



A two-phase, non-isothermal model for water management in the cathode gas diffusion layer of polymer electrolyte membrane fuel cells

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Abstract

Water management is essential because of its effect on the performance and durability of polymer electrolyte membrane (PEM) fuel cells. This paper uses a non-isothermal two-phase model to study the flow in the cathode gas diffusion layer (GDL) of a PEM fuel cell. For this purpose, the conservation equations of mass, momentum, energy, and other auxiliary equations have been solved numerically and validated with data available from papers with an error of less than 2%. The results show that the pressure variation of the gas mixture (P_g) along the cathode GDL is negligible, while the capillary pressure (P_c) is significant. An increase in the pressure of the cathode channel as well as the porosity of GDL leads to an increase in the concentration of oxygen in the cathode catalyst layer, but by increasing the porosity coefficient of the electrodes from 0.4 to 0.7, the effective thermal conductivity of the fuel cell decreases and the maximum temperature of the fuel cell increases by about 1K. The flow of liquid water and the consequent saturation are higher in the vicinity of the cathode catalyst layer, but due to evaporation, their amount decreases as the channel approaches. In the current density range of $0.6 < j < 1 \text{ A/cm}^2$, the α parameter (which is defined as the ratio of the water entering from the membrane to the catalyst to the water produced due to the reaction) tends to a constant value of 1.2

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1. Introduction

The adverse environmental impact of fossil fuels and their role in the greenhouse effect and pollution are still being studied by governments. Hydrogen, an alternative fuel that can be prepared from renewable and non-renewable energy sources, and fuel cells, efficient and environmentally friendly energy-converting devices with a wide range of applications, can be promising fuel alternatives for the future. Among the different types of fuel cells, PEM fuel cells are considered a suitable option for use in cars and portable devices due to their high power density, low emissions, low operating temperature, maintenance, and low noise [1, 2]. Despite these advantages, heat and water management is challenging in this type of fuel cell. The presence of liquid water plays an essential role in increasing the ionic conductivity of the polymer electrolyte membrane, as well as reducing the initial energy required to activate the electrochemical reaction of hydrogen and oxygen in the catalysts [3]. On the other hand, the presence of liquid water partially fills the pores of the electrodes and increases the resistance to mass transfer, reducing the fuel cell's performance. The filling of the electrode pores with liquid water is called water flooding, a harmful phenomenon that can occur with high current density in the cathode electrode and low current density in the anode electrode [4].

During the operation of the PEM fuel cell, the heat produced by the electrochemical reaction in catalyst layers, the heat generated by the transfer of electrons and ions from the electrodes and membrane, respectively, and the latent heat caused by the condensation and evaporation of water lead to the temperature gradient in the PEM fuel cell. Operating at high temperatures reduces water absorption in the fuel cell membrane and thus reduces its durability. In addition, as the temperature increases, the voltage and ideal efficiency of the fuel cell decreases. In contrast, working at low temperatures reduces the kinetic rate of electrochemi-

cal reactions. Moreover, working at low temperatures reduces the water saturation pressure and consequently increases the possibility of water flooding. As a result, water and heat management play an influential role in the performance and durability of PEM fuel cells [5].

In the past decades, several single-phase models have been studied to investigate the performance of PEM fuel cells [6-9]. For example, Bernardi et al. [6, 7] were among the first one-dimensional single-phase and isothermal models published in the 1990s. In these models, it was assumed that the liquid water flows through the small pores of the electrodes and the gas mixture flows through the larger pores. Therefore, liquid water and steam flow in separate paths, so there is no contact and mass exchange between them. Also, Rowe and Li [8] investigated the performance of polymer fuel cells in a one-dimensional, single-phase, and non-isothermal model. Djilali and Lu's model [9] is one-dimensional, single-phase and non-isothermal. Their results show that the gas pressure along the GDL is negligible compared to liquid water. In addition, the effect of temperature gradient and pressure gradient on mass penetration is insignificant. These models are simple and provide valuable information to help understand the phenomena in the polymer fuel cell; however, the results of these models are not compatible with the experimental results [10] in the range of practical current density and higher. Therefore, it is necessary to model the flow, especially on the cathode side, in a two-phase manner.

In the past decade, different two-phase models have been published with different levels of complexity, each of which has studied the PEM fuel cell from a specific aspect, some of which are mentioned here. Pasaogullari and Wang [11] presented a two-phase and analytical model to investigate the effect of flooding on oxygen transfer and fuel cell performance. The results show that water flooding has a significant effect on reducing oxygen concentration and fuel cell performance. Khajeh-Hosseini et al. [12] presented a

one-dimensional and isothermal model of the cathode side of a PEMFC (including cathode GDL, cathode catalyst layer, and membrane) to investigate water management problems. Their results show that electro-osmotic drag contributes to the net water flux transported through the membrane, and the amount of water condensation becomes much greater at the GDL/CL interface than in other regions of GDL. Habibalahi et al. [13], investigated water management in the cathode GDL using the Lattice-Boltzmann method. Results show that using hydrophobic GDL with a porous gradient accelerates water drainage, but this model is isothermal.

Zhan et al. [14] investigated the importance of the non-uniform distribution of the porosity coefficient in the GDL in a two-phase, isothermal, and one-dimensional model. In this research, the effect of two-phase contact is considered with α assigned a hypothetical value and the effect of mass exchange between the two phases in the GDL ignored. Hu et al. [15] presented a two-phase model of a polymer fuel cell. These researchers have considered only the contact effect in their model and have drawn the fuel cell polarization diagram for two temperatures of 323 K and 353 K. The strength of that article was that it presented the three-dimensional modeling of fuel cells; however, their modeling was done with the assumption of constant temperature, and the effect of pressure changes on both sides of the cathode and anode was not investigated. Yu and Liu [16] investigated the phenomenon of water transfer in different fuel cell components in a two-phase, isothermal, and two-dimensional model. In that research, a range of current densities in which the catalyst layer remains unused was presented, and the effect of pressure on the output voltage of the fuel cell was investigated. In their modeling, the researchers considered the effect of contact caused by the occurrence of a two-phase flow but neglected the effects of mass exchange between the two phases. In addition, their modeling cannot investigate the effects of temperature in gradient parts of the fuel cell because

it is isothermal.

Pasaogullari and Wang [17] compared two methods of two-phase flow modeling in GDL. The UTF method was based on the assumption of constant pressure in the gas phase. The method was obtained from the reformulation of the usual models, in which instead of solving two sets of equations of motion for the liquid and gas phases, one set of equations is solved. In this model, the mass exchange between the two phases is ignored, and they assign α as a hypothetical number. Das et al. [18] investigated the water flow in the cathode catalyst layer of a polymer fuel cell in a two-phase, one-dimensional, and transient model. The effect of the contact angle on the water flow in the catalyst layer, which has not received much attention before, was investigated; however, this analytical model is based on many simplifying assumptions. In this model, a hypothetical value for α is used. Baschuk and Li [19] investigated the effects of variable degrees of water flooding in the cathode catalyst layer and/or cathode GDL on cell performance. The results show that the flooding of the cathode GDL and catalyst layer increases the resistance to mass transfer, and as a result, the oxygen concentration in the reaction sites decreases.

In addition to the contact effect, Song et al. [20] have considered the effect of mass exchange between two phases of gas and liquid in two-phase and non-isothermal modeling. The assumption of instability in modeling distinguishes this research from other discussed models. In this research, the parameter β is defined as the ratio of water vapor entering the GDL to the total water entering, and the effects of variation β in the modeling were investigated.

Vynnycky [21] presented a new two-dimensional and two-phase model by considering both contact and mass exchange effects. Assuming thermodynamic equilibrium between the gas and liquid phases, he defines a quantity called δ as a place in the GDL where the phase change stops. Therefore, by writing single-phase flow equations for the single-phase re-

gion and two-phase flow equations for the two-phase regions, the accuracy of the modeling has been increased. However, the complexity of meshing is one of the research's weak points. In all the above models, in addition to the mentioned cases, only the cathode GDL has been modeled; therefore, approximate boundary conditions have been used for modeling.

Yu and Liu [22], in a two-phase, isothermal, and two-dimensional model, considered the equations of water transport in different components of a fuel cell and investigated the effect of increasing current density on parameters such as oxygen concentration, membrane water content, and output voltage from a fuel cell. In this research, the value has been calculated for the specific current density at the boundary of the membrane and the catalyst layer. This research considers the effect of contact between two phases, but the effect of mass exchange between two phases is ignored. Hassanzadeh et al. [23, 24] presented a two-phase model in which contact and mass exchange effects are considered. Also, due to the importance of the exact value of α on the water content of the membrane and the ohmic drop, they calculated a relatively accurate value for it by modeling other fuel cell components. However, the disadvantage of this model is that it is constant temperature and constant pressure. Hassanzadeh and Golkar [25] modeled and optimized a non-isothermal two-phase flow in the cathode GDL of a PEM fuel cell and found the optimal values of porosity, electrode thickness, and relative humidity in an essential condition by optimization algorithms.

Zhao et al. [26] recently presented a one-dimensional, two-phase, non-isothermal model to investigate the performance of a PEM fuel cell, in which a semi-implicit algorithm was used to increase the execution speed of the SIMPLE algorithm. This model has been validated with good accuracy by data from an automobile manufacturer. Some of the results show that it is necessary to use the two-phase model to study the

performance of the fuel cell at the high relative humidity of reactants, but in low relative humidity, two single-phase and two-phase models provide the same results. Due to the importance of increasing computational efficiency, a one-dimensional, two-phase, non-isothermal model was recently presented by Pan et al. [27]. The new model is two orders faster than conventional one-dimensional models with an error of less than 4%. Ijaudola et al. [28] published a paper on the effect of flooding in polymer fuel cells that operate at relatively low temperatures, in which they investigated the effect of water accumulation on the cathode and anode side and on the performance of the fuel cell, in addition, provides methods to prevent flooding and proper management in PEM fuel cells. Rahmani pour and Harleh [29] presented a three-dimensional model and investigated the effect of the contact angle on water management in a polymer fuel cell. The results show that higher GDL liquid removal values lead to better water management, and the highest amount of water removal occurs at an angle of 102.63.

As seen, several articles have been published in the field of two-phase flow in PEM fuel cells; however, all aspects have not been considered and simplifying assumptions have been used in the modeling. In this article, the non-isothermal two-phase flow in the cathode GDL is modeled, and the effect of liquid water presence and non-uniform temperature distribution on fuel cell performance is investigated. In order to use accurate boundary conditions at the interface between the cathode catalyst layer and the cathode GDL, as well as to determine the relatively accurate value of α , other PEM fuel cell components are also modeled. In addition to the effect of contact and mass transfer between the two phases, this modeling considers the positive effect of the pressure difference between the two channels, as well as the effect of temperature, pressure, and saturation on fluid properties on fuel cell performance.

2. Two-phase flow in the cathode GDL

In two-phase flow modeling, liquid water and gas mixture are in contact with each other, and this contact affects both the movement and mass exchange between the two phases. The effect of the contact of two phases and the mass exchange between them distinguishes two-phase modeling from single-phase modeling. The following assumptions were used to derive the governing equations:

The flow is steady state, incompressible, and non-isothermal.

- The GDL is uniform and homogeneous.
- A gas mixture is ideal.
- The amounts of gases dissolved in water are negligible.

2.1 Mass conservation equations in the cathode GDL

Figure 1 shows the schematic of the cathode GDL. According to the figure, moist air enters from the channel, and liquid water enters from the catalyst layer.

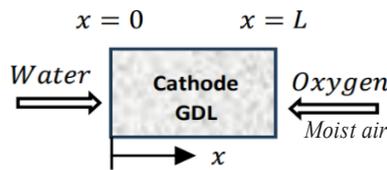


Fig. 1. Schematic of the cathode GDL.

The moist air entering the GDL contains oxygen, nitrogen, and water vapor. In the steady state condition, the oxygen molar flux in the GDL is constant and depends on the current density. So, the oxygen molar flux is equal to:

$$N_{o_2} = \frac{J}{4F} \tag{1}$$

Because oxygen is not consumed along the GDL, its mass flux is also constant and its gradient is equal to zero:

$$\nabla \cdot (M_{o_2} N_{o_2}) = 0 \tag{2}$$

Oxygen is not consumed in the cathode GDL, so the net flux due to its convection and diffusion is constant, and its flux gradient is equal to zero:

$$\nabla \cdot (\rho_g U_g Y_{o_2} - \varepsilon \rho_g (1-s) \nabla Y_{o_2}) = 0 \tag{3}$$

In this relation, ρ_g is the density of the gas mixture, U_g is the apparent velocity of the gas mixture in the GDL, Y_{o_2} is the mass fraction of oxygen, ε is the porosity of the GDL (which is defined as the ratio of the volume of the pores space to the total volume of the electrode), s is the saturation quantity (which is defined as the ratio of the volume of liquid water in the pores of the GDL to the total volume of the pores), and $D_{eff}^{o_2}$ is the effective diffusion coefficient of oxygen in the porous medium, which is modified as follows by considering the porosity and the saturation amount in the GDL [20]:

$$D_{eff}^{o_2} = D_{mix}^{o_2} (\varepsilon(1-s))^{1.5} \tag{4}$$

In this equation, $D_{mix}^{o_2}$ is the diffusion coefficient of oxygen in a gas mixture in a non-porous medium, which depends on temperature and pressure as follows [1, 20]:

$$PD_{mix}^{o_2} = 0.1775 \times 10^{-4} (T / 273.15)^{1.823} \tag{5}$$

Unlike oxygen, the mass flux of water vapor in the cathode GDL is not constant (due to mass exchange

with liquid water), and its gradient is equal to:

$$\nabla \cdot (M_{H_2O} N_{H_2O}) = -\dot{m}_{H_2O} \quad (6)$$

Where \dot{m}_{H_2O} is the mass rate of water vapor per unit volume that has turned into liquid water. \dot{m}_{H_2O} is a function of saturation, the mole fraction of water vapor, and gas mixed pressure.

At any point of the GDL that $\dot{m}_{H_2O} \geq x_{H_2O}^{sat}$ condensation occurs, the rate of which is equal to [21]:

$$\dot{m}_{H_2O} = k_{cond} \varepsilon (1-s) \frac{M_{H_2O} P_g}{RT} (x_{H_2O} - x_{H_2O}^{sat}) \quad (7)$$

Also, at any point of the GDL that $x_{H_2O} \leq x_{H_2O}^{sat}$ evaporation occurs, the rate of which is equal to [21]:

$$\dot{m}_{H_2O} = k_{vap} \varepsilon s \rho_L p_g (x_{H_2O} - x_{H_2O}^{sat}) \quad (8)$$

In these relations, the quantities k_{cond} , k_{vap} , ρ_L and $x_{H_2O}^{sat}$ are the condensation constant of water vapor, the evaporation constant of water, the density of liquid water, and the mole fraction of water vapor in saturation, respectively. The mole fraction of water vapor in the saturated state is calculated from the following equation [20]:

$$x_{H_2O}^{sat}(T, atm) = \exp(13.3815t - 1.9760t^2 - 0.6445t^3 - 0.1299t^4) \quad (9)$$

In this relation, $t = 1 - 373/T$.

In the cathode GDL, the flux of liquid water is not constant due to mass exchange with water vapor, and its gradient is equal to:

$$\nabla \cdot (\rho_l U_l) = \dot{m}_{H_2O} \quad (10)$$

2.2. Momentum conservation equations in the cathode GDL

Darcy's relation can be used to calculate the velocity of liquid water in a porous media [2]:

$$U_l = -k_{abs} (\nabla \cdot \rho_l) / \mu_l \quad (11)$$

In this relation, U_l , P_l , and μ_l are the apparent velocity (volume flow rate per unit surface area), pressure, and absolute viscosity of liquid water, respectively. The viscosity of water depends on temperature and is expressed as follows [20]:

$$\mu_l = 0.6612(T - 229)^{-1.562} \quad (12)$$

In the Darcy relation, k_{abs} represents the absolute permeability of the porous medium, which is an inherent property of the porous medium and is independent of the type of fluid passing through it.

In the two-phase flow in a porous medium, part of the pores is filled by gas mixture and part by liquid water. The presence of gas in the pores affects the movement of liquid water, so Darcy's equation is modified by the saturation quantity, s [20]:

$$U_l = -k_{abs} s^3 (\nabla \cdot \rho_l) / \mu_l \quad (13)$$

In the same way, for the gas phase, we can write:

$$U_g = -k_{abs} (1-s)^3 (\nabla \cdot \rho_g) / \mu_g \quad (14)$$

The mass flux of the mixed gas is equal to the sum of the mass flux of its component species. Therefore, for the gas mixture on the cathode side, which includes oxygen, nitrogen, and water vapor species, U_g is equal to:

$$U_g = \frac{1}{\rho_g} (M_{O_2} N_{O_2} + M_{N_2} N_{N_2} + M_{H_2O} N_{H_2O}) \quad (15)$$

Nitrogen is not consumed, so its flux is zero. Assuming that the gas mixture is ideal, the density of the gas mixture can be calculated from the perfect gas equation:

$$\rho_g = P_g \frac{M_g}{R_u T} \quad (16)$$

Where R_u and M_g are the universal gas constant and the molar mass of the mixed gas, respectively. Nitrogen and oxygen, as well as water vapor, are present in the cathode GDL, whose mass fraction varies along the GDL, so the molecular mass of the gas mixture M_g is calculated as follows:

$$M_g = \left(\frac{Y_{O_2}}{M_{O_2}} + \frac{Y_{N_2}}{M_{N_2}} + \frac{Y_{H_2O}}{M_{H_2O}} \right)^{-1} \quad (17)$$

In this relation, M_i and Y_i represent the molecular mass and mass fraction of the gas species i , respectively. To determine the apparent velocity of liquid water, U_l , it is necessary to first calculate the pressure distribution P_l . Since the radius of the pores in the GDL is about micrometers, the effect of the capillary pressure P_c is significant. As a result, the determination of pressure P_l requires determination of capillary pressure. Therefore, it is necessary to calculate the capillary pressure first. Capillary pressure refers to the pressure difference between the liquid phase and the gas phase in paths with a small diameter, which is expressed as follows:

$$P_c = P_g - P_l \quad (18)$$

Leverett's empirical relation is used to calculate capillary pressure in a two-phase flow. Leverett's relation expresses the relationship between capillary pressure and saturation value. In addition to the amount of saturation, the capillary pressure also depends on the porosity and the contact angle of liquid water with the surface [2].

$$P_c = \delta \cos \theta \left(\frac{\epsilon}{k_{abs}} \right)^{0.5} j(s) \quad (19)$$

Where θ is the angle that the water drop makes with the surface, according to Figure 2, it is $\theta > 90^\circ$ for hydrophobic surfaces and $\theta < 90^\circ$ for hydrophilic surfaces.

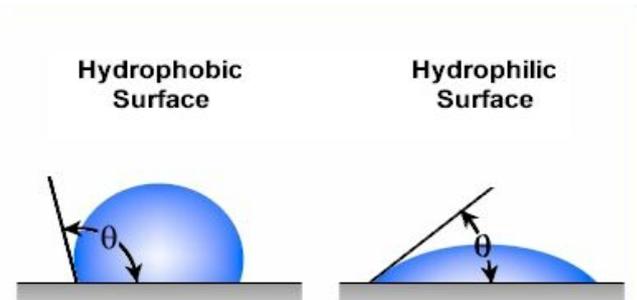


Fig. 2. Contact angle on hydrophilic and hydrophobic surfaces.

In hydrophilic environments, capillary pressure is positive; in hydrophobic environments, its value is negative, increasing with increasing contact angle. In hydrophobic surfaces, the saturation distribution is lower than in hydrophilic surfaces, and this justifies the waterproofing of the GDL with Teflon because less saturation quantity reduces the possibility of flooding in GDL.

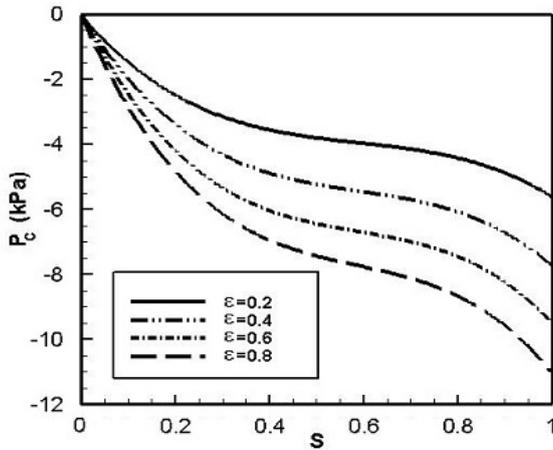


Fig. 3. Capillary pressure variation curve with saturation in a hydrophobic medium.

Figure 3 shows the curve of capillary pressure variation for saturation quantity in a hydrophobic environment. It is clear that the value of capillary pressure increases with decreasing porosity.

In Leverett’s relation, the surface tension δ is dependent on temperature and is expressed as a relation (20):

$$\delta = -1.78 \times 10^{-4} \times T + 0.1247 \tag{20}$$

In Lorette’s relation, $j(s)$ is a quantity that depends on saturation quantity, and for hydrophilic surfaces ($\theta > 90^\circ$) is calculated from equation (15) [2]:

$$j(s) = 1.417(1-s) - 2.21(1-s)^2 + 1.263(1-s)^3 \tag{21}$$

And if the surface is hydrophobic ($\theta < 90^\circ$), $j(s)$ is calculated from equation:(16)

$$j(s) = 1.417(s) - 2.21(s)^2 + 1.263(s)^3 \tag{22}$$

2.3. Energy conservation equation for the cathode GDL

According to Figure (4), the energy conservation equation is obtained by choosing a control volume and specifying the energy transfer processes in the GDL. In the GDL, heat is transferred through convection and conduction. Also, heat is generated due to the electron transfer and phase change, so these two factors are finally considered as two heat sources in the energy equations of the cathode GDL.

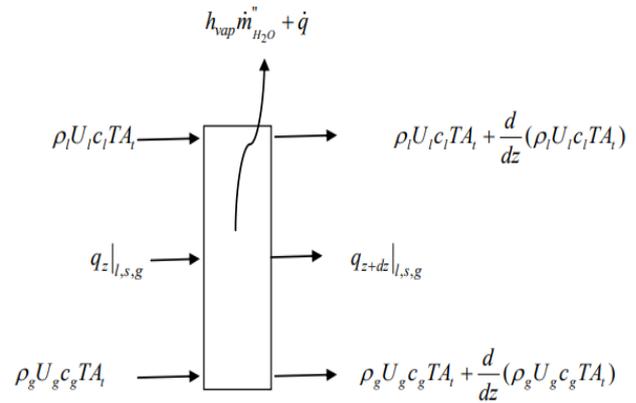


Fig. 4. Control volume in the cathode GDL.

Finally, the energy equation is obtained by writing the energy balance equation for the control volume and simplification.

$$\nabla \cdot \left[-(s \epsilon k_l + (1-s) \epsilon k_g + (1-s) k_g) \nabla T \right] + \left[\rho_l U_l c_l + \rho_g U_g c_g \right] \nabla T = h_{vap} \dot{m}_{H_2O} + \dot{q} \tag{23}$$

In this equation, h_{vap} is the enthalpy of evaporation, which is equal to the difference between the enthalpy of liquid water and water vapor:

$$h_{vap} = h_g - h_l \tag{24}$$

Evaporation enthalpy is a function of temperature and is expressed as follows [20]:

$$h_{vap} = 3.0709 \times 10^{-4} (647.15 - T)^{0.35549} \quad (25)$$

\dot{q} in the energy equation is also a heat production source due to ohmic loss, which is calculated as follows:

$$\dot{q} = j^2 / \sigma_e \quad (26)$$

In this relation, σ_e represents the electrical conductivity of the solid phase of the cathode GDL.

In the energy equation, the quantities k_g , k_l and k_s are the thermal conductivity of the gas, liquid, and solid phases, respectively. Also, c_g and c_l are the specific heat capacity of gas and liquid water phases are calculated as follows [20]:

$$c_l = -4.0699 \times 10^{-8} (T - 273.15)^5 + 1.3113 \times 10^{-5} (T - 273.15)^4 - 1.629 \times 10^{-3} (T - 273.15)^3 + 1.0536 \times 10^{-1} (T - 273.15)^2 - 3.2989 (T - 273.15) + 4216.4 \quad (27)$$

The specific heat capacity of the gas mixture is calculated based on the mass fraction of the species in the gas mixture [20]:

$$c_g = c_{O_2} Y_{O_2} + c_{H_2O} Y_{H_2O} + c_{N_2} (1 - Y_{O_2} - Y_{H_2O}) \quad (28)$$

In the same way, the thermal conductivity of the gas mixture is calculated by the mass fraction of the species in the gas mixture [20]:

$$k_g = k_{O_2} Y_{O_2} + k_{H_2O} Y_{H_2O} + k_{N_2} (1 - Y_{O_2} - Y_{H_2O}) \quad (29)$$

For accurate modeling of the cathode GDL, other fuel cell components such as anode GDL, membrane, and

catalyst layers have also been modeled. However, in the practical current density ranges, the flow in the anode GDL is a single phase. As a result, the flow in the anode GDL is modeled as a single phase.

3. Solution method and validation

3.1. Boundary conditions and solution method

The present model is a non-isothermal two-phase model. In order to accurately determine the amount of water entering the cathode GDL and using more accurate boundary conditions, other fuel cell components (membrane and anode GDL) have also been modeled. In the practical current density range, the flow in the anode electrode is single-phase, so the flow in the anode electrode is modeled as single-phase. According to the scope of the solution, the boundary conditions have been applied only at the interface of channels and the cathode and anode GDLs. Based on this, accurate boundary conditions at the interface of the cathode GDL and the membrane are obtained to model the two-phase flow of the cathode GDL.

The temperature at the interface of the channel and the cathode GDL is considered to be 333K. In order to know the exact amount of saturation in the interface between the channel and the cathode GDL, it is necessary to model the flow in the cathode channel. However, considering that the flow in the gas cathode channel is not modeled in the current research, a hypothetical value of 0.05 has been attributed to saturation in this boundary.

The molar flux of water vapor in the interface between the channel and the cathode GDL is unknown; therefore, it is necessary to assign a value to it as an initial educated guess. The correctness of this guess is determined by the molar flux of water in the interface between the membrane and the cathode GDL. In addition, it is necessary to determine the temperature

gradient at the interface between the channel and the cathode GDL. By assigning an initial educated guess to it, the boundary conditions on the cathode side are completed. The correctness of this guess is determined by calculating the temperature at the interface between the anode channel and the anode GDL.

The finite difference method has been used to solve the governing equations of fuel cell components. Derivatives in the equations are converted to a numerical code in Fortran using the first-order Taylor progression method and integrals using the method of the sum of the product of the term inside the integral in the spatial step.

3.2. Validation

In Table 1, the values of the quantities in the primary condition are given.

Table 1. Modeling Base Values [20]

| | | |
|----------------------------------|-------------------|-----|
| Working temperature | T (k) | 333 |
| Anode and cathode pressure | P (atm) | 1 |
| Relative humidity of the cathode | RH (%) | 85 |
| Relative humidity of the cathode | RH (%) | 75 |
| Membrane thickness | t_m (μm) | 175 |
| Thickness of electrodes | t_e (μm) | 300 |
| Contact angle | θ° | 110 |
| Porosity coefficient | ϵ | 0.4 |

To validate the numerical solution, according to Figures (5) and (6), the temperature distribution curves and saturation quantity in the GDL cathode have been compared with the numerical solution results of Song et al., and the results have good accuracy.

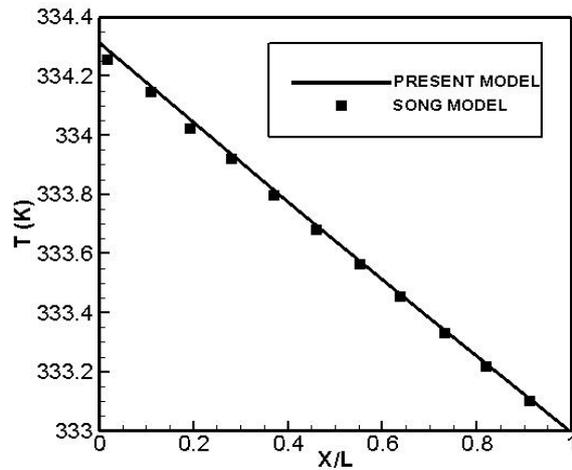


Fig. 5. Comparing the present numerical results for temperature with the results of Song et al.[20].

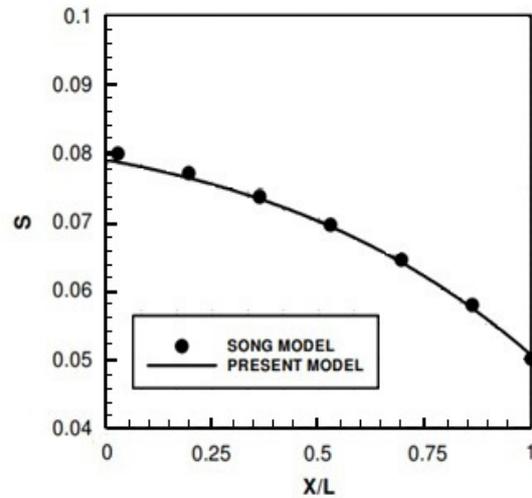


Fig. 6. Comparing the present numerical results for the saturation with the results of Song et al.[20]

4. Results and discussion

This paper investigates the effect of various factors on the amount of liquid water in the cathode GDL. The distribution of liquid water in the GDL is affected by various factors, which can be referred to as current

density, operating temperature of the fuel cell, pressure and relative humidity in the cathode and anode channels, porosity coefficient, etc. The impact of some of these parameters has been investigated in this section.

4.1. Effect of current density

As mentioned earlier, one of the features of the current research is the calculation of the coefficient α . The variation curve of the coefficient α for current density is drawn in Figure 7. As shown, with increasing current density, the coefficient α increases because as the current density increases, the rate of water transfer due to electroosmotic drag is higher than the rate of water production in the cathode catalyst layer. Therefore, the electroosmotic drag increases. An increase in electroosmotic drag is also associated with an increase in the coefficient α . Another essential point in this figure is that the coefficient α remains constant in the high current density because proton ions in the membrane can only carry a limited number of water molecules with them. Therefore, as the water content of the membrane increases at high current densities, the electroosmotic drag coefficient remains constant, which also leads to the constant coefficient α .

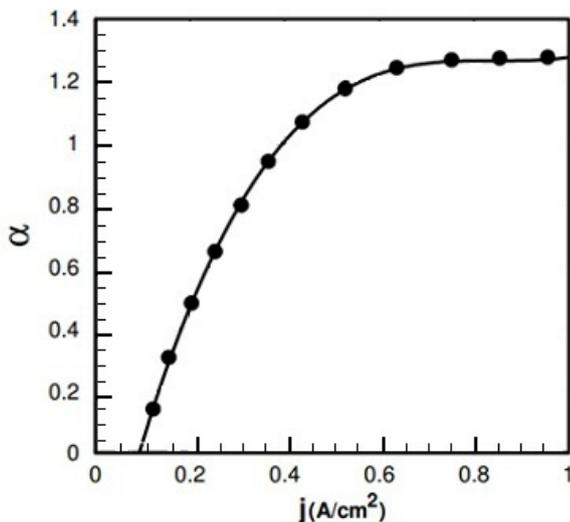


Fig7. Distribution curve of coefficient α with current density.

Figure 8 shows the liquid water flux distribution curve along the cathode GDL. According to the figure, the amount of liquid water flux is higher on the side of the cathode catalyst, and due to the evaporation of water, its amount gradually decreases as it approaches the cathode channel. As the current density increases, the amount of water produced and entering the cathode catalyst increases; therefore, the flux of liquid water exiting the catalyst increases. In addition, by increasing the current density, the temperature of the cathode catalyst also increases; however, its effect on water evaporation is not significant compared to the amount of liquid water entering the catalyst.

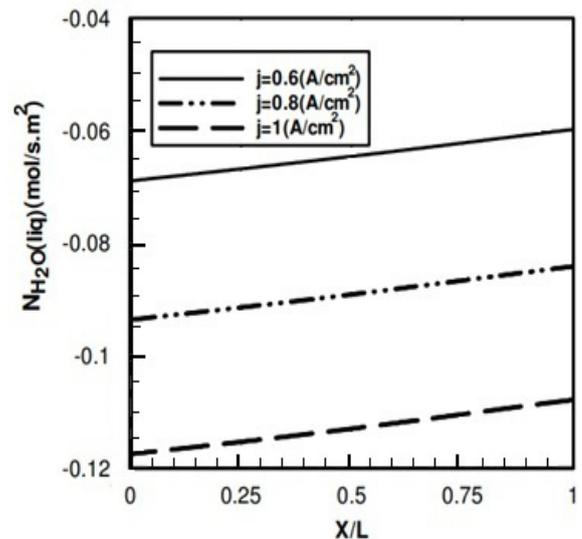


Fig.8. Liquid water flux distribution along the GDL cathode at different current densities.

Figure 9 shows the curve of the saturation value along the cathode GDL. According to the figure, the saturation value is higher in the vicinity of the catalyst layer. Due to the evaporation of liquid water, as it approaches the cathode channel, the saturation value decreases and finally reaches the value of 0.05 at the boundary. As the current density increases, the amount of water entering the cathode GDL increases, and more pores are filled with liquid water. As a result, the saturation value increases.

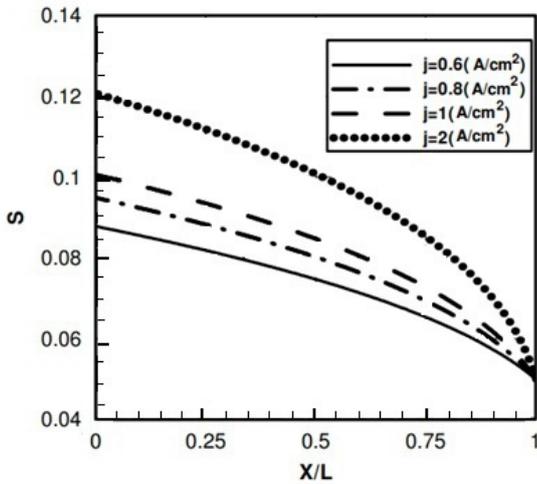


Fig. 9. Saturation distribution along the GDL cathode at different current densities.

Another point that can be seen about the coefficient α in Figure 10 is that the value of the coefficient α increases as the cell temperature increases because increasing the cell temperature increases the evaporation rate of liquid water in the cathode GDL. Therefore, the amount of liquid water in the interface of the membrane and the cathode catalyst layer decreases. This leads to an increase in the electroosmotic force, and as a result, the α coefficient slowly increases.

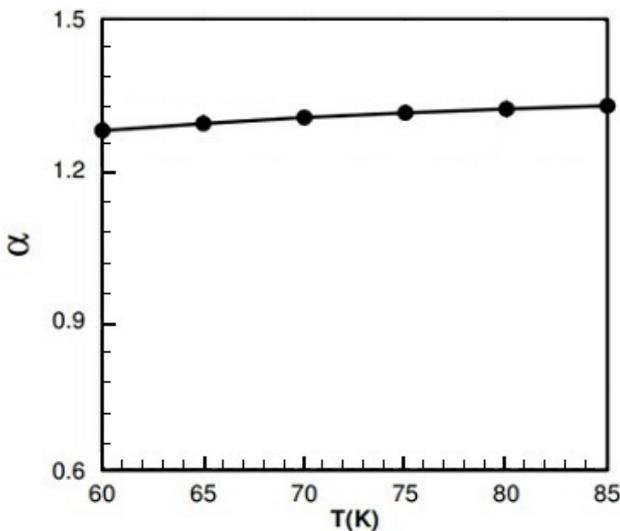


Fig. 10. Distribution curve of coefficient α at different fuel cell temperatures.

4.2. Effect of relative humidity variation in the cathode channel

As mentioned, the ionic conductivity of the membrane depends on its water content. Therefore, the reactants are humidified before entering the fuel cell. Figure 9 shows the variation curve of the water evaporation rate in the cathode GDL at different relative humidities of the cathode channel. It can be seen that when the relative humidity of air in the cathode channel increases, the evaporation rate decreases. In fact, increasing the relative humidity of the air in the cathode channel decreases the water vapor absorption capacity of the gas mixture in the cathode GDL. The changes in the evaporation rate curves at low relative humidity show that the water evaporation rate is lower near the channel and increases as it approaches the catalyst layer (where there is more liquid water). However, when the saturated air (100% relative humidity) enters the cathode channel, the evaporation rate is positive, indicating that condensation occurs along the entire length of the cathode GDL. Its rate also increases when approaching the cathode channel, which has a lower temperature and amount of liquid water.

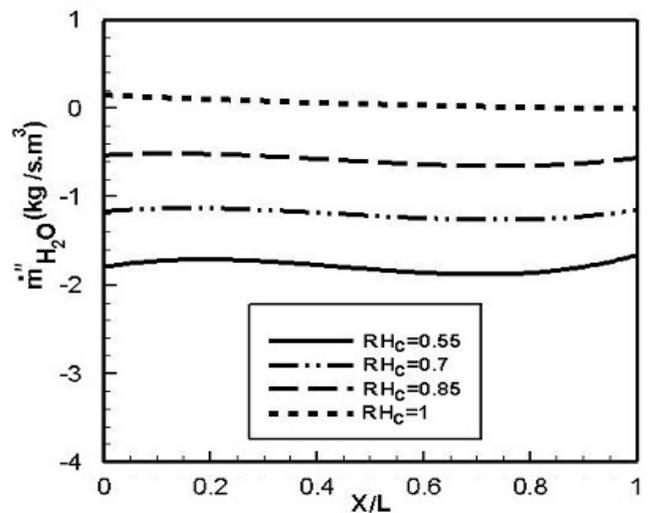


Fig. 11. Water evaporation rate curve along the GDL cathode at different relative humidities of the cathode channel.

As the relative humidity of the air in the channel increases, the rate of evaporation decreases, and as a result, the amount of water vapor entering the cathode GDL increases. Figure 12 shows the relative humidity variation of liquid water along the gas cathode GDL in different relative humidities of the air entering the cathode channel. According to the Figure, the increase in the amount of incoming water vapor due to the increase in the relative humidity of the channel has the dominant effect, and as a result, the relative humidity in the cathode increases. If the incoming air is extremely humid (100% humidity), the relative humidity will be greater than unity throughout the GDL of the cathode, and condensation will occur throughout it.

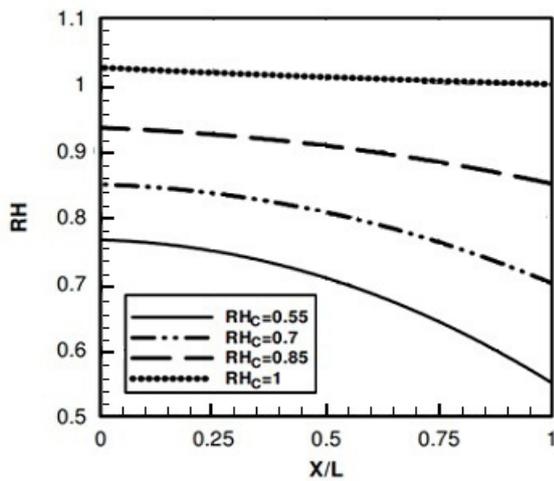


Fig. 12. Distribution of relative humidity along the cathode GDL for different relative humidities of the cathode channel.

4.3. The effect of the cathode GDL porosity

According to Figure 13, increasing the porosity coefficient of the cathode GDL increases the volume of empty spaces. As the volume of empty spaces increases, the resistance to oxygen mass transfer decreases, and as a result, the concentration of oxygen in the GDL increases. Due to the negligible changes in mixture gas pressure along the cathode GDL (according to Figure 12), the concentration of water vapor decreases with increasing oxygen concentration.

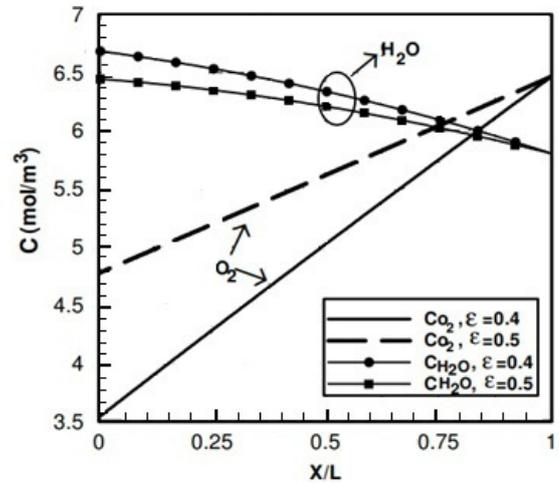


Fig.13 .Oxygen and water vapor concentration distribution along the cathode GDL at different porosity coefficients.

Figure 14 shows the gas mixture and capillary pressure changes along the GDL cathode. As seen, the gas pressure changes along the cathode GDL are insignificant, so the gas pressure can be assumed to be constant with high accuracy. The capillary pressure across the fuel cell's cathode is also negative, so water flows from the catalyst side to the cathode channel. Additionally, the negative capillary pressure due to the increase in the porosity coefficient shows that the water produced in the cathode catalyst is pushed toward the cathode channel with a higher pressure.

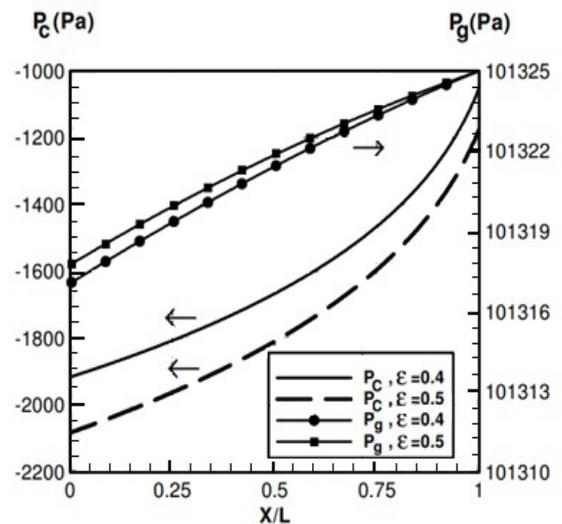


Fig. 14. Capillary and gas mixture pressure distributions along the cathode GDL at different porosity coefficients.

By increasing the porosity coefficient of the GDL cathode, the percentage of empty volume to the total volume of the GDL cathode has increased. Therefore, the value of the thermal conductivity coefficient is expected to decrease. According to the Fourier conduction law, it is expected that the temperature gradient in the fuel cell will increase as the thermal conductivity decreases. Figure 15 shows the temperature distribution curve throughout the fuel cell for different porosity coefficients. It can be seen that increasing the porosity coefficient will decrease the effective solid surface of the GDL and increase the resistance to heat transfer. As a result, the temperature difference between the cathode catalyst and the channel temperature increases.

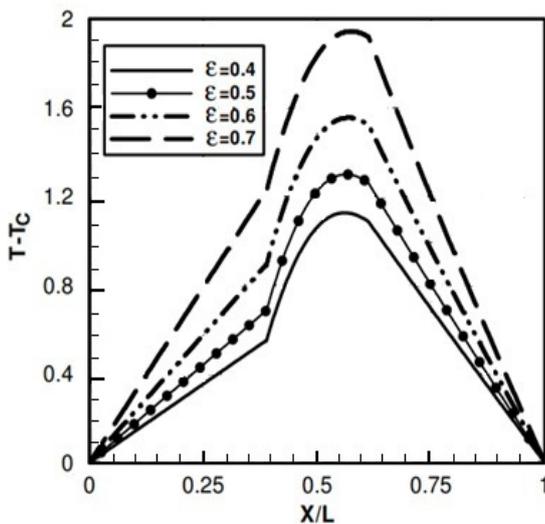


Fig. 15. Temperature distribution along the cell at different porosity coefficients.

4.4. Effect of the cathode channel pressure

It is clear that the lower the voltage loss, the higher the output voltage of the fuel cell. One of these factors is the slow reaction in the cathode catalyst layer, so the losses of the reduction reaction on the cathode side are significantly higher than on the anode side. Various factors affect the slow kinetics of the reduction reaction, one of which is the oxygen concentration in the reaction sites. The low oxygen concentration in the

cathode catalyst has various factors, one of which is using air instead of pure oxygen. Although using air instead of pure oxygen has a negligible effect on the reversible voltage, its effect on the reaction kinetics is significant. One way to increase the oxygen concentration is to increase the gas pressure in the cathode channel. Although increasing the pressure of the cathode channel does not change the oxygen concentration in the cathode channel much, it has two essential roles. Secondly, according to Henry's relation, the dissolution of oxygen in water depends on the pressure, which increases oxygen concentration in the reaction sites. As a result, the cathode activation loss decreases. Figures (16) and (17) show the curves of changes in oxygen concentration and water vapor concentration in the cathode GDL for different pressures in the cathode channel, respectively. The concentration distribution shows that with the increase of gas pressure in the cathode channel, the concentration of oxygen and water vapor increased along the cathode GDL, which caused an increase in the concentration of oxygen and water vapor at the place of the electrochemical reaction. Secondly, with the increase in the gas pressure of the cathode channel, the difference in the concentration of oxygen and water vapor in the infiltration layer of the cathode gas increased.

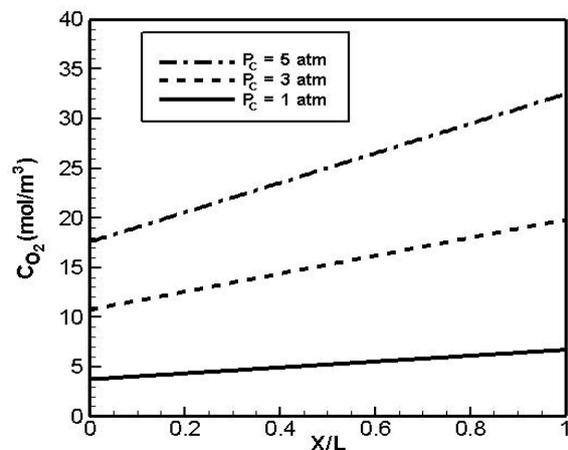


Fig. 16. Oxygen concentration distribution along the cathode GDL at different cathode channel pressures.

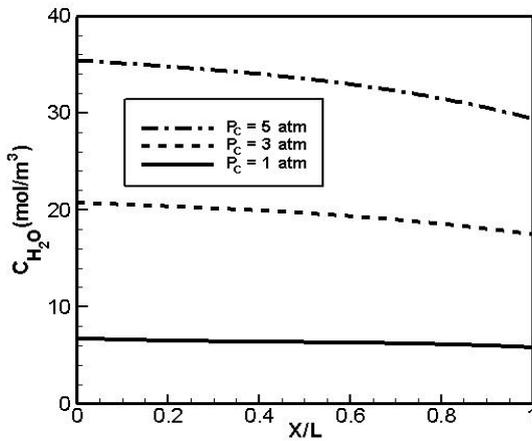


Fig. 17. Water vapor concentration distribution along the cathode GDL at different cathode channel pressures and anode pressure of 1 atm.

In Figure 18, the curve of variation of relative humidity in the cathode GDL is drawn for different pressures of the cathode channel. According to the Figure, as the gas pressure of the cathode channel increases, the amount of relative humidity in the cathode GDL increases. However, the changes from the pressure of 1 to 3 atmosphere are much greater than the increase in pressure from 3 to 5 atmosphere. Therefore, increasing the pressure more than this amount does not significantly affect the amount of moisture and only increases the sealing problems of the fuel cell components.

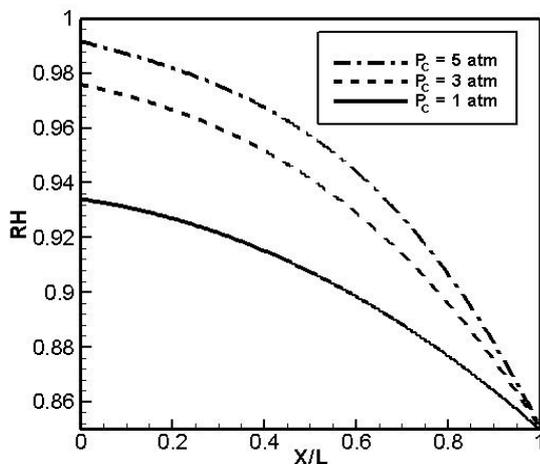


Fig. 18. Relative humidity distribution along the cathode GDL at different cathode channel pressures and anode pressure of 1 atm.

Summary and conclusion

This paper aimed to investigate the effect of different issues on the amount of liquid water distribution in the cathode GDL. The distribution of liquid water in the cathode GDL depends on various parameters. So, the effect of current density, cathode channel humidity, cathode channel pressure, and porosity coefficient on fuel cell performance was discussed. For this purpose, a non-isothermal two-phase model was used, and conservation and auxiliary equations were solved and validated. The results showed that it is necessary to control several factors simultaneously to manage water in the cathode GDL properly. Considering that both the humidity of the cathode channel and the transfer of water from the membrane to the catalyst and the temperature affect the amount of saturation in cathode GDL, it is necessary to control the other parameter by increasing each of these parameters to avoid the phenomenon of water flooding which prevents the transfer of gases reactants to the catalyst. Also, even though the gas and liquid water are in contact and exchange heat and mass, the gas pressure is constant throughout the GDL. However, the variation in liquid water pressure is significant due to surface tension. Increasing the porosity coefficient increases the concentration of oxygen in the catalysts, and due to the decrease of the effective thermal conductivity coefficient, the temperature of the cell increases.

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