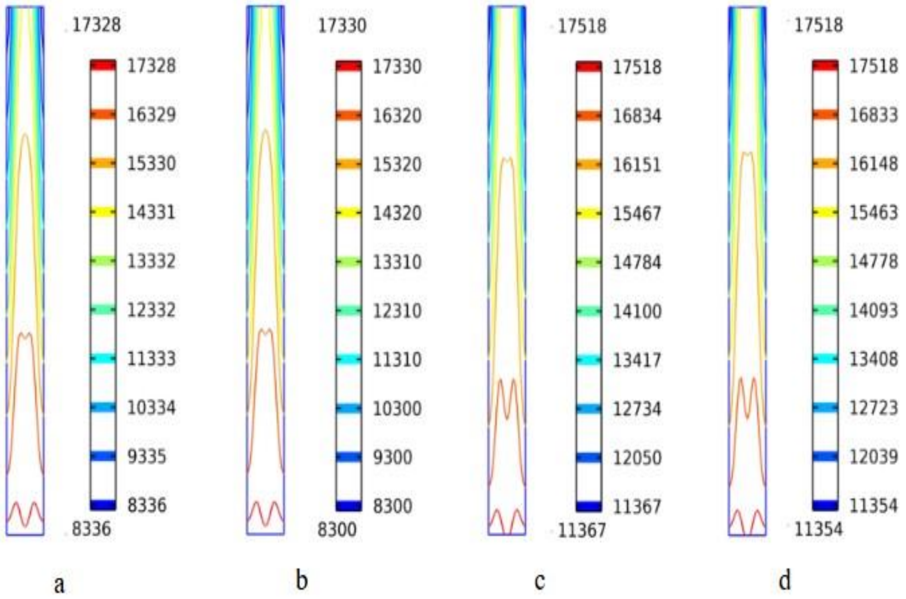

Figure 4. *Current density change in polymeric membrane: (a) Investigation of changes in PEMFC by application of initial parameters; (b) Investigation of changes in the PEMFC with the increase of the hydrogen input velocity; (c) Investigation of changes in the PEMFC with the increase of the oxygen input velocity; (d) Investigation of changes in the PEMFC with the increase of the hydrogen and oxygen input velocities.*

A. INVESTIGATION OF CHANGES IN PEMFC DUE TO THE INCREASING HYDROGEN INPUT VELOCITY

With increasing hydrogen velocity, hydrogen concentration in anode, oxygen concentration in cathode, water formation in anode, water formation in cathode and current density change in electrolyte membrane were respectively examined for PEMFC operated at 62 °C and 1 atm. All simulation results were evaluated for 0.4 V. Hydrogen input velocity was increased from 0.2 $m.s^{-1}$ to 0.3 $m.s^{-1}$ and no changes were made for oxygen velocity $m.s^{-1}$. Simulation results of changing the hydrogen input velocity at the anode input are shown in Figure 5 and Figure 4b.

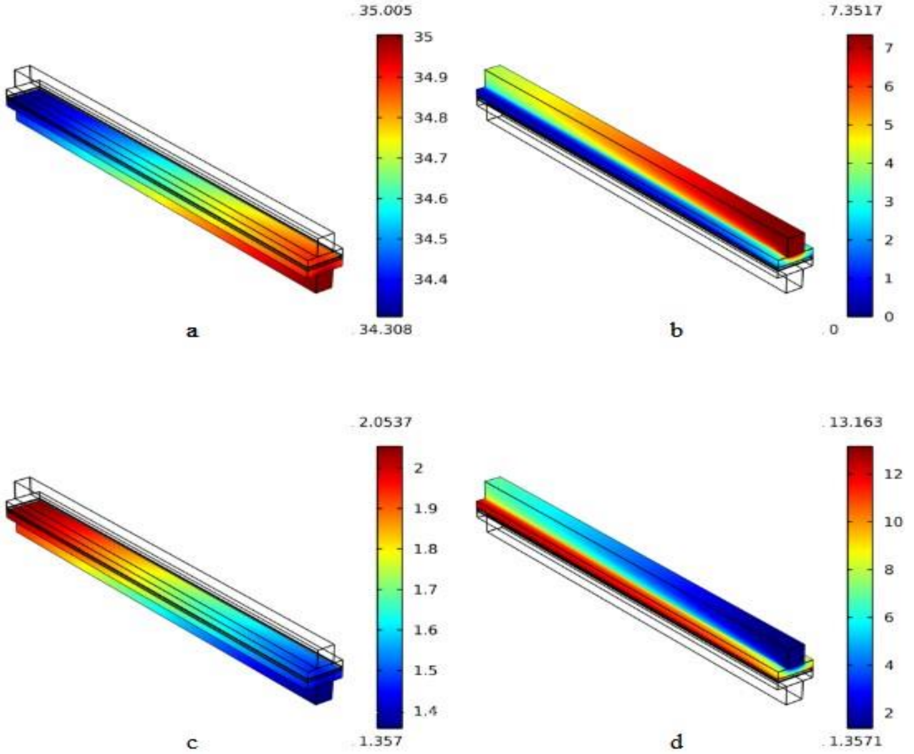

Figure 5. *Investigation of changes in the PEMFC with the increase of the hydrogen input velocity a) hydrogen concentration in the anode, b) oxygen concentration in the cathode, c) water concentration in the anode, d) water concentration in the cathode.*

For the initial parameters hydrogen inlet velocity was 0.3 $m.s^{-1}$ and oxygen inlet velocity was 0.5 $m.s^{-1}$; hydrogen concentration in anode electrode was between 34.308 and 35.005 $mol.m^{-3}$, oxygen concentration in cathode electrode was between 0 and 7.3517 $mol.m^{-3}$, water concentration in anode electrode was between 1.357 and 2.0537 $mol.m^{-3}$, water concentration in cathode electrode was between 1.3571 and 13.163 $mol.m^{-3}$, current density in the polymeric membrane was between 8300 - 17330 $A.m^{-2}$. When hydrogen distribution at anode was examined, input concentration was the same for two simulations and it is 0.3 $m.s^{-1}$. When investigated the hydrogen distribution in anode, beginning concentration was 35.1 $mol.m^{-3}$ for the two simulations. This value is in the anode input region and decreases as it moves away from the input region. A decrease in minimum hydrogen amount at anode electrode was observed. Since the anode inlet region was constant size, the amount of hydrogen fed increased by the ratio of 3/2. This rise increased the minimum amount of hydrogen in the concentration. Conversely, all of these values are valid for molecular hydrogen. No such reduction was observed for ionic hydrogen. While molecular hydrogen was decreasing, ionic hydrogen increased. The ionic hydrogen moved away from this region to the cathode electrode. Negatively charged electrodes, which begin to accumulate in the anode, were sent to a load by means of a low resistance conductor. In this case, it was expected that when the input velocity of hydrogen increases, the amount of hydrogen input in the anode and the amount of electrons to be released will increase. As the flow velocity increased, initially the ionic hydrogen tended to increase in the perspective of concentration, although remained at a constant concentration after a certain point. The regions where the minimum hydrogen amount existed in anode part were cell boundary and hydrogen output points. The hydrogen distribution was 33.751 $mol.m^{-3}$ for 0.2 $m.s^{-1}$, while the concentration was around 34.308 $mol.m^{-3}$ where the velocity was 0.3 $m.s^{-1}$. These data showed that the concentration amount would increase when the input rate of hydrogen increased. Any change was not observed in the oxygen concentration simulation at the cathode. A reduction in the water concentration at the anode was observed when hydrogen input velocity was increased. Maximum water concentration was 2.6099 $mol.m^{-3}$ for $m.s^{-1}$ (hydrogen input velocity), while water concentration was 2.0537 $mol.m^{-3}$ for 0.3 $m.s^{-1}$ (hydrogen input velocity). The reason for the decrease in water concentration was that the amount of hydrogen increases while the amount of oxygen remains constant. The insufficient amount of oxygen for the new situation causes insufficient oxidation.

Conversely, this is a pioneering information for controlling water in the anode region [4]. The increase was numerically examined in cell performance by controlling water transport in PEMFC. With their CFD analysis, they modeled the change in current density caused by different temperature values. In addition, the studies were performed to create a high efficiency PEMFC by controlling the variables such as pressure, temperature, relative humidity and channel size that may occur along a flow channel in PEMFC [18]. In conclusion, they suggested that thermal and water control within the cell affect performance. This study is showing that the amount of hydrogen fed into the cell is an important factor for this control. In the simulation of increasing hydrogen input velocity, any change in both water concentration in the cathode region and current density on the polymeric membrane was not observed. This was expected situation when considered that there are two separate electrodes. In addition, any change was not observed in the Contour diagram when the hydrogen input velocity was increased. The value of current density varied between 8300 and 17730 $A.m^{-2}$ in both simulations. The minimum current density was 8336 $A.m^{-2}$ for the other simulation and decreased to 8300 $A.m^{-2}$ in this simulation. Conversely, the maximum current density was 17328 $A.m^{-2}$ for the other simulation and increased to 17330 $A.m^{-2}$ in this simulation. Since the simulations were performed under constant voltage 0.4 V, the power density was determined to be constant. When the amount of fuel and oxygen increased, the current density increased slightly, conversely, after a certain level, no matter how much the amount of fuel and oxygen increase, current density did not increase since water would not be formed. For a consistent increase in current density, only hydrogen speed increase or oxygen rate increase is not effective. The feed rates of both molecules should increase at a certain rate.

B. INVESTIGATION OF CHANGES IN PEMFC DUE TO THE INCREASING OXYGEN INPUT VELOCITY

The concentration change on the anode and cathode and the change in the current density in the membrane were investigated with the increase of oxygen input velocity in the PEMFC. The oxygen input velocity was changed from 0.5 $m.s^{-1}$ to 0.8 $m.s^{-1}$. The hydrogen velocity was taken to the initial value of 0.2 $m.s^{-1}$ and all simulation results were evaluated for 0.4 V. The simulation results for changing the oxygen input velocity at the cathode input are given in Figure 6 and Figure 4c.

For the initial parameters hydrogen inlet velocity was 0.2 $m.s^{-1}$ and oxygen inlet velocity was 0.8 $m.s^{-1}$; hydrogen concentration in anode electrode was between 33.54 and 35.005 $mol.m^{-3}$, oxygen concentration in cathode electrode was between 0.0048 and 7.3521 $mol.m^{-3}$, water concentration in anode electrode was between 1.357 and 2.8211 $mol.m^{-3}$, water concentration in cathode electrode was between 1.3572 and 13.101 $mol.m^{-3}$, current density in the polymeric membrane was between 11367 - 17518 $A.m^{-2}$. In the simulations carried out by increasing the oxygen input velocity in the cathode, any change for the amount of hydrogen concentration in the anode and water concentration in the anode was not observed. The concentration of water and hydrogen were in balance for both two simulations. Conversely, the situation varied for the cathode electrode. By increasing the oxygen input velocity, the minimum oxygen concentration increased from 0 $mol.m^{-3}$ to 0.0048 $mol.m^{-3}$. The maximum oxygen concentration increased from 7.3517 $mol.m^{-3}$ to 7.3521 $mol.m^{-3}$. Simulations also showed that the maximum oxygen concentration was in the input region for both cases. As we moved away from the inlet region and came near the membrane surface, the oxygen was brought together with hydrogen. Conversely, in the simulation of the increase in oxygen velocity, it was observed that this will occur to a saturation and be stabilized when the hydrogen molecules are depleted.

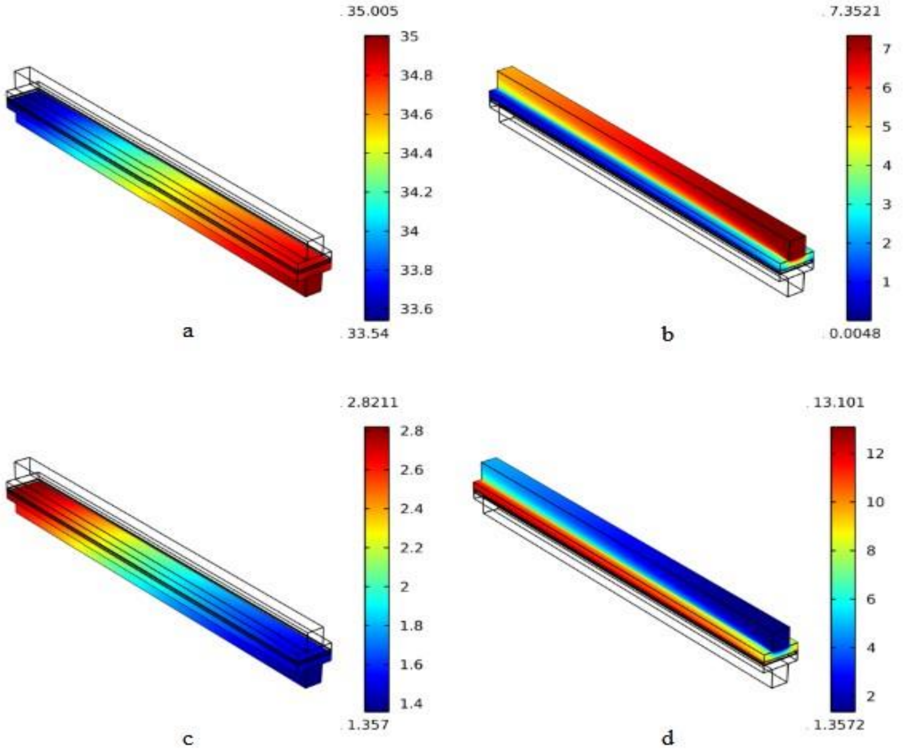

Figure 6. *Investigation of changes in the PEMFC with the increase of the oxygen input velocity: a) hydrogen concentration in the anode, b) oxygen concentration in the cathode, c) water concentration in the anode, d) water concentration in the cathode.*

The simulation of examining the water concentration in the cathode region clearly demonstrated this situation. Observations on Figure 4c show that the minimum water concentration is 1.3572 $mol.m^{-3}$ in both two simulations. Conversely, there was a reduction in the maximum water concentration. This value decreased from 13.163 $mol.m^{-3}$ to 13.101 $mol.m^{-3}$ compared to the initial state. This value indicated that all of the hydrogen was oxidized and there was any hydrogen to oxidize anymore. After this, it is known that water cannot be formed and will remain completely as oxygen for every speed increase in the cathode region. In addition, for both two simulations, the formation of water firstly started quickly and steadily continued when it reached saturation. The polymeric membrane current density in this modeling differs according to the initial parameters and simulations of only the increase in hydrogen velocity. This difference is the minimum current density. The minimum current density was 8336 $A.m^{-2}$ for the other simulation and increased to 11367 $A.m^{-2}$ in this simulation. With this simulation, it is clear that more current could be obtained at constant voltage and thus more energy could be produced. In addition to this, water transport will be facilitated and cell life will be prolonged by a decrease in water concentration. Conversely, the strength properties of membrane material are among the limiting factors in energy production. Simulation of only changing the rate of oxygen input showed that an increase in the amount of oxygen impinging on the membrane surface. In this simulation, any more water could not be formed because all of the hydrogen were depleted, and the oxygen that has excess molecular weight was constantly contacting the membrane causing physical erosion [30]. In their work with NCPEM fuel cell (NC:Nanocomposite), membranes produced from different types of nanocomposite materials have been examined. Studies showed that cell life increases with increased membrane strength. With the only change of the oxygen input velocity simulation, it was observed that the amount of unreacted oxygen decreased to minimum and subsequently the membrane life prolongs. In addition to all of them, temperature rise in the cell will occur due to the decrease in water concentration in the cathode electrode and thermal control will be difficult [31]. The negative effects of temperature rise were examined on PEMFC. For PEMFC, it was determined that the cell yield increases with increasing temperature although cell life was shortened. Our study shows that thermal control on PEMFC can be changed only by changing the oxygen input velocity. Consequently, the advantages and constraints of the new situation should be taken into account for more energy production.

C. INVESTIGATION OF CHANGES IN PEMFC DUE TO THE INCREASING HYDROGEN AND OXYGEN INPUT VELOCITY

Various observations have been made by simultaneously increasing the hydrogen velocity entering the anode and oxygen velocity entering the cathode in the PEMFC. In this simulation, hydrogen inlet velocity was measured for 0.3 $m.s^{-1}$ and oxygen inlet velocity was 0.8 $m.s^{-1}$. Simulations of hydrogen distribution in the anode, oxygen distribution in the cathode, water formation in the anode, water formation in the cathode, current density change in the polymeric membrane were examined and simulation results were shown in Figure 7 and Figure 4d.

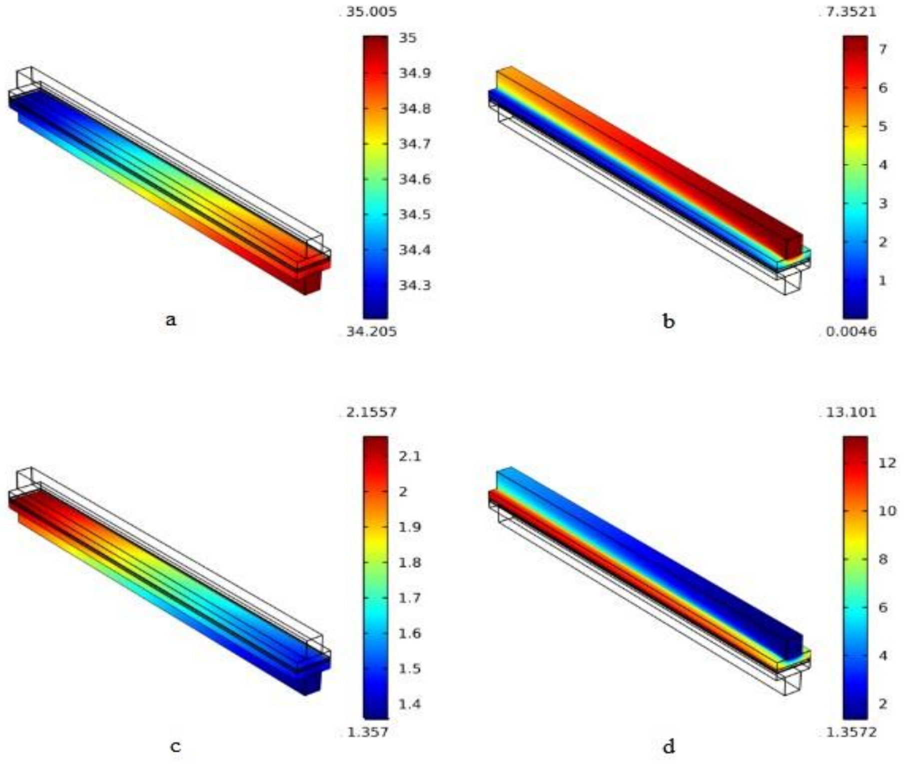

Figure 7. *Investigation of changes in the PEMFC with the increase of the hydrogen and oxygen input velocities: a) hydrogen concentration in the anode, b) oxygen concentration in the cathode, c) water concentration in the anode, d) water concentration in the cathode.*

For the initial parameters hydrogen inlet velocity was 0.3 $m.s^{-1}$ and oxygen inlet velocity was 0.8 $m.s^{-1}$; hydrogen concentration in anode electrode was between 34.205 and 35.005 $mol.m^{-3}$, oxygen concentration in cathode electrode was between 0.0046 and 7.3521 $mol.m^{-3}$, water concentration in anode electrode was between 1.357 and 2.1557 $mol.m^{-3}$, water concentration in cathode electrode was between 1.3572 and 13.101 $mol.m^{-3}$, current density in the polymeric membrane was between 11354 - 17518 $A.m^{-2}$. A simultaneous concentration change in the anode and cathode electrodes were observed in the simulation of the simultaneous changing of the hydrogen and oxygen inlet velocities. In addition, this concentration change directly influenced the current density in the polymeric membrane. The minimum hydrogen concentration in the anode electrode increased to 34.205 $mol.m^{-3}$. For this case, the maximum hydrogen concentration at the anode remained constant at 35.005 $mol.m^{-3}$. The minimum oxygen concentration in the cathode electrode increased from 0 $mol.m^{-3}$ to 0.0046 $mol.m^{-3}$, while the maximum oxygen concentration in the cathode electrode increased from 2.6099 $mol.m^{-3}$ to 2.1557 $mol.m^{-3}$. Simulations showed that the increases in the velocity of hydrogen fed by the anode and the oxygen fed by the cathode did not affect the maximum hydrogen in the anodes. Conversely, it caused an increase in the minimum hydrogen concentration in the anode electrode and the minimum oxygen concentration in the cathode electrode at feed velocities. This increase showed that hydrogen and oxygen were fed more than it should be.

For this case, the minimum water concentration at the anode remained constant at 1.357 $mol.m^{-3}$. This value was the same as the minimum water concentration in the simulation of changing the only hydrogen inlet velocity. The maximum water concentration in the anode electrode decreased from 2.6099 $mol.m^{-3}$ to 2.1557 $mol.m^{-3}$. These values were a pioneer for minimization of floods in the anode electrode which occurred by simultaneously changing the hydrogen and oxygen inlet velocities. The minimum water concentration in the cathode electrode increased from 1.3571 $mol.m^{-3}$ to 1.3572 $mol.m^{-3}$. The maximum water concentration decreased from 13163 $mol.m^{-3}$ to 13101 $mol.m^{-3}$. These values were at the same level as the simulation of changing the only oxygen input velocity. The minimum current density in the polymeric membrane increased from 8336 $A.m^{-2}$ to 11354 $A.m^{-2}$ and the maximum current density increased from 17328 $A.m^{-2}$ to 17518 $A.m^{-2}$. This change indicates the increase in current density with simultaneous increase of hydrogen and oxygen inlet velocities. The results showed that the simulation of simultaneous changing of hydrogen and oxygen inlet velocities is more stable than simulations of changing the only hydrogen inlet velocity and changing the only oxygen inlet velocity. The hydrogen concentration in the anode region increased with the increase of the only hydrogen input velocity. Since the input velocity of oxygen fed by the cathode remained constant, the water formation velocity in the cathode increased first and then remained constant. The fact that the rate of water formation stayed in balance indicates that the reaction is no longer equilibrium and cannot generate more currents. From this simulation, it was observed that only the increase in the velocity of hydrogen input increases the amount of pure hydrogen used, although it was not effective in power generation. The oxygen concentration in the cathode region increased only with the increase of oxygen input velocity. Since the rate of hydrogen supplied by the anode stayed in balance, the rate of water formation in the cathode increased first and then were in balance. The fact that the rate of water formation was in balance indicates that the reaction is no longer equilibrium and cannot generate more currents. The increase in the minimum current density was resulted from the initial parameters. The hydrogen inlet velocity in the initial parameters was accepted as 0.2 $m.s^{-1}$ and the oxygen inlet velocity was accepted as 0.5$m.s^{-1}$. In the ideal combustion equation, 2 moles of hydrogen and 1 mol of oxygen are sufficient for the formation of water. Conversely, irreversibility occurs in real combustion. Here, it was desired to burn all of the reacted hydrogen by obtaining an excess of oxygen in order to achieve complete combustion. The excess oxygen content in the initial parameters was assumed to be 25%. It was expected that an increase in the minimum current density is initially expected when the amount of oxygen given to burn 1 mol of hydrogen is increased only in the simulation of increasing the oxygen velocity. Conversely, the simulation also showed an increase in the amount of oxygen in the cathode. This result indicated that there was any more hydrogen not to react and that oxygen was supplied at an excessive rate. This increase in velocity would cause wear on the membrane surface during operation, thus shortening the cell life. Simulation of simultaneous changing of hydrogen and oxygen input velocities increased the hydrogen concentration in the anode electrode and the oxygen concentrations in the cathode electrode. This simulation showed that the rate of water formation could be changed depending on the ratio of the hydrogen and oxygen input velocities. Floods and water leaks could be controlled by controlling the water in the cell. By controlling water with a certain temperature value, thermal control could be facilitated. In order to perform this process, it was determined that the hydrogen velocity at the anode inlet and the oxygen velocity at the cathode inlet should be simultaneously changed in PEMFC. Using the obtained results, the amount of excess oxygen to be used for a PEMFC having 1 atm pressure, 62 $^{\circ}$C temperature and 0.4 V voltage value was calculated as 23.62%. In a PEMFC with an anode inlet velocity of 0.2 $m.s^{-1}$, the oxygen inlet velocity should be 0.4945 $m.s^{-1}$. When these speed values were applied, the power density that could be obtained from PEMFC was 3820 $W.m^{-2}$ and the cell yield was 58.77%. Since the different materials were not needed in the developed modellings and all velocity tests could be done in simple ways, it is superior to the existing studies. Since HTPEMFCs operating at high temperatures have a high vapor loss which leading to erroneous results, alternative solutions should be sought for using these modellings. Developed modellings could be easily applied in all fuel cells operating at low temperatures and forming water as a product. A numerical analysis for hydrogen and oxygen feed velocities has been developed to minimize the use in a PEMFC that feeds pure hydrogen at the anode inlet and pure oxygen at the cathode inlet, to ensure water control, thermal control and prolong cell life by reducing membrane wear. In this analysis, the results of different speed parameters from COMSOL programme were used. Then, we aimed to check its accuracy by indirectly optimizing this model with a numerical method such as Golden Section Method. The error analysis was performed by comparing the results in each analysis with the previous one. By repeating the processes performed, current density and power density were obtained for optimum hydrogen and oxygen rates. The golden ratio number is an irrational number and is considered to be approximately 0.61803.

$$\frac{\sqrt{5}-1}{2} \cong 0.61803 \tag{7}$$

Representation of the Golden Section Method:

$$d = \left(\frac{\sqrt{5}-1}{2}\right) \times (X_U - X_L) \tag{8}$$

In here, U = upper, L= low

$$X_1 = X_L + d \tag{9}$$

$$X_2 = X_U - d \tag{10}$$

If $f(X_1) > f(X_2)$, X_2 is new X_L, If $f(X_2) > f(X_1)$, X_1 is new X_U (11)

The Golden Section Method was possible to see the reality value of convergence by making error analysis after all the operations. It could be said that convergence is sufficient by ensuring continuity in error analysis. When the current density of the hydrogen velocity at the anode in PEMFC was examined, the limit values were determined first. In these values, X_L was equal to stoichiometric combustion. Then, the hydrogen inlet velocity at the anode was gradually increased on COMSOL. It has been observed that, after a certain increase, only the increase of the hydrogen input velocity at the anode has any effect on the current density. The reason for this was that there is less oxygen than the amount that could burn hydrogen. The speed value in the province with this process constituted the X_U value and referred to the maximum hydrogen value that could be burned with a limited amount of oxygen. X_1 and X_2 values were obtained by applying the 1st step of the Golden Section Method for the current limit values. The optimum hydrogen velocity in the anode was determined by performing error analysis on the required processes. The same processes were valid for the oxygen rate at the cathode. With all these processes, the analysis made for the hydrogen inlet velocity at the anode and oxygen inlet velocity at the cathode had the most realistic results. The change obtained as a result of the transactions is shown in Figure 8. Total combustion Equation (12) occurred in PEMFC;

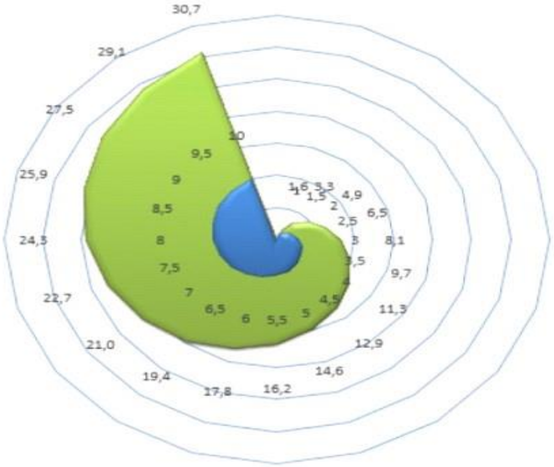

Figure 8. *Hydrogen and oxygen feed velocity graphic obtained with Golden Section Method.*

$$H_2 + \frac{1}{2}\, O_2 \rightarrow H_2O \tag{12}$$

For this equation, the coefficient of the hydrogen in the molecular state is (a) and the coefficient of the molecular oxygen is (b), and the ideal combustion is 1 and ($\frac{1}{2}$) respectively, at total combustion. Conversely, it is not possible to achieve this balance in reality. For this reason, it is desired to realize total combustion with excess air by using a large amount of oxygen. For this process to take place, it must be $b > \frac{1}{2}$. Conversely, a restrictor is needed for the desired value. In addition, it is desired to preserve the (a) coefficient in minimum for the (b) coefficient to be obtained. Both of these sequential processes directly affect the combustion efficiency in the reaction. For this reason, it is possible to provide combustion under the best conditions by changing the number of (a) and (b) coefficients. Under the current PEMFC study conditions, numerous iterations have been performed by choosing coefficients upper or down the ideal (a) and (b) coefficients for combustion of hydrogen. By applying the golden ratio on the equation obtained from all these iterations, the ranges of (a) and (b) coefficients were restricted. As a result of each iteration carried out, error analysis was performed and optimum study efficiency was calculated. Velocity equations created for PEMFC operating in optimum conditions are shown below. Of these equations, first one is valid for the anode and second one is valid for the cathode.

$$U_{a_{in}} = \lambda_a \times \frac{I}{2F} \times X_{H_2} \times \frac{R \times T}{P \times S} \tag{13}$$

$$U_{c_{in}} = \lambda_a \times \frac{I}{4F} \times X_{O_2} \times \frac{R \times T}{P \times S} \tag{14}$$

In these equations, $U_{a_{in}}$ and $U_{c_{in}}$ are anode and cathode input velocities, respectively. λ_a is stoichiometric ratio and S is cross-sectional area while I is current density and F is Faraday constant. R is ideal gas constant, P is pressure and T is absolute temperature. In first equation X_{H_2} points the hydrogen mass fraction, while X_{O_2} Equation 13, while f_2 function represents Equation 14.

In Figure 9 the polarization curve for the reference model and the optimum model is given. Based on this curve, it is possible to comment on power density and cell resistance. The polarization curve was made for the results obtained for a voltage between 0.4V - 0.9V. While creating the graph, the average current density change in a cell was evaluated. The results show that the current density and the voltage changed inversely in the cell. At the beginning, any current did not flow through the cell. The potential difference in this case shows the maximum voltage V_{max}. As the current density increases within the cell, the voltage shows a logarithmic decrease. As the area under the polarization curve increases, the power density obtained increases. The data obtained shows that the power density obtained for the optimum model was higher. It also showed the value $R^2 = 0.9287$ for the regression analysis for this process. This result shows that when combined with our decreasing graph in error analysis, we have made an accurate modeling.

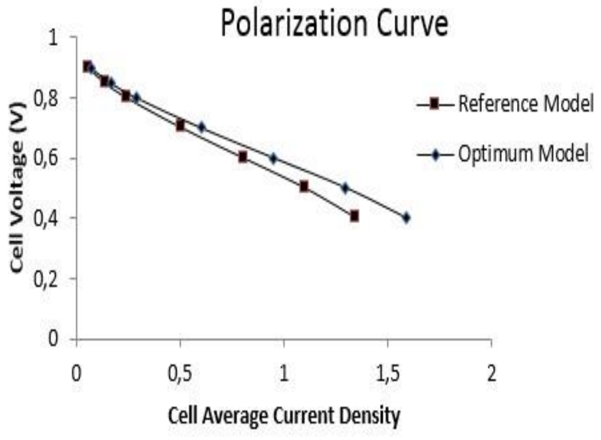

Figure 9. *Polarization curve for the reference model and the optimum model.*

IV. CONCLUSIONS

In this study, a 3D PEMFC was examined using COMSOL Multiphysical Programme. The studies have been simulated based on mathematical and numerical models using COMSOL. For PEMFC, stoichiometric total combustion, partial combustion, total combustion states were examined respectively. According to the results obtained here, minimum use of hydrogen and oxygen was aimed and achieved for maximum cell performance. The compliance of the findings in the future studies is very easy to perform. Moreover, it is certain that this model for a cell will show similar characteristics as quality in the stalk structure. Modeling approaches were performed to minimize the loss of activation, ohmic and concentration in the cell. Modeling was compatible with mathematical data and other studies. By applying model approaches, velocity effect was investigated to prolong membrane life by preventing membrane wear due to excessive speed. The pressure changes were tried to minimize in the cell by simulation. It was tried to optimize the amount of water that may occur in the cathode. (Too much leads to flooding, and less causes the membrane to heat up, adversely affecting performance). By simulation, it was aimed to preserve the molecular hydrogen in the anode to a minimum ensuring maximum current density. Determining the optimum PEMFC performing conditions by simulations, it was obtained to minimize the use of pure hydrogen which is present in trace amounts for pure form in nature and is generally derived from other hydrocarbon compounds. Thanks to simulations, maximum cell performance was achieved by providing water management and thermal management within the cell. Gas leaks, which might occur, could be minimized with a stable combustion. As mentioned before, confirming the simulations by Golden Section Method makes an important contribution to the literature.

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