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Simulation study for 3D dynamic characteristics of voltage losses in PEM fuel cell

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Abstract

Fuel cells, providing an advanced alternative energy source, are devices that can convert chemical energy into electrical energy. Modeling of a fuel cell provides improvements to the design of the fuel cells as well as providing cheaper, better and more efficient fuel cells. Three basic voltage losses occur in the fuel cell: activation polarization, ohmic polarization and concentration polarization. In this study, simulation of voltage losses in PEM (proton exchange membrane) fuel cells was performed by using Matlab@Simulink program. Polarization and power curves were obtained for different operating temperatures by considering these losses.

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1. Introduction

Energy consumption is one of the most important requirements of countries with high levels of development and has been continuously increasing. In fact, most of the energy we consume is supplied from fossil fuel sources such as coal, oil and natural gas [1, 2]. However, there are basically three problems in the use of such fuels worldwide [3]. The first problem is that fossil fuels will be depleted in the near future, and the second problem is the increase in environmental pollution, and finally the increase in human health. It is possible to define renewable energy as an energy source that can be obtained from natural resources and renews itself continuously [4]. The most important feature that distinguishes renewable energy from other types of energy is that it can renew itself naturally and does not disappear. In addition, renewable energy types are very important in terms of reducing the carbon emissions that can harm the environment [5, 6].

Fuel cells are one of the renewable energy sources that will become the power source of the near future. Fuel cells have energy efficiency, low environmental pollution and unlimited fuel supply, as well as the potential to meet environmental expectations while moving confidently towards commercialization [7, 8]. Fuel cells can power everything from cell phones to tools at home and even cars.

Polymer electrolyte membrane (PEM) fuel cells, one of the most popular, are available in a variety of fuels, from hydrogen to ethanol to biomass-derived materials [9]. A PEM type fuel cell [10] consists of two electrodes one is positively charged (cathode), another is negatively charged (anode), and an electrolyte membrane. Oxygen is reduced to the cathode while hydrogen is oxidized to the anode. Transportation of protons from the anode to the cathode occurs through the electrolyte membrane, whereas electrons are transported to the cathode above the outer circuit. Hydrogen protons in fuel cells remain ionic by passing from molecule to molecule using special materials. Protons circulate through a polymer membrane consisting of persulfonic acid groups with a Teflon backbone. Electrons are attracted by conductive materials and go to the charge if necessary. In the cathode, oxygen reacts with protons and electrons to form water and generate heat. The stabilization of the electrode structure and minimization of the catalyst particle play important role for future material developments. The studies on the highly efficient electrocatalysts for the oxygen evolution reaction (OER) were presented in [11-14]. A basic PEM fuel cell stack consists of a proton exchange membrane, catalyst and gas diffusion layers, flow field plates, gaskets, and end plates. A stack with multiple cells has "membrane electrode assembly (MEA)" sandwiched between bipolar flow field plates and only one set of end plates.

Fuel cells are still showing intense development. The combination of new and optimized materials, advanced

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product development, new architectures, more efficient handling processes, design optimization and integration are expected to result in significant gains in performance, efficiency, reliability, productivity and cost effectiveness. Computational Fuel Cell Engineering (CFCE) tools that allow systematic simulation, design and optimization of fuel cell systems may facilitate the integration of such advances, allow less reliability of hardware prototyping, and reduce development cycles. A new model for combined protonics and water transport in polymer membranes is presented in [15]. A method for reducing the model of a nonlinear dynamic fuel cell stack suitable for control and diagnostic studies is performed in Ref. [16]. In order to meet the increasingly stringent application requirements in the PEM type fuel cell, performance gains and productivity gains are crucial. Computational fluid dynamics (CFD) is an ideal tool for achieving these improvements. A comprehensive CFD-based vehicle that can accurately simulate the main transport event occurring in a PEM fuel cell was presented in Ref. [17]. The results of the study were compared with the numerical model results and the results of Ref. [18]. It is seen that the study performed at low current values shows better agreement. A study on the modeling, simulation and analysis of the dynamic behavior of the 5kW PEM fuel cell system [19]. The model used in the study includes hydrogen fuel regulator and PEM fuel cell stack. The model was used to investigate the effect of temperature on fuel cell voltage and power flow at various temperatures. A series of fuel cell studies have been performed to investigate heat and mass transfer in reactive gas channels and water supply to protect the moisture of the membrane [20-26].

Although operating conditions are important for a fuel cell performance, the main factors in this performance are the structure, material and performance of the elements used in each unit of the fuel cell. For this reason, studies on materials and equipment used in fuel cells are of great importance. In this study, performances of fuel cell elements were simulated using Matlab@Simulink simulation program.

2. Materials and Methods

A typical PEM fuel cell has the following reactions:

Anode reaction: $H_2 \rightarrow 2H^+ + 2e^-$ (1)

Cathode reaction: $1/2O_2 + H^+ + 2e^- \rightarrow 2H_2O$ (2)

General reaction: $H_2 + 1/2O_2 \rightarrow 2H_2O + electrical\ energy + heat$ (3)

The reactants are carried by diffusion and/or convection to the catalyzed electrode surfaces where electrochemical reactions take place. Water and waste heat generated by the fuel cell must be removed continuously. Otherwise, PEM may cause critical problems for fuel cells. The maximum electrical energy output and the voltage difference between the cathode and the anode are obtained when the fuel cell is operated under thermodynamically reversible conditions. This maximum possible cell potential is called "reversible cell potential". The net output voltage of a fuel cell at a given current density is the reversible potential minus the irreversible potential and can be written as:

$$V(i) = V_r - V_{irr} \quad (4)$$

Here V_r is the maximum voltage of the fuel cell (i.e., = E_r) and V_{irr} is non-reversible voltage loss (i.e, over-voltage) occurring in the fuel cell. The actual work in the fuel cell is less than the maximum useful work due to other irreversible processes in the process. The irreversible voltage loss is indeed the summation of activation potential (υ_{act}), ohmic over-voltage (υ_{ohmic}) and concentration over-voltage (υ_{consan}) and it is represented by the following equations:

$$V_{overvoltage} = V_{irr} = \upsilon_{act} + \upsilon_{ohmic} + \upsilon_{consan} \quad (5)$$

$$V(i) = V_r - \upsilon_{act_a} - \upsilon_{act_c} - \upsilon_{consan_a} - \upsilon_{consan_c} - \upsilon_{ohmic} \quad (6)$$

As can be seen from Eqn. 6, activation polarization ($\upsilon_{act_a}$and υ_{act_c}) and concentration polarization (υ_{consan_a} and υ_{consan_c}) occur at both in the anode and cathode, while the resistive polarization (υ_{ohmic}) represents ohmic losses across the fuel cell. The equation for the fuel cell polarization curve is the relationship between fuel cell potential and current density. It can be written as follows:

$$E = E_r - \frac{RT}{\alpha_c F} ln\left(\frac{i}{i_{0,c}}\right) - \frac{RT}{\alpha_a F} ln\left(\frac{i}{i_{0,a}}\right) - \frac{RT}{nF} ln\left(\frac{i_{L,c}}{i_{L,c}-i}\right) - \frac{RT}{nF} ln\left(\frac{i_{L,a}}{i_{L,a}-i}\right) - iR_i \quad (7)$$

where E_r is the standard reversible voltage, R is the ideal gas constant, T is the absolute temperature, F is the Faraday constant, n is the number of moles of electrons transferred per fuel consumed, α is the charge transport constant, $i_{L,a}$ and $i_{L,c}$ are the limiting current density at the anode and cathode, and i is the operating current density of fuel cell, respectively.

3. Results and Discussion

3.1. Voltage losses from activation

Although many progresses have been achieved in the area of electrode kinetics, however, it is clear that methods still need to be developed to fully understand the anode and cathode kinetics. The electrochemical reactions that occur in the anode and cathode when modeling fuel cells need to be understood as they control the power generation rate and cause activation voltage losses. The over-voltage required to cross the energy barrier for the electrochemical reaction to take place is called polar activation polarization. Such polarization dominates losses at low current density and measures catalyst activity at a given temperature. The catalyst lowers the height of the activation barrier but causes voltage loss due to the slow oxygen reaction. The total activation polarization over-potential generally ranges from 0.1 to 0.2 V, which reduces the maximum potential to less than 1.0 V even in open circuit conditions. Activation over-potential expressions can be derived from the Butler-Volmer equation. In PEM fuel cells, the anode for hydrogen oxidation is very high compared to the cathode for oxygen reduction. Therefore, the contribution of the cathode to activation polarization is often neglected.

The parameters in the equations to be used in polarization and power curves modeling for the fuel cell are: cell area, hydrogen pressure, air pressure, temperature, Faraday constant, ideal gas constant, internal resistance and Gibbs energy in liquid state (J/mol). The parameters and their values used in the present study for the simulation of polarization and power curves are given in Table 1.

Table 1. The parameters and their values used in the present study for the simulation of polarization and power curves

Parameters	Values
Ideal gas constant (R)	8.314 J/molK
Faraday's constant (F)	96487 Columbs
Hydrogen pressure	2 atm
Air pressure	2 atm
Cell area	55 cm^2
Number of cells	1
İnner resistance	0.245 Ohm-cm^2
Charge transport constant	0.4
Amplification constant	0.1
Exchange current density	$10^{-9.486}$ (A/cm^2)
Limiting current density	1.5 (A/cm^2)
Gibbs energy	-228170 (J/mol)
Mass transport constant	1.1
Ideal gas constant (R)	8.314 J/molK

In this study, activation losses in anode and cathode as function of temperature and current density were simulated with Matlab® Simulink program. The variation of activation loss was investigated for 4 °C increased temperature values in the range 40 to 80 °C and increased current density values in the range 0 to 1.1 A / cm^2. As shown in Figure 1, the loss resulting from activation increases linearly with temperature, while a functional change as in the graph is observed with the current density. The increased temperature appears to cause a voltage drop in the activation polarization zone.

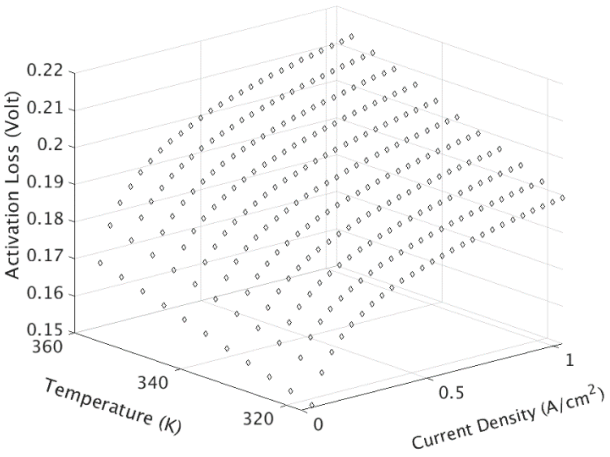

Figure 1. Change of activation loss with respect to current density (A/cm^2) and temperature (K).

3.2. Ohmic losses

The voltage loss due to the charge carrying resistance of electrons and ions, which are charged particles, is defined as "ohmic losses". General methods of reducing ohmic losses are to make the electrolytes as thin as possible and to use high conductivity materials that are well connected to each other. In this study, the ohmic loss was simulated by using the effective surface area of the fuel cell, the thickness of the electrolyte layer and electrical conductivity parameters. The obtained result is shown in Figure 2. The change in ohmic loss was investigated by increasing the cell area with 10 in the range of 50 to 100 cm^2 and the current density with 0.1 in the range of 0.1 to 1.1 A. As shown in the graph, ohmic loss is very sensitive to current density and surface area of the cell. At the same time 5 different thickness electrodes were used to see how this sensitivity of ohmic loss changes with the thickness of the electrode. In order to see the effect of electrolyte thickness in detail, the change in ohmic loss according to the current density for a 100 cm^2 cell is shown in Figure 3. It is clear that ohmic loss increases with respect to electrolyte thickness.

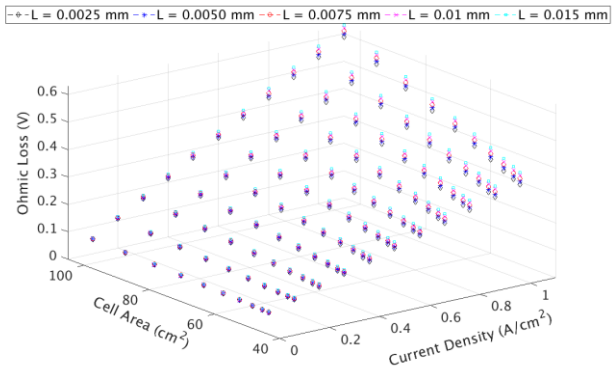

Figure 2. Change of ohmic loss as a function cell area (cm^2) and current density (A/cm^2)

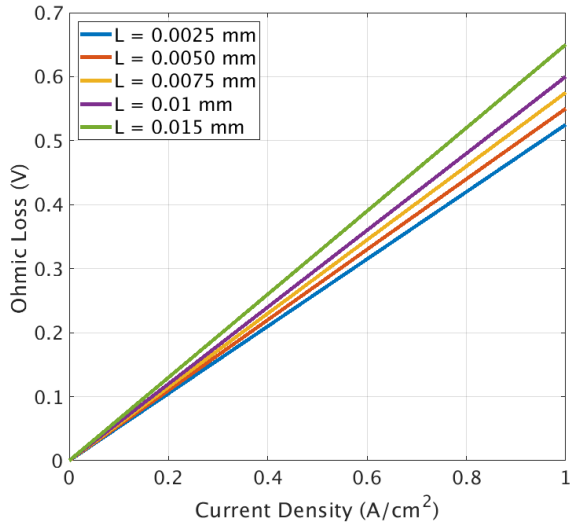

Figure 3. Change of ohmic loss (V) with respect to current density (A/cm^2) for an electrolyte having different thicknesses.

3.3. Voltage losses from concentration

When a fuel cell is filled by fuel and oxygen generates electricity, the product water must be continuously removed to maintain efficiency and provide appropriate fuel and oxidant in the catalyst layers. Another source of voltage losses is mass transport constraints, which can significantly affect fuel cell performance. Losses caused by mass transport are also called "concentration losses". In the simulations performed in this study, the limiting current density values in the cathode and anode were taken as $1.5A/cm^2$.

The polarization curve and the power curve with respect to the different operating temperatures obtained using the Matlab® Simulink program are shown in Figure 4.

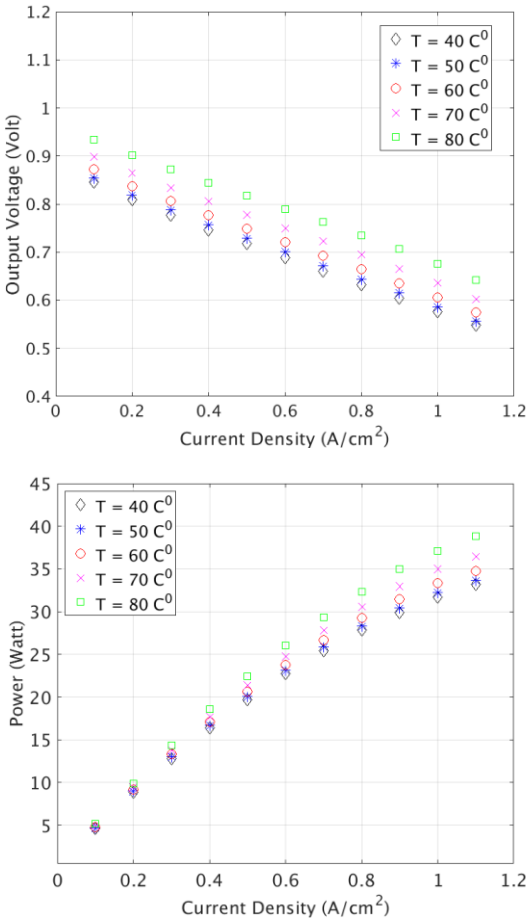

Figure 4. a) Polarization curves and b) power curves obtained for a PEM type fuel cell at different temperatures

These curves may not exactly match the actual curves obtained for a fuel cell stack. However, it is a good start to perform simulation of a PEM fuel cell. Individual modeling of the structure of the proton exchange, the gas diffusion layer, the catalyst layers and the fuel flow plates for a complete PEM fuel cell simulation will allow for more realistic polarization and power curves.

4. Conclusion

With a wide range of applications, from dynamic mobile systems to stationary systems, PEM fuel cells are one of the potential tools for generating clean energy. Although it has important features such as wide usage range and high efficiency, it has a disadvantage in terms of durability and cost. In order to compete with other power systems today, many studies focus on reducing PEM fuel cell costs and better durability. It is important to model and simulate these technological developments before the application.

In this study, our aim is to simulate voltage losses that can occur in PEM fuel cells by considering the various operating temperatures and thickness of electrodes.

According to the simulation, the increased temperature leads to a voltage drop in the activation polarization. As a result, to derive a final decision on the PEM fuel cell properties, all the parameters need to be taken into account during the simulation.

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Conflicts of interest

The authors state that did not have conflict of interests.

References

[1] Miller B. G., Clean coal engineering technology, Coal as fuel: past, present, and future, 1st ed. Boston: Butterworth-Heinemann, (2011) 1-51.

[2] Zou C., Zhao Q., Zhang G., Xiong B., Energy revolution: From a fossil energy era to a new energy era, *Natural Gas Industry B*, 3(1) (2016) 1-11

[3] Staffell I., Scamman D., Abad A.V., Balcombe P., Dodds P.E., Ekins P., Shah N., Ward K.R., The role of hydrogen and fuel cells in the global energy system, *Royal Society of Chemistry-Energy Environ. Sci*., 12(1) (2019) 463-491.

[4] Harting C., Jörissen L., Kerres J., Lehnert W., Scholta J., Polymer electrolyte membrane fuel cells, Materials for Fuel Cells, *Woodhead Publishing Series in Electronic and Optical Materials*, 8(3) (2008), 101-184.

[5] Panwar N.L, Kaushik S.C., Kothari S., Role of renewable energy sources in environmental protection: A review, *Renewable and Sustainable Energy Reviews*, 15 (2011) 1513–1524.

[6] Fahmy F.H., Abdel-Rehim Z.S., Hydrogen gas production an dutilization as electricity using a renewable energy source. *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*, 21(7) (1999) 629–641.

[7] Bauen A., Foradini F., Hart D., Fuel Cell-Based Renewable Energy Supply: Sustainable Energy for Isolated and Island Communities. In: Afgan N.H., Carvalho M.G., (Eds). New and Renewable Technologies for Sustainable Development. 1st ed. Boston: Springer, (2002) 421-428 .

[8] Bauen A., Hart D., Assessment of the environmental benefits of transport and stationary fuel cells, *Journal of Power Sources*, 86 (1-2) (2000) 482-494.

[9] Wang Y., Chen K.S., Mishler M., Cho S.C., Adrohera X.A., A review of polymer electrolyte membrane fuel cells: Technology, applications, and needs on fundamental research, *Applied Energy*, 88(4) (2011) 981-1007.

[10] Peighambardoust S.J., Rowshanzamir S., Amjadia M., Review of the proton exchange membranes for fuel cell applications, *International Journal of Hydrogen Energy*, 35 (17) (2010) 9349-9384

[11] Elmacı G., Ertürk A.S, Sevim M., Metin Ö., MnO2 nanowires anchored on mesoporous graphitic carbon nitride (MnO2@mpg-C3N4) as a highly efficient electrocatalyst for the oxygen evolution reaction, *Journal of Hydrogen Energy* 44 (33) (2019) 17995-18006.

[12] Elmacı G., Frey C.E., Kurz P., Zümreoğlu-Karan B., Water oxidation catalysis by using nano-manganese ferrite supported 1D-(tunnelled), 2D-(layered) and 3D-(spinel) manganese oxides, *Journal of Materials Chemistry* A 4 (22) (2016) 8812-8821.

[13] Elmacı G., Frey C.E., Kurz P., Zümreoğlu-Karan B., Water Oxidation Catalysis by Birnessite@Iron Oxide Core–Shell Nanocomposites, *Inorganic Chemistry*, 54 (6) (2015) 2734-2741.

[14] Elmaci G., Microwave Assisted Green Synthesis of Ag/AgO Nanocatalyst as An Efficient OER Catalyst in Neutral Media, *Hittite Journal of Science & Engineering*, 7 (1) (2020) 61-65.

[15] Djilali N., Computational modelling of polymer electrolyte membrane (PEM) fuel cells: Challenges and opportunities, *Energy* 32 (2007) 269–280.

[16] Najafi N., Dipenta D., Bencherif K., Sorine M., Modeling and simulation of a reformate supplied PEM fuel cell stack, application to fault detection, *HAL Applications and Tools of Automatic Control*, 21 (1) (2007) 1-18.

[17] Kone J.P, Zhang X., Yan Y., Hu G., Ahmadi G., CFD modeling and simulation of PEM fuel cell using OpenFOAM, *Energy Procedia*, 145 (1) (2018) 64-69.

[18] Yuan W., Tang Y., Pan M.Q., Li Z.T., Tang B., Model prediction of effects of operating parameters on proton exchange membrane fuel cell performance, *Renewable Energy*, 35 (2010) 656-666.

[19] Salam A.A., Mohamed A., Hannan M.A., Modeling and Simulation of a PEM Fuel Cell System Under Various Temperature Conditions, 2nd WSEAS/IASME International Conference on Renewable Energy Sources (Res'08) Corfu, Greece, October 2008, 26-28.

[20] Djilali N., Lu D., Influence of Heat Transfer on Gas and Water Transport in Fuel Cells, *Int. J. Therm. Sci.,* 41 (1) (2002) 29-40.
[21] Musser J., Wang C.Y., Heat Transfer in a Fuel Cell Engine, Proceedings of NHTC'00, 34th National Heat Transfer Conference, Pittsburgh, 2000, 1-7.
[22] Verbrugge M.W., Hill R.F., Transport Phenomena in Perfluorosulfonic Acid Membranes During the Passage of Current, *J. Electrochem. Soc*., 137 (4) (1990) 1131-1138.
[23] Springer T.E., Zawodzinski T.A., Gottesfeld S., Polymer Electrolyte Fuel Cell Model, *J. Electrochem. Soc.*, 138 (8) (1991) 2334-2342.
[24] Fuller T.F., Newman J., Water and Thermal Management in Solid-Polymer-Electrolyte Fuel Cells, *J. Electrochem. Soc*., 1993, 140 (5) (1993) 1218-1225.
[25] Nguyen T.V., White R.E., A Water and Heat Management Model for Proton-Exchange-Membrane Fuel Cells, *J. Electrochem. Soc.,* 140 (8) (1993) 2178-2186.
[26] Wohr M., Bowlin K., Schnurnberger W., Fischer M., Neubrand W., Eigenberger G., Dynamic Modeling and Simulation of a Polymer Membrane Fuel Cell Including Mass Transport Limitation, *Int. J. Hydrogen Energy,* 23 (2), (1998) 213-218.