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Modeling and simulation of PEM Used for Automotive Applications

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ABSTRACT

Not only are Fuel cell vehicles one of the significant options to replace gasoline engines, but they also come with a multitude number of benefits; For instance, fuel cell efficiency is more than about three times the efficiency of engines with internal combustion. According to the specific complexities of modeling the behavior of PEMFC, determining the performance of this system in case of its structural characteristics is considered as one of the parameters needed to better know of behavior the PEMFC. The present study attempts to find and examine a polymer membrane fuel cell for utilizing in a vehicle. To examine the performance of fuel cells, the modeling process was done by addressing diverse production-consumption heat in the anode and cathode positions and waterflood conditions. Using quadratic method, the flow channels were meshed and based on the finite difference method the mathematical equations were numerically discretized in the steady-state. Based on the simulation results, all heat values decrease over the channel of flow. By evaluating the relative humidity effect, it was obvious that the cathode relative humidity didn't change considerably along the channel of flow and at the same time, the relative humidity of the anode decreased along the channel of flow. There was a significantly low membrane layer velocity given the fact that this layer had a lower permeability coefficient in comparison with reactant layers and gas diffusion (Average Reynolds number: 612).



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1) Introduction

Energy and various approaches to achieve it are among the most important concerns of humans in the new century. Today, many researchers are working on new sources of energy. The sources of energy must be accessible easily, renewable, environment-friendly, dense energy source, inexpensive, and easy to store and transport. Still, there is a very small list of energies in this category. One of the widely studied sources of energies is fuel cell energy. No hydrocarbon is burned in a fuel cell and to generate electricity, hydrogen, and oxygen of the air interact with no need for any combustion. Therefore, the generation of electricity happens with much higher efficiency through combining the oxidizer and fuel with no noise or pollution. The hydrogen required in the fuel may be supplied from different sources like coal, oil, biogas, natural gas, water electrolysis, syngas from processing biomass materials, and the like. Direct generation of electricity is a good replacement for thermodynamics cycles used in internal combustion engines, where fuels chemical energy is turned into mechanical energy through the combustion process, and then ultimately converted to electrical energy [1]. In general, there are special complexities to model the proton exchange behavior of membrane fuel cells (PEMFC). Determining the conductivity of membrane proton based on the properties of the structure is one of the parameters required to have a deeper insight into the PEMFC function. The fuel cell pack consisting of all the elements like cathode, gas diffusion layers, anode, catalytic layers, membrane, and flow channels have been examined in most modeling processes. Currently a great deal of research works has been conducted to reduce the limitations and price simultaneously. Although significant advances have been made in recent years to improve the total performance of fuel cell, of water transfer issue is accompanied by heat transfer [2,3].

In 2007, a model based on two phases were introduced for a PEMFC working at high temperature. The model had met all the polarization and transfer phenomena with a great consistency with lab data at temperature range of 150 to 170 °C.

In an account of the fuel cell dependence on catalyst activity, membrane doping surface, and supplying dissolved gases to the electrolyte medium, it was found that key limitations of transfer existed in the two electrodes when the use of catalyst is between 0.1 to 1%. It is worth. This means that at high temperature, there is a risk or membrane drying, which leads to a lower ionic conductivity, higher and higher thermal stresses, and rupture of membrane eventually [4]. However, at lower temperatures, the rate of the reaction decreases and the losses inside the cell increase. In addition, a decline in the temperature of cell decreases the pressure of saturation and this increases distillation of water and leads to floating. Thus, there are restrictions in terms of temperature in fuel cell in both directions of increasing and decreasing and less variation in cell temperature could be desirable. Other important issues in this regard are using fuel cell in ambient condition in a car, diverse operation condition, and wide changes in the operating temperature of fuel cell, small temperature difference in the environment and the fuel cell, which is not comparable to that of internal combustion engine, and challenges of keeping the fuel cell cool, and desire to use inlet gases with low moisture to lower the power needed to keep the inlet gases humid [5-10].

It is necessary to study the inlet conditions and its effect on the performance of the fuel cell input and other functional factors such as flow rate. There have been several studies on diverse fuel cells to and performance of fuel cell. Specifically, the cell membrane characteristics, the effect of inlet temperature, electrochemical poles, and humidity [6-8]. The purpose of analyzing fuel cell systems is studying different fuels, examining hybrid systems using fuel cell, examining functional variables like pressure and their and temperature effect on performance, and develop an optimized system to lower the weight and price. There are studies as well on diagrams of current-voltage of fuel cell mass for use in the vehicle [1-10].

To evaluate the fuel cell mass in these studies, each cell piece in the fuel cell has not been studied, because of the complexities of the system, long calculation, and the role of hard mass in each other. As a result, researcher have to consider restrictions like fixed cell temperature. The effects of flow channel geometry were examined by Lobato et al. using a 3D model for PEMFC and three diverse geometries of four-stage parallel, helical, and pin type flow channel. A specific density of current is assigned to each geometry, which indicated а direct dependency of the distribution of current density on the reactant's diffusion method on the electrode surface [6]. Based on the model, it was predicted that parallel flow channels exhibit a lower efficiency. due to the presence of preferred paths that cause the reactive gases fail to have a good distribution on the entire electrode surface. The role of gas inlet intensity and temperature was examined in this study. The model also showed better performance of fuel cell with higher temperatures [7]. As to steady and transient behavior of PEMFC, a 1D dynamic isotherm model was introduced. Transient mass transfer of components of bipolar plates was taken into account by the model along with gas diffusion layers and discharging electric double layers. As well, the behavior of the fuel cell in the steadystate and the resistance spectra were obtained in this study [11].

Literature survev revealed that some researchers have modeled PEMFC and determined the factors influencing fuel cell efficiency such as operating conditions, gas flow rate, and flow channel geometry [12-18]. Thus, we need an accurate mathematical model to estimate performance of cell and manage water and heat in a PEMFC. In addition, the role different parameters like relative pressure, humidity, temperature on fuel cell performance must be examined using such models. Here, an model and membrane efficient proton conductivity condition was introduced as a function of diverse variable and management of water and health in polymer fuel cell using sulfone polymers-based membranes.

2) Polymer Membrane Fuel Cell

Currently, scientific research works are conducted on the commercial scale production of PEMFCs. Some authors have used renewable sources of energy as a fuel to lower pollutions. The membrane in such designs is polymer based and transfer protons generated in the anode to cathode. Thus, the membrane must be a good proton conductive medium. The PEM fuel cell functions consists of fuel (hydrogen) ethanol, formic acid, and methanol solution entering the anode and oxidized into protons and electrons or other products like carbon dioxide. The overview of a PEMFC is illustrated in Fig.1.

Hydrogen is oxidized at the anode, which is shown as follows:

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

Following oxidation, the proton moves to the cathode using the polymer membrane while the electron moves to the cathode using the outer circuit. Through adding air or oxygen to the cathode, a reaction takes place on the cathode catalyst surface, which yields water.

$$\frac{1}{2}O_2 + 2H^+ + 2e \tag{2}$$
$$\Rightarrow H_2O$$

The cell's lifespan is higher than 5×10^5 hours (as the cell's temperature growth, the longevity of the cell decreases). Furthermore, the density of the output flow exceeds that of all cells we know. Therefore, the PEMFC is the most commonly used cell for small electrical appliances and vehicles. Generally, around 50% of the power is available at ambient temperature and it reaches it max power in just three minutes. The heat created by the cell can be further used to warm up a room or water [19].



Figure 1: Overview of a PEM fuel cell

3) Fuel Cell Vehicle System

To generate mechanical force, we need more than a fuel cell. Figure 2 illustrates a schematic of a vehicle powered by a fuel cell system. These vehicles are used electrical engines that are operating with alternating current. The direct current type of electrical energy from a fuel cell cannot be used to run an engine. Thus, the current must be converted into alternating form using an inverter converter. After that, the engine can be started to move the vehicle.



Figure 2: Fuel cell vehicle system.

4) Mathematical Equations

4.1) Equations Governing Species Transport

Air, oxygen, or hydrogen is feed to cathode and anode flow channels. To obtain the molar rate of oxygen and hydrogen to the cathode and anode, the following equations can be used [3].

$$\dot{N}_{Q_2}^{cell} = \frac{S_C A_{cell} \overline{I}}{4\Gamma} \tag{3}$$

$$\dot{N}_{H_2}^{\dot{c}ell} = \frac{S_a A_{cell} \overline{I}}{2F} \tag{4}$$

where, S_a is the anode stoichiometric coefficient, S_c is the cathode stoichiometric coefficient, A_{cell} is the cross-section, I represent the current density, and F represent the Faraday constant. Further, $\dot{N}_{H_2}^{cell}$ and $N_{O_2}^{cell}$ are molar flow rate of input to flow channels for hydrogen and oxygen, respectively.

The density of current in a polymer fuel cell with steady state is given through the transport rate of the species taking part in the reactions. That is, the density of current can be obtained using the rate of oxygen/hydrogen fuel transport from anode and cathode flow change to reaction sites [2]. Taking into account the cross-section dimensions cathodes and anode flow channels are in millimeters, a small concentration gradients can be expected for diverse types of the gase phase in y,z direction, which is negligible. Thus, the gradients of concentration for diverse types of gas phase are only needed for direction x. Assume x as a point in Fig.3, where the production/consumption rate of the species in the reaction and the local current density, I, is obtained as follows:

$$\frac{dN_i}{Dx} = \xi_i \frac{wI(x)}{4F} \tag{5}$$

where, N_i is the molar flow rate related to species i, *w* is the channel width, I(x) is the local current density, and ξ_i represent the stoichiometric parameter related to the local species [2].



Figure 3: Schematic of a cell in a fuel cell [2].

4.2) Flood State Equations

The volume of water in liquid form obtained in a polymer fuel cell and the flooding condition are functions of the difference of water saturation pressure (P_W^{sat}) and partial pressure of water vapor (P_W^V) in the cell.

Vapor condensing happens in the cavities in the gas flow distributor when water vapor partial pressure is higher than the pressure of water saturation. In the same way, when water vapor partial pressure is less than the saturation pressure of water, the liquid form water in cell is evaporated and turns into water vapor. Thus, the occurrence of two-phase conditions flooding state in the cathode/anode flow channels is a function liquid form water in the channels and vapor form water that enter and leave the membrane, which is obtained as follows [2,12].

$$\frac{dN_{w,k}^i}{dx} = \left(\frac{k_c wh}{RT}\right) \left(P_W^V - P_{w,k}^{sat}\right) \tag{6}$$

$$\frac{dN_{w,a}^{\nu}}{dx} = -\frac{dN_{w,a}^{L}}{dx} - w\frac{aI(x)}{F}$$
(7)

$$\frac{dN_{w,c}^{\nu}}{dx} = -\frac{dN_{w,c}^{l}}{dx} + w\frac{(1+s\alpha)I(x)}{2F}$$
(8)

So that, v represent the vapor phase index, lrepresents the liquid phase index, w is the water index, 2 represents the universal gas represents constant. ? constant of homogeneous for rate condensation/evaporation of water, and h is the channel height, [2]. The process of condensing water vapor occurred at interface 24 of gases diffusion layer (GDL) and the catalytic, which forms droplets of water in the empty pores of the layer. These liquid droplets reached the boundary of move along the airflow and the GDL-flow channel inside the channel. Regarding capillary forces, liquid water is moved to the pores of the gas diffusion layer. Based on Darcy's law, we can calculate the liquid water velocity in the gas flow distributor layer N_w^i . Therefore, we have:

$$v_i = -\frac{k_w}{\mu w} \nabla P_i \tag{9}$$

$$N_w^i = -\frac{p_w k_w}{M_w \mu_w} \nabla P_I \tag{10}$$

where, P_I is the liquid water pressure, k_w is the liquid water permeability in the GDL, μw is the viscosity of liquid water viscosity, p_w is density of liquid water, and M_w is the molecular weight of water [2].

4.3) Governing Equations of Cell Electrochemistry

A cell's output voltage, *Ecell*, in a polymer fuel cell can be achieved by deducting the value of potential drop in the cell from the amount of cell open-circuit voltage. Now, we have:

$$E_{cell} = E_{oc} - \eta_{act} - \eta_{ohm} - \eta_{conc}$$
(11)

where *Eoc* is the open-circuit voltage (v). Moreover, η_{act} , η_{ohm} , and are the η_{conc} ohmic activation overpotential (v), overpotential (v), and concentration overpotential (v), respectively. The voltage of open-circuit is given as follows:

$$E_{oc} = 1.229 - 0.85 \times 10^{-3} (T - 298.15)$$
(12)
+ 4.31
× 10⁻⁵T(lnP_{H₂}
+ 0.5lnP_{O₂})

where, P_{O_2} and P_{H_2} are partial pressures related to oxygen and hydrogen. Through omitting the activation overpotential of the anode, we can utilize equation (13) to omit the activation overpotential of cathode:

$$\eta_{act}(x) = \frac{RT}{0.5F} ln\left(\frac{I(x)}{I_0 P_{o2}^{cat}(x)}\right)$$
(13)

where, I_0 is the exchange current density in a reference pressure (A/m^2) and P_{o2}^{cat} is the oxygen partial pressure in the catalytic layer (Pa) [2]:

$$P_{0_2}^{cat}(x) = C_{02}^{cat}(x)RT$$
(14)

where, C_{o2}^{cat} is the oxygen concentration at the catalyst level, which is pertinent to the concentration of oxygen in the flow channel $C_{0_2}^{bulk}(x)$:

$$C_{0_{2}}^{cat}(x) = C_{0_{2}}^{bulk}(x) - \frac{l(x)}{4F} \left(\frac{1}{h_{02}} + \frac{t_{GDL}}{D_{02-g}^{eff}}\right)$$
(15)

where, h_{02} is the oxygen mass transfer coefficient and D_{02-g}^{eff} is the effective diffusion coefficient of oxygen in a mixture of gases. The later coefficient is needed for transferring oxygen within pores of the gas diffusion layer. The cathode and anode flow channels in polymer fuel cells have a square cross-sectional area and the fluid flows steadily within these channels [2].

The amount of membrane conductivity is:

$$k_m(x) = (0.5139\lambda_m)$$
(16)
- 0.3260)exp $\left[1268(\frac{1}{303} - \frac{1}{T}) \right]$

With a given voltage, the mean current density of a polymer fuel cell, \overline{I} , is calculated through integrating the value of local current density, I(x) along the flow channel.

$$\bar{I} = \frac{1}{L} \int_{0}^{L} [1 - \bar{S}(x)] I(x) dx$$
(17)

4.5) Equations Governing Thermal Energy

As to the millimeter dimension of the anode and cathode current channels cross-section, the temperature gradient created in directions y and z in a current channel is small and can be neglected. The general equation controlling the thermal energy in a flow channel in a polymer fuel cell is [2]:

$$p_{mix}C_{p,mix}v_x\frac{\partial T}{\partial x}$$

$$= k_{mix}\frac{\partial^2}{\partial x^2} + Q_{total}^{source}$$
(18)

where, p_{mix} is the gaseous mixture density, $C_{p,mix}$ is the gaseous mixture heat capacity, v_x is the flow velocity of gas in \mathbb{Z} direction, and k_{mix} is the thermal conductivity of gas mixture. Furthermore, *T* is the gas flow temperature and *Qsource* is all exchanged/produced/consumed heat energy. Regarding the reaction in a polymer fuel cell, we consider that the generate water is liquid. In addition, desorption/ absorption heat of water molecules at the electrode surface should be considered. The balance of the gas phase (excreted) and the liquid phase (absorbed) at the two phases interface governs the absorption phenomenon. The changes in the enthalpy affect the absorption heat, which can be obtained using equation (19):

$$\Delta H_{sorp} = \Delta H_{H_{20,ad}}^f - \Delta H_{H_{20,ad}}^f$$
(19)
$$- \Delta H_{H_{20,gas}}^f$$

According to previous research, the enthalpy of water absorption in Nafion 117 changes by varying the membrane hydration degree. Recently, experiments have been performed on Nafion 112 and their values were highly similar to that of latent heat of water [11]. It is not easy to determine the energy generated by a polymer fuel cell and the electrochemical reactions. Generally, the energy level electrical work is obtained using enthalpy or entropy changes in electrochemical systems. This research uses entropy changes to determine the amount of heat created in the reaction. The entropy of species *i* with pressure of P and temperature of *T* is obtainable as follows (20):

$$S_{i}(T,P) = S_{i}^{O} + \int_{T_{0}}^{T} \frac{C_{p,i}}{T} dT + \int_{P_{0}}^{P} (-\frac{\partial v_{i}}{T}) dP$$
(20)

where, v_i represents species i the specific volume and S_i is the absolute entropy of species \square under standard conditions of $T_0 = 298.15 K$ and $P_0 = 1 bar$.

While, there is a specific entropy change related to the overall reactions occurring in a polymer fuel cell, it is not easy indicate to which part of the entropy, the cathode half-reaction or anode half-reaction is related. In the case of anode and cathode electrodes, the entropy values are used in thermodynamic equilibrium equations for charged species, and these values have been determined with approximate values in other studies. That is, it is not possible to create a cationic solution empty of entropy ions. Assuming that the water obtained is liquid in the reactions, the desorption/ absorption of water molecules heat at the electrodes surface must be included in the consideration. Using Equation (21) it is possible to determine the total heat created/used in the anode and cathode flow channels [13,2]:

$$Q_{total}^{C} = Q_{sorp}^{c} + Q_{cond/evap}^{C}$$

$$+ Q_{reac}^{C} + Q_{act}^{c} + Q_{conv}^{c}$$

$$Q_{total}^{a} = Q_{sorp}^{a} + Q_{cond/evap}^{a}$$

$$+ Q_{reac}^{a} + Q_{conv}^{c}$$

$$(21)$$

$$+ Q_{reac}^{a} + Q_{conv}^{c}$$

5) Results and Discussion 5.1) Solution

In this research, the system consisted of liquid and gas phases on the two sides of the cathodes and anode. In addition, the flow regime in the flow channels was steady type. The gas phase on the cathode is a mixture of nitrogen, water vapor and oxygen and the gas phase are mixture of water vapor and hydrogen on the anode side. The liquid phase on the two side of anode and cathode is water. The dimensions of the gas flow channels is millimeter range. Different types of production-consumption heat in the cathode and anode positions (such as halfreactions heat, absorption/desorption heat, activation heat, etc.) and water flood conditions are taken into account. Consequently, the fuel cell performance was investigated. The flow channels were networked by the quadratic method and based on the finite difference method the equations were discretized numerically for a steady-state. Eventually, the equations were solved in MATLAB. The bipolar plates consist of several gas flow channels in the fuel cell, which are called grooves, and oxygen and hydrogen gases enter these grooves.

A spiral form was assumed for the flow channels in this simulation. As illustrated in Figure 4, the bipolar plane is featured with grooves. Ws and Wg represent the height and width of the bipolar plate, respectively. The flow channels have a rectangular cross-section. In addition, the cross-sectional area is represented with a Hg and Wg. To solve the governing equations using numerical methods, we need to network the geometry of the problem. Takin into account the dimensions of the flow channels, which are in millimeters, we can simplify the geometry of the problem from a 3D state into a 1D state because of the trivial changes of the variables in the two directions. Having the nodes number, the flow channels are networked. The min nodes number is a number that does not change significantly the results if the number of nodes exceeds that limit.



Figure 4: A schematic of a bipolar plane with grooves

Table 1: Names and types of some parameters used
in modeling

Number	Variable name	Parameter type
1	Groove and bipolar plate dimensions	Constant
2	nodes number	Variable
<u>∠</u>		Vallable
3	The temperature of cathodes and anode and cathode bipolar plate membrane, surface, and electrode	Variable
4	Thickness, weight, and porosity of dry membrane anode and	Constant
5	cathode heat transfer and the diffusion coefficient	Constant

5.3) Numerical Pattern Validation

The simulation results showed that cathode activation heat, anode half-reaction heat, and the anode absorption heat are positive, and the desorption/absorption cathode heat and half-reaction heat are cathode negative. Ultimately, the amount of all heat declines along the flow channel. By examining the effect of inlet pressure, it is clear that an increase in the pressure improves cell performance at low current density, although the performance deteriorates at high current density. The study of the effect of relative humidity shows that increasing the cathode relative humidity trivially affected cell performance, while an increase in the anode relative humidity can improve cell performance [12-15]. Figure 6 shows the cell voltage diagram based on current density average, which is related to the results of this programming. Table 2 provides the data on program information/input parameters that are set in the Input Variables section of the program. Figure 6 also demonstrates the diagram of cell voltage based on current density average taken from experiments.

	p	
Parts	Parameter	Amount
	w	1(mm)
	h	1(mm)
	Sc	1.8
Flow	Sa	1.2
channel	T_c^{in}	70(°C)
	T_a^{in}	70(°C)
	RH_a^{in}	1.0
	RH_c^{in}	1.0
Membran	+	0.1 (mm)
e	ι _m	0.1 (11111)
Bipolar	W	10(cm)
plates	L	10(cm)

Table 2: Values considered for 'Input Variables'

Comparing Figures 5. highlight that the general trend of these two graphs corresponds well with the experimental results. Further, changes in current density affect oxygen distribution and vice versa, i.e., the slope of changes in oxygen concentration along the channel is similar to changes in current density. The difference between model and laboratory results is related to activation losses and ohmic losses, model accuracy as well as experimental tests accuracy. Voltage drop is observed more rapidly.



Figure 5: Cell voltage diagram in terms of current density provided (Model and Experimental results) [24].

Table 3: Cell	voltage in terms of current density
provided	Model and Experimental results)

Current DENSITY	Cell Voltage	(v)
(A/cm²)	Experimental results	Model results
0	1.07	1.08
0.1	0.8	0.86
0.2	0.77	0.83
0.3	0.74	0.80
0.4	0.7	0.72
0.5	0.65	0.65
0.6	0.6	0.58
0.7	0.54	0.5
0.8	0.48	0.41
0.9	0.4	0.33
1	0.24	0.1

5.4) Effect of Inlet Temperature

The temperature of surface of the electrodes and bipolar plates on the two sides of anode and cathode are assumed as constant. Whereases, the temperature of polymer fuel cell ranges from 65 to 120°C. Therefore, the constituent elements of the cell are assumed to have the same range of temperature [20]. The distribution of cell temperature might be affected by changes in current density as the key source of heat in the polymer membrane cell is caused by the electrochemical reactions heat and the fact that such reactions are irreversible. The heat is also a function of the density of current based on Eq(22). Given that rate of the generation of local heat along with the channel decreases, it can be said that the generation rate of the heat and the channel decreases. In addition, the max heat level happens close to the inlet of the cathode channel. Changes in the temperature along the channel are listed in Table 4. As we move to the end of the channel, a decline in the temperature takes place and the highest temperature appears in all sections at the interface between the catalyst layer and the membrane. The highest temperature of the anode is 83°C and along the channel it declines to 78°C The temperature on n the cathode demonstrates a different trend so that it declines to 58°Cat first and then rises to around 62°C Thus, the mean temperature on the cathode side is lower than that of the anode side. The observed change in the temperature is significant mostly when the cells are in serial arrangement.

Table 4: The temperature changes along the channel

x/L	Temperature(C)	
	T in Cathode	T in Anode
0	73	73
0.2	54	83
0.4	55	79
0.6	57	78
0.8	60	77
1	61	76

At medium densities of current with considerable drops of ohm in fuel cell, an increase in the temperature raises the membrane ionic conductivity and increases the performance of cell. With high densities of current, temperature increases lead to an increase in vapor pressure, which stops the negative influence of flotation on the performance of cell. With higher temperatures (90 °C); while the increase in temperature of cell lowers the transfer losses and increases the rate of electrochemical reactions, the cell potential decreases because of small increases in water vapor pressure and the membrane dry out. In addition, with drying, the ionic conductivity decreases and thermal stresses incrases; which results in rupture of membrane [24]. Thus, the diagram of performance is tests only at 82°C and lower.

5.5) The Effect of Humidifying The Inlet Gases

Note that the inlet gas flow should be humidified because of the operating conditions of the polymer fuel cells. The relative humidity in these cells for the fed gases into the cathode and anode flow channels is normally assumed in 70-100%. The inlet gases pressure also must be the same or slightly difference as high differences in pressure increases the risk of damage to the components of the cell on anode and cathode sides [13]. It is also assumed that the fuel fed to the cathode flow channel is a mixture of nitrogen, oxygen, and water vapor. In some cases of fuel cell, humid air is fed to the cathode and anode channels to make sure of hydration and minimize the ohmic loss in the membrane. In this case, the gas entering the cathode electrode becomes extremely saturated during the operation and floating might happen with very small current densities. Moreover, the

expense of humidifying inlet gas and power needed must be taken into account [19].

Recently, there has been a tendency to use low relative humidity at the cathode inlet in the industry. Tables 5 and 6 show the quality of water vapor relative humidity in the cathode and anode flow channels. Clearly, there is a fast decrease in the relative humidity on the anode side along the flow channel and at its beginning and then, decreases with a more balanced trend. Still, the relative humidity remains saturated on the cathode side. The water condenses when its concentration passes the saturation concentration and liquid is formed. In the case that the input gases are totally humidified, condensations initiate at the start point of the channel and water vapor condensation starts all over the cathode gas diffusion layer. Through closing the pores of gas diffusion layer, floating happens at the layer resulting in decreasing the rate of electrochemical reactions and a decline in the performance of the cell [24].

x/L	Relative humidity and quality	
	Quality of	RH of Cathode
	Cathode	
0	1	1
0.2	0.95	1
0.4	0.88	1
0.6	0.83	1
0.8	0.74	1
1	0.65	1

Table 5: Quality of water vapor and relative humidity in the cathode flow channels

Along the growth in the density of current, a decrease happens in the performance because of the higher moisture content. With increase in the inlet humidity, flotation happens on a wider area of the cathode gas diffusion layers. However, flotation happens on the gas diffusion layer of cathode when the input gases are thoroughly wet.

The pores of gas diffusion layer are blocked by this phenomenon and thus the level oxygen reaching gas diffusion layer decreases, which results in a decline in the performance of cell. Because the power of cell is outcome of voltage multiplied by current density, these phenomena affect the diagram of power density in the same way. In addition, the highest power is achievable when the cathode has a weak relative humidity [24,25].

x/L	Relative humidity and quality	
	Quality of Anode	RH of Anode
0	1	1
0.2	1	0.67
0.4	1	0.65
0.6	1	0.64
0.8	1	0.63
1	1	0.59

Table 6: Quality of water and relative humidity and vapor in the anode flow channels

5.6) Reynolds Number

Inertial to viscous forces ratio, as indicated by the Reynolds number, is created by fluid motion. Since the turbulence or stratification of a flow depends on these forces, we can use the Reynolds number to determine the regime (stratification or turbulence) of a flow. It is predicted that the size of fuel cells will decrease in the future and the Reynolds number of flows in cooling channels will reduce as well. A decrease in the Reynolds number hurts the cooling of the cell. As shown in Table 7, it is observed that the flow number is steady on the anode side and the flow is not disturbed in all channels on the anode and cathode sides. The difference of the minimum surface temperature and maximum temperature declines in all models along with an increase in inlet Reynolds. With higher concentrations, the parameter ΔT becomes a specified number for all models, which is a function of the Reynolds number.

Table 7:	Reynolds	number	of flows.
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x/L	Reynolds number of flow	
	Re of Cathode	Re of Anode
0	590	100
0.2	610	100
0.4	611	100
0.6	612	100
0.8	613	100
1	614	100

6) Conclusions

The modeling introduced in this work includes diverse types of production-consumption heat in the cathode and anode positions (e.g. activation heat, half-Reaction heat, absorption/desorption heat) and the condition of waterflooding to examine the fuel cell performance. To network the flow channels a quadratic method was used. In addition, based on the finite difference method, the equations were discretized numerically in a steady-state. Then, the equations were solved in MATLAB. According to the simulations results:

Anode half-reaction heat. the anode absorption/desorption heat. and cathode activation heat were positive. In addition, cathode half-reaction heat the cathode absorption/desorption heat were negative. Along the flow channel, there was a decrease in anode half-reaction heat, the amount of anode absorption/desorption heat, and cathode activation heat. Relative humidity effect showed that the cathode relative humidity does not change significantly along the flow channel. In addition, the relative humidity of anode declined along the flow channel. There was a significantly lower velocity in the membrane layer compared to that of reactant (cathode) layers and gas diffusion, which was because of lower permeability coefficient of the layer. The velocity was expanding at the star point of the channels.

List of Symbols

E	Cell voltage
D	Infiltration coefficient
GDL	Gas penetration layer
H_g	Groove depth
I_ave	Average current density
К с	Constant condensate / water
K_L	evaporation rate
L	Bipolar plate height
Р	Pressure
S	Stoichiometric coefficient
RH	relative humidity
Т	Temperature
W	Bipolar plane width
W_g	Groove width
W_s	The width of the solid part
Ecell	Cell voltage
К	Hydraulic permeability
T_c^{in}	Cathode inlet temperature
T_a^{in}	Anode inlet temperature

P_a^{in}	Anode inlet pressure
P_c^{in}	Cathode inlet pressure
Р	Density
σ	Surface tension
ν	Cinematic viscosity
T_s^c	Cathode surface temperature
T_e^a	Anode surface temperature
T _{mem}	Membrane temperature
t _m	Membrane thickness
+	The thickness of the gas
lGDL	penetration layer

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مدلسازی و شبیه سازی پیل سوختی غشا پلیمری مورد استفاده در خودرو پیل سوختی

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چکیدہ

اطلاعات مقاله

تاریخچهٔ مقاله: دریافت: ۲۸ مهر ۱۴۰۰ پذیرش: ۱۳ تیر ۱۴۰۱ *کلیدواژهها:* خودرو سامانه پیل سوختی مدل سازی

پیل سوختی بهترین پیشنهاد برای جایگزینی موتورهای درونسوز میباشد. سیستمهای پیل سوختی هیچ گونه آلودگی نداشته و اجزای متحرک ندارند. بازده پیلهای سوختی بیش از سه برابر موتورهای درونسوز است. مدلسازی رفتار پیل سوختی غشای تبادل پروتون دارای پیچیدگیهای ویژهای می-باشد و تعیین عملکرد آن بر حسب ویژگیهای ساختاری آن یکی از پارامترهای مورد نیاز برای شناخت بیشتر رفتار پیلهای سوختی غشای تبادل پروتون میباشد. در این مطالعه، یک نوع پیل سوختی غشا پلیمری برای کاربرد در خودرو تحلیل گردید. در این مدلسازی، انواع حرارتهای تولیدی-مصرفی در سمت های آند و کاتد (از قبیل: حرارت نیمواکنشها، حرارت اکتیواسیون، حرارت جذب/دفع و ...) لحاظ گردید و تحت این شرایط عملکرد پیل سوختی بررسی شد. نتایج حاصل از شبیهسازیها نشان داد که مقدار همهی احرارتها در طول کانال جریان کاهش پیدا میکند (با متوسط عدد رینولدز ۲۱۲). بررسی تاثیر رطوبت نسبی نشان داد که رطوبت نسبی آند در طول کانال جریان کاهش میباید .سرعت در لایه غشا به دلیل کوچکتر بودن ضریب نفوذپذیری این لایه نسبت به لایه های پخش گاز و واکنشگرها (کاتد) بسیار کمتر می باشد.



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