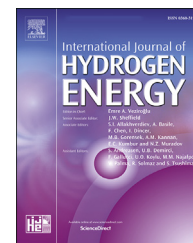


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Model based water management diagnosis in polymer electrolyte membrane fuel cell

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HIGHLIGHTS

- A modified segmented model for water management diagnosis in PEMFC is illustrated.
- Fuel cell performance and flow regime in channel is studied simultaneously.
- Pressure drop is as a criteria in diagnosis only at inlet saturated condition.
- Flow regime is main factor in water management diagnosis at low current density.

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ABSTRACT

Water management diagnosis in polymer electrolyte membrane fuel cell is of great importance. The water produced in the fuel cell affects its performance and lifetime through the current distribution and the two phase flow pattern in the channel. The aim of the present study is to modify a segmented model in order to investigate a model-based water management diagnosis at different operating conditions. Simulations are conducted in three current densities: low (0.2 A/cm^2), medium (0.6 A/cm^2) and high (1 A/cm^2), four temperatures ranged from 40 to 70, two stoichiometries (2 and 3) and four inlet humidities (25%, 50%, 75% and 100%). The results show that at fully saturation inlet condition, there is a uniform local current density for all three considered current densities. Also, two-phase pressure drop and output voltage have similar trends. Hence two phase pressure drop can be considered as a suitable criterion for water management diagnosis. At inlet humidities less than 50%, non-uniformity of local current density increases that leads to reduction of output voltage, especially at high current density. Generally, for non-saturated inlet condition, two phase pressure drop and output voltage may show different trends. Therefore, two-phase pressure drop can be used only as a criterion for the formation of water and not for water management diagnosis.

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Three main water flow regimes in PEMFC channels are mist, film and slug regimes in which pressure drop of two phase flow can be used to predict flow regime [9–11]. In addition to two phase pressure drop, visualization techniques have been used to study water content and flow regime in PEMFC [12]. Visualization of flow pattern in PEMFC has shown that in slug flow, PEMFC has an unstable behavior due to flooding in GDL and channel [13]. Based on two phase pressure drop, if its value exceeds a normal range, flooding is supposed to happen. However, drying of membrane is unpredictable in this approach. Therefore, a lower limit of two phase pressure drop can be considered to guarantee membrane humidification. Assessment of these upper and lower pressure drop limits in fuel cell has been the aim of several studies [7,8]. Hussaini and Wang [14] have investigated experimentally cathode side flooding using flow visualization technique. Their results show that flooding occurs when two phase pressure multiplier is greater than 3. Banerjee et al. [15] have examined experimentally the two phase flow pressure drop and have applied the pressure drop multiplier successfully to conduct water fault diagnosis. They have presented ranges of pressure drop multiplier in normal condition, flooding and drying out. However, due to difficulty and complexity in on-line experimental work in PEMFC, some researchers have been utilized simulation model to calculate pressure drop [8]. Almost all of the microscopic numerical simulations exert an interface capturing method to study the behavior of droplet [16,17]. Since electrochemical reactions are not considered in these microscopic models, straight relation between two phase pressure drop and cell performance cannot be obtained. In addition, the estimation of pressure drop in a cell or a stack using a CFD simulation is not practical because of its high computational cost [18]. Hence, a number of macroscopic

The main idea and novelty of this work is to develop a model which can consider simultaneously flow pattern in channels and fuel cell performance. To the best of our knowledge, our model can overcome weakness of other models and open a new insight in PEMFC diagnostic tools. Based on two phase pressure multiplier and flow map in channel, water management diagnosis in PEMFC is conducted.

The proposed model of Ref. [21] is modified in the present study in which active surface of PEMFC is divided into several segments that are connected based on the flow field. Properties of reactants and membrane are assumed to be uniform at each segment. The lumped method has been used along the channel while one-dimensional model has been applied perpendicular to the channel in the membrane. By solving governing equations of each segment, pressure, humidity, gas flow rate and water content have been calculated at the outlet of each segment which is implemented as the input of the later segment. Fig. 1 shows the connection between different segments for serpentine flow field. Co-flow arrangement is considered in the present study. Although in several previous studies [22], it is shown that a better uniformity of the current is obtained in counter-flow arrangement, since the main aim of the present study is to diagnose the water management in PEMFC, type of arrangement doesn't have any great effect on

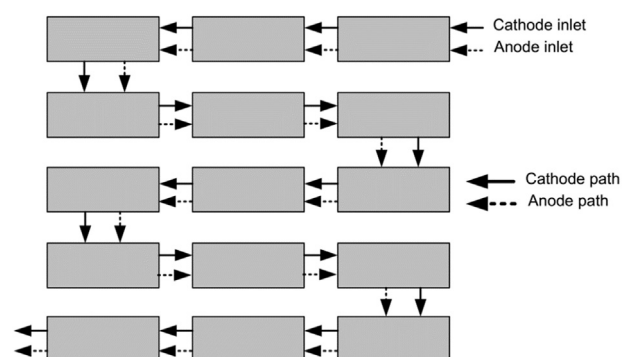


Fig. 1 – Schematic of connection of different segments in the simulation.

this aim. The governing equations of a single cell with constant temperature in steady condition are provided in the following section.

Channel equations

Gas and product water are exchanged between the channel and the GDL. The mass flow rate of each species at the outlet is calculated from the mass balance equation. As mentioned above, the liquid water in the channel can cover the interface between channel and GDL and hinder gas transport towards membrane. Two phase pressure drop in the channel is a function of channel water content. Hence, the flow regime in channel can be related to two phase pressure drop by the superficial velocity of each phase.

Mass balance equation

The molar flow rate of species at the outlet is calculated as:

$$N_{j,out} = N_{j,in} + N_{j,reaction} + N_{j,mem} \quad (1)$$

where j implies to hydrogen and water at the anode side and to oxygen, water and nitrogen at the cathode side. $N_{j,reaction}$ is a function of electric current in each segment, I_{seg} , and is given by:

$$N_{j,reaction} = \frac{I_{seg}}{nF} \quad (2)$$

where F is Faraday constant. n is stoichiometric coefficient that is equal to 2 for water and hydrogen and 4 for oxygen. Also, $N_{j,mem}$ is the transfer rate of water from the membrane to the channel and is calculated by the membrane model described in the following sections.

Two phase pressure drop

The produced water in the catalyst layer flows from GDL towards the channel and then discharges to the channel outlet. Although a portion of the water is evaporated with regard to cell temperature and inlet gas humidity, a considerable amount of water content remains in liquid form in channels. Therefore pressure drop must be calculated based on two phase flow correlations. According to Lockhart and Martinelli model [23], two phase flow pressure drop, $\left(\frac{dP}{dy}\right)_{TP}$, is related to

single phase flow pressure drop, $\left(\frac{dP}{dy}\right)_l$, by defining two phase multiplier, Φ_L , as follows:

$$\Phi_L = \sqrt{\left(\frac{dP}{dy}\right)_{TP} / \left(\frac{dP}{dy}\right)_l} \quad (3)$$

where single phase flow pressure drop is estimated by well-known Darcy–Weisbach equation [13].

For cases without heat transfer phenomena, Lockhart and Martinelli [23] have proposed Φ_L as follows:

$$\Phi_L^2 = 1 + \frac{C}{X} + \frac{1}{X^2} \quad (4)$$

where

$$X = \sqrt{\left(\frac{dP}{dy}\right)_l / \left(\frac{dP}{dy}\right)_g} \quad (5)$$

Also, C is Chisholm parameter which is equal to 5 for laminar flow [24]. Since water is added gradually to gas flow along the channel, the pressure drop can be viewed as a channel with water condensation. In these cases, Nelson–Martinelli's correlation [25] can be used to calculate pressure drop multiplier, Φ_{LO} , when both gas and liquid flow regimes are laminar.

$$\Phi_{LO} = \frac{\left(\frac{dP}{dy}\right)_{TP}}{\left(\frac{dP}{dy}\right)_{LO}} = (1 - \chi) \Phi_L^2 \quad (6)$$

where χ is the quality and $\left(\frac{dP}{dy}\right)_{LO}$ is pressure drop when mass flow flux of fluid is equal to the sum of mass flow flux of gas, G_g , and fluid, G_l . Assuming a linear variation of χ along the channel, the ratio of pressure drop is obtained from the following expression:

$$\frac{\Delta P_{TP}}{\Delta P_L} = \frac{1}{L} \int_{\chi_{inlet}}^{\chi_{outlet}} \Phi_{LO} dy \quad (7)$$

In the present study, the mass flow rate of gas and liquid is calculated by the mass balance equation in each segment. Therefore, the outlet quality can be estimated as:

$$\chi_{outlet} = \frac{G_{g,outlet}}{G_{l,outlet} + G_{g,outlet}} \quad (8)$$

As a result, two phase pressure multiplier in each segment and pressure of flow at the outlet can be calculated from Eqs. (6) and (7).

GDL equations

Gas diffusion layer has the role of exchanger of reactants, water and electrons between the channel and the catalyst layer. Stephen-Maxwell equation is used to describe the diffusion of multi-component gas mixtures in the GDL [26]. Mole fraction gradient of i th species is given by:

$$\nabla x_i = RT \sum_{j=1}^n \frac{x_i N_{j,gdl} - x_j N_{i,gdl}}{PD_{i-j}^{eff}} \quad (9)$$

where D_{i-j}^{eff} is effective diffusion coefficient of the mixture of two phase flow inside porous media that is linked with single phase flow inside non-porous media diffusion coefficient, D_{i-j} , as given in Eq. (10):

$$D_{i-j}^{eff} = D_{i-j} f(\epsilon) g(s) \quad (10)$$

where s is saturation and ϵ is porosity of GDL. $f(\epsilon)$ shows effect of the porosity on diffusivity, calculated using a polynomial relationship as follows:

$$f(\epsilon) = \epsilon^{1.5} \quad (11)$$

Effect of saturation on diffusivity is modeled by $g(s)$ function defined by a polynomial function as follow:

$$g(s) = (1 - s)^m \quad (12)$$

where $m = 2$ has been extracted from Ref. [27].

In saturated conditions, it is assumed that the steam pressures in the channel and in the porous layer are both equal to the saturation vapor pressure. The vapor pressure is proportional to the molar fraction; hence the molar fraction of water vapor in the GDL is equal to the mole fraction of saturated vapor.

$$x_{v,gdl} = \frac{P_{v,sat}}{P_{seg}} \quad (13)$$

Liquid water is driven by the capillary pressure through the GDL. Value of this capillary pressure is calculated by:

$$P_c = P_g - P_w = \sigma \cos(\theta_c) \left(\frac{\varepsilon}{K} \right)^{0.5} J(S) \quad (14)$$

where P_g and P_w are gas and water pressure within GDL, respectively. θ_c is the contact angle and K is permeability of GDL porous material. Surface tension, σ , between air and water has been considered to be 0.625 Nm^{-1} . Also $J(S)$ is Leverett's function, defined as [28]:

$$J(S) = 1.417S - 2.120S^2 + 1.263S^3 \quad (15)$$

where S is reduced water saturation, given by:

$$S = \frac{s - s_{im}}{1 - s_{im}} \quad (16)$$

In the above equation, s_{im} is the immobile saturation that is equal to 0.1 [5].

One dimensional transfer of liquid flow through porous layer from channel to membrane (z) due to capillary pressure, $N_{w,gdl}$, is defined by Ref. [28]:

$$N_{w,gdl} = - \frac{\rho_w K K_{rw}}{M_w \mu_w} \left(\frac{dP_c}{dS} \right) \frac{dS}{dz} \quad (17)$$

where ρ_w , μ_w and M_w and K are density, viscosity, molecular weight of water and absolute permeability, respectively. k_{rw} is relative permeability of GDL and is related to reduced water saturation as follows [28]:

$$K_{rw} = S^3 \quad (18)$$

$N_{w,gdl}$ is net water transferred between anode and cathode side through membrane calculated by membrane model. Also, in cathode side, produced water must be added to its value. Hence, by combining and solving Eqs. (14–18), variation of saturation in GDL can be obtained.

Membrane equation

Water transfer is carried out by two main phenomena of diffusion and electro osmosis through the membrane between anode and cathode. The transfer of the proton from the anode to the cathode results in the movement of water, known as electro osmosis drag modeled by:

$$N_{w,osmotic} = k_{osmotic} \frac{I_{seg}}{F} \quad (19)$$

where $K_{osmotic}$ is electro osmosis drag coefficient [18]:

$$K_{osmotic} = \frac{2.5 \lambda_{mem}}{22} \quad (20)$$

λ_{mem} is the water content in membrane and its value is a function of water activity, a_{mem} , obtained as:

$$\lambda_{mem} = \begin{cases} 0.043 + 17.8a_{mem} - 39.85a_{mem}^2 + 36.0a_{mem}^3 & 0 < a_{mem} < 1 \\ \frac{14 + 1.4(a_{mem} - 1)}{1 < a_{mem} < 3} \end{cases} \quad (21)$$

where a_{mem} is the average of water activity of membrane in both anode and cathode sides. Diffusion is another process that causes the transfer of water between anode and cathode sides. The rate of water transfer due to diffusion is a function of difference of dissolved water concentration in the nafion between anode and cathode, calculated by:

$$N_{w,diff} = K_{diff} \frac{C_{w,ca} - C_{w,an}}{t_{mem}} \quad (22)$$

where t_{mem} is the membrane thickness and C_w is the concentration of water, given by:

$$C_{w,i} = \frac{\rho_{mem}}{M_{mem}} \lambda_i \quad (23)$$

where i index refers to anode or cathode. Also M_{mem} and ρ_{mem} are membrane molecular weight and density, respectively. Diffusion coefficient of the membrane, K_{diff} , is a function of temperature and water content of membrane [29]:

$$K_{diff} = K_\lambda \exp \left(2416 \left(\frac{1}{303} - \frac{1}{T_{seg}} \right) \right) \quad (24)$$

where K_λ is:

$$K_\lambda = \begin{cases} 10^{-10} \lambda_{mem} < 2 \\ 10^{-10} (1 + 2(\lambda_{mem} - 2)) & 2 < \lambda_{mem} < 3 \\ 10^{-10} (3 - 1.167(\lambda_{mem} - 3)) & 3 < \lambda_{mem} < 4.5 \\ 1.25 \times 10^{-10} \lambda_{mem} & \lambda_{mem} \geq 4.5 \end{cases} \quad (25)$$

The net molar mass flux of water from cathode to anode, $N_{w,mem}$, is evaluated as:

$$N_{w,mem} = N_{w,diff} - N_{w,osmotic} \quad (26)$$

The specification of PEMFC used in this study is listed in Table 1.

Voltage calculation in each segment

Theoretical reversible voltage in the fuel cell, E_{rev} , is reduced due to activation overvoltage, V_{act} , ohmic overvoltage, V_{ohm} ,

Table 1 – Parameters of PEMFC.

Parameter	Value
Cell active area (cm^2)	100
Channel depth (mm)	1
Channel width (mm)	1.6
Rib width (mm)	1.7
Number of channel	6
Segment length (cm)	3.33
GDL thickness (μm)	184
GDL porosity	0.725
Dry membrane thickness (μm)	25
Dry density (kgm^{-3})	2000

and concentration overvoltage arising from lack of reactant gas in catalyst layer, V_{conc} .

$$V_{seg} = E_{rev} - V_{act} - V_{ohm} - V_{conc} \quad (27)$$

In a specific current, reversible voltage of each segment is calculated based on the partial pressure of hydrogen and oxygen, membrane water content and cell temperature, as follows [21]:

$$V_{rev} = 1.229 - 0.85 \times 10^{-3} (T_{seg} - 298.15) + 4.3085 \times 10^{-5} T_{seg} \left[\ln(P_{an,H_2,g/m}) + \frac{1}{2} \ln(P_{ca,O_2,g/m}) \right] \quad (28)$$

where T_{seg} is in Kelvin and $P_{an,H_2,g/m}$ and $P_{ca,O_2,g/m}$ are obtained from diffusion layer model in anode and cathode sides. The activation overvoltage is given by:

$$V_{act} = v_0 + v_a [1 - \exp(-c_1 i_{seg})] \quad (29)$$

where constants v_0 , v_a and c_1 are used from Ref. [30]. Also, the ohmic overvoltage is calculated by:

$$V_{ohm} = I_{seg} R_{seg} \quad (30)$$

where R_{seg} is sum of all internal resistances in the electron transfer pathway resulting from the gas diffusion layer, R_{gdl} , bipolar plates, $R_{bipolar}$, membrane, R_{pem} , and contact resistance, $R_{contact}$:

$$R_{seg} = R_{pem} + R_{gdl} + R_{bipolar} + R_{contact} \quad (31)$$

Because of high electrical conductivity of bipolar plates and GDL, their resistances are negligible. Also, R_{pem} is calculated by:

$$R_{pem} = \frac{t_{pem}}{\sigma_{pem}} \quad (32)$$

where σ_{pem} is conductivity of membrane that depends on temperature and membrane water content [18]:

$$\sigma_{pem} = (b_{11} \lambda_{pem} - b_{12}) \exp \left[b_{13} \left(\frac{1}{303} - \frac{1}{T_{cell}} \right) \right] \quad (33)$$

In Eq. (33) constants, b_{11} , b_{12} , b_{13} , are determined from experimental data [30]. In addition, the contact resistance, $R_{contact}$ is assumed 0.047Ω [21].

The concentration overvoltage is important only at high current density. Its value is a function of current density and water saturation calculated using modified empirical equation proposed in Ref. [31]:

$$V_{conc} = b_{21} i_{seg}^{b_{22}} \ln \left(1 - \frac{i_{seg}}{i_{limit}(1-s)} \right) \quad (34)$$

where the coefficients b_{21} , b_{22} and i_{limit} are reported in Ref. [21].

Results and discussion

Governing equations of each segment are solved in Matlab-Simulink software. In order to verify the present simulation, results for parallel channels in both sides are compared with those of Chen et al. [21] in the same conditions and equation constants in Fig. 2. As shown, a good agreement is obtained that emphasizes the accuracy of the present simulation.

Polarization curve

In order to comprehensive investigation, simulations have been carried out for three current densities including low ($0.2 \frac{A}{cm^2}$), moderate ($0.6 \frac{A}{cm^2}$) and high ($1 \frac{A}{cm^2}$), four different inlet relative humidities (case 1: both anode and cathode are 25%, case 2: both anode and cathode are 50%, case 3: both anode and cathode are 75%, case 4: both anode and cathode are 100%) and two different stoichiometries in the cathode side, 2 and 3. All simulations were conducted with stoichiometry 1.3 in the anode side. The operating temperature of the fuel cell is another important parameter affecting its performance. Hence, the simulations are performed in four different operating temperatures ranged from 40 to 70°C.

Polarization curve at different stoichiometries, operating temperatures and inlet humidities are depicted in Fig. 3a–h. As can be observed, the effect of ohmic resistance on fuel cell performance is negligible in cases 1 (Fig. 3a and b) and 2 (Fig. 3c and d) at low current density. Therefore, the variations of ohmic resistance due to temperature change do not significantly affect the output voltage of the cell. By increasing the current density, the slope of the polarization curve increases at higher temperatures because of higher ohmic resistance of the membrane at lower humidities. Indeed, membrane drying is higher in higher stoichiometries. Hence, the maximum drying phenomenon emerges for the inlet humidity of 25%, operating temperature of 70°C, stoichiometry 3 and at the current density of $1 A/cm^2$ that leads to zero cell voltage (Fig. 3 b).

It can be observed that the cell performance is improved with an increase in temperature in the case 4 (Fig. 3g and h). Since the cell is in the full saturation condition, stoichiometric increment from 2 to 3 has little effect on its performance. In other words, under this condition, the membrane's water content is sufficient and there will be no membrane drying with the increasing of stoichiometry, current density and operation temperature.

In the case 3, an increase in temperature, especially at higher temperatures, doesn't show much effect on the output

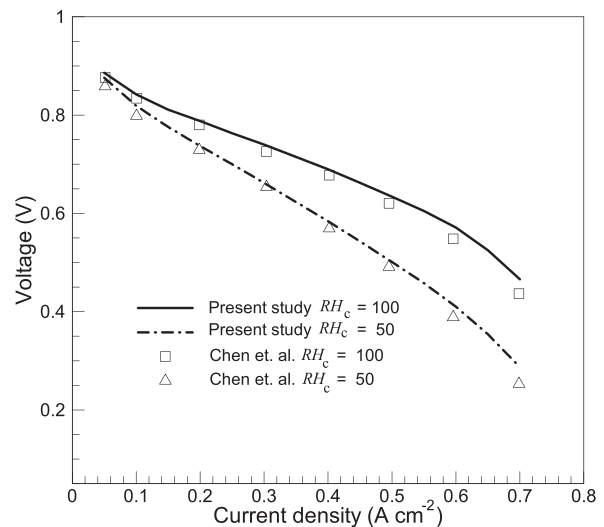


Fig. 2 – Comparison of simulation results with Ref. [21].

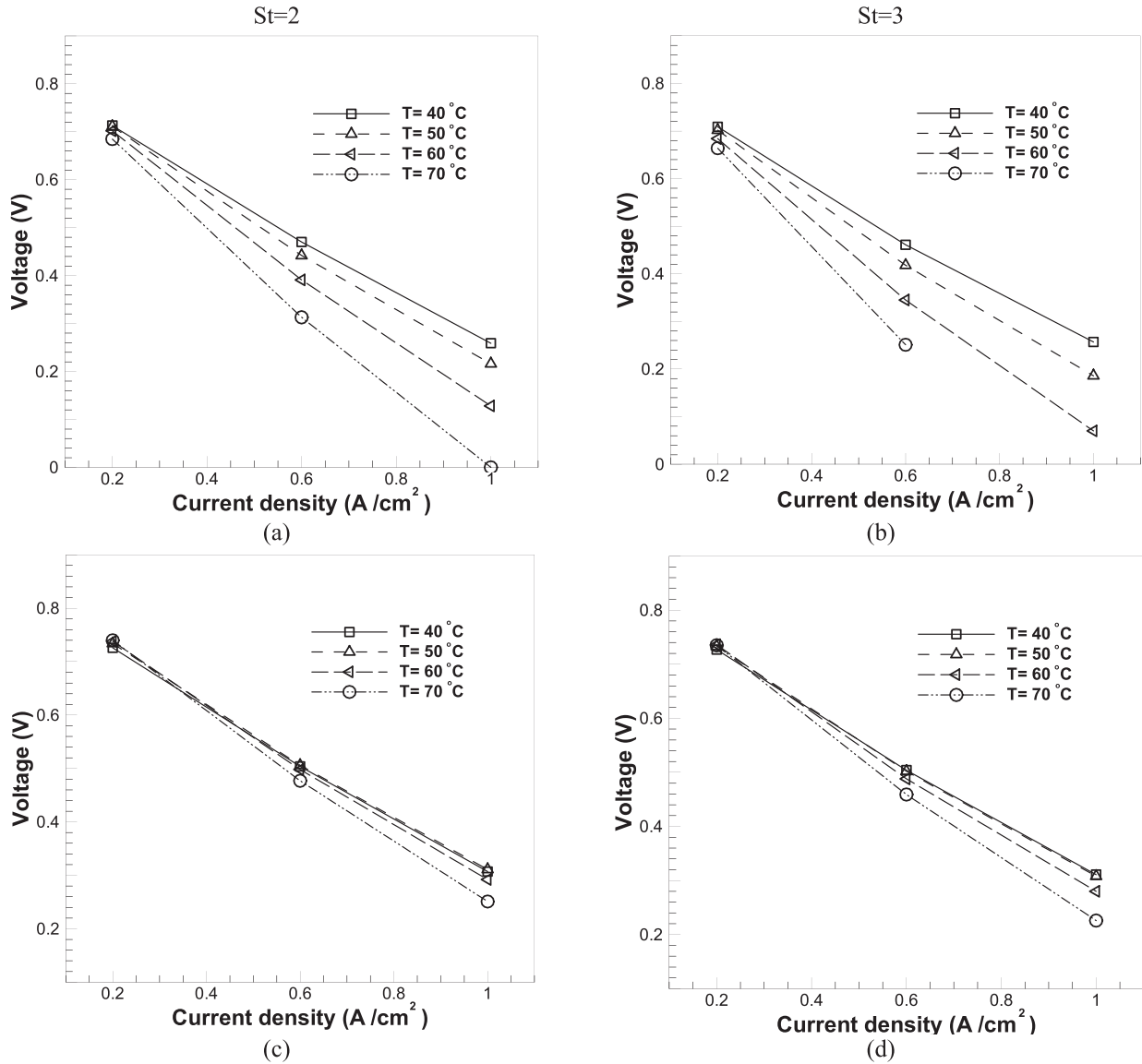


Fig. 3 – Polarization curve at different cell temperatures for inlet humidity of (a) and (b) $\phi_{in} = 25\%$, (c) and (d) $\phi_{in} = 50\%$, (e) and (f) $\phi_{in} = 75\%$, (g) and (h) $\phi_{in} = 100\%$, (left column $St = 2$, right column $St = 3$).

voltage. Higher operating temperature enhances open circuit voltage of the cell. On the other hand, Electro-osmotic drag increases with the increment of current density that leads to reduction of humidity in anode side and consequently a decreasing in cell voltage. Because of these two opposite effects, the operating temperature does not significantly affect the performance of the cell, as shown in Fig. 3e and f.

Two phase multiplier

The polarization curves, shown in Fig. 3, prove that the inlet humidity and operating temperature play an important role in the performance of fuel cell. In previous experimental studies, the pressure drop is used as an index to determine the status of the cell due to simple measuring [8]. Two phase pressure drop in channels can be used as a criterion for estimation of water content within fuel cell. Thus, drying or flooding inside

fuel cell can be deduced by its values. Furthermore, water content is one of the most important parameters in cell performance. Hence it is expected that there is a relation between two phase pressure drop and cell output. Thus, some researchers utilize pressure drop to predict water content in cell [19].

Polarization curves have shown that membrane drying occurs at low inlet humidity, high operating temperature and also high stoichiometry that lead to reduction of cell voltage. In order to investigate the relation between the output voltage and two phase pressure drop, simulation results in all cases are illustrated in Fig. 4a–d.

At low inlet humidity (25% and 50%), both the pressure drop coefficient and the cell voltage are reduced with the increasing of operating temperature due to membrane drying. The decreasing rate is higher at stoichiometry of 3. In all cases, two phase multiplier values are close to 1.2 and decrease with

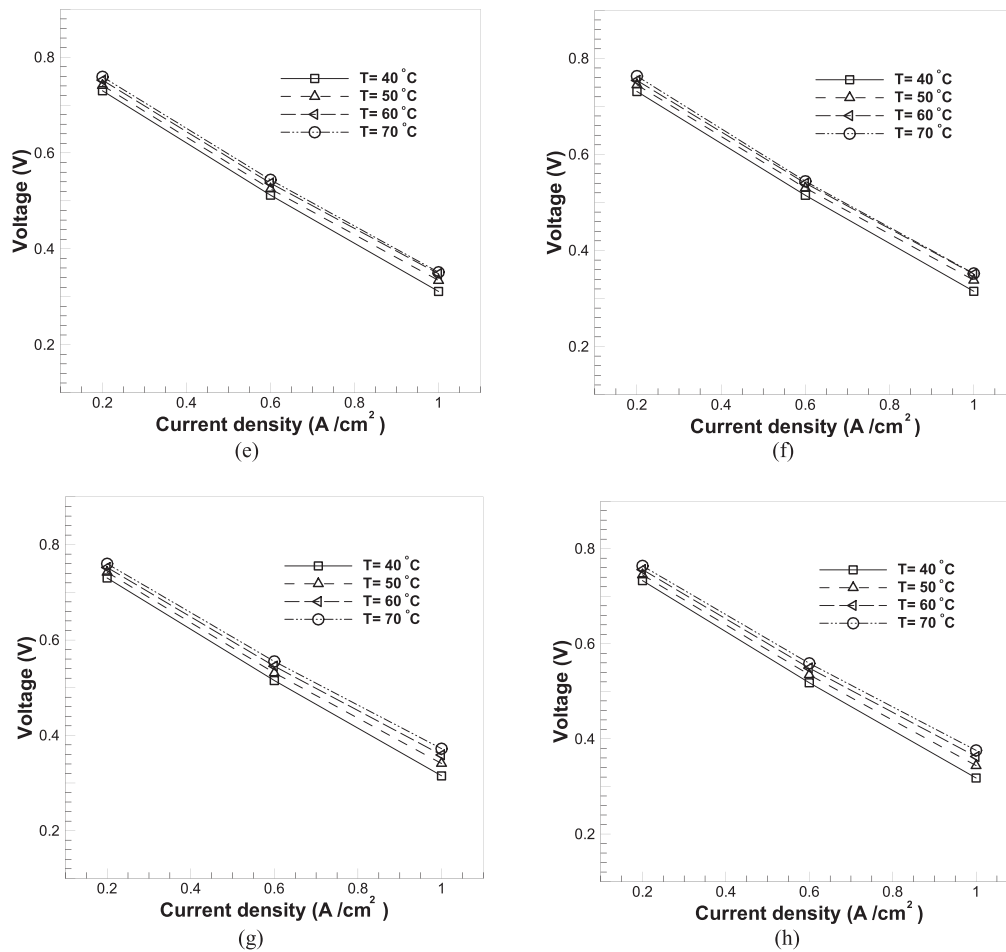


Fig. 3 – (continued).

an increase in temperature down to 0.8. Also, reduction behavior is more intense at higher current densities. Unlike cases with low inlet humidities, there is a different trend in

case 4 (Fig. 4d) versus operating temperature increment. Because of high water content, cell voltage increases with the increasing of temperature. Since high amount of water is

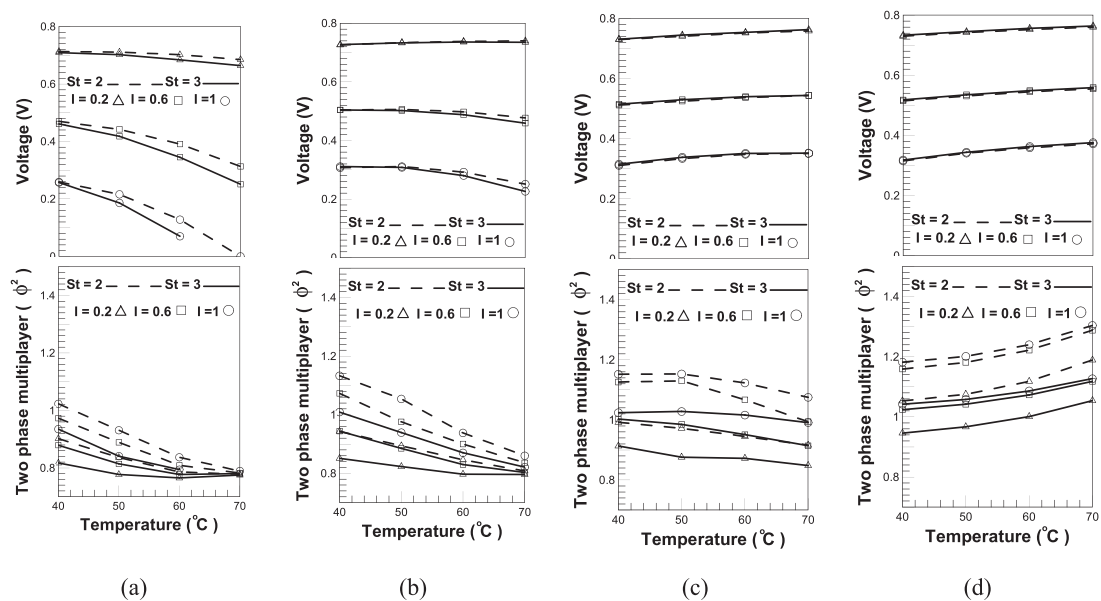


Fig. 4 – Variation of two phase multiplier and cell voltage for inlet humidity (a) 25%, (b) 50%, (c) 75% and (d) 100%.

created owing to high output voltage, two phase multiplier is enhanced.

In case 3 (Fig. 4c), unlike pressure drop, cell voltage shows an increment with temperature increasing. Due to low humidity at the entrance of the channel, membrane is not saturated. Therefore, a lower local current is generated in this region. But the local current density is enhanced along the channel owing to higher level of humidity arising from produced water in the cell reaction. In other word, the entrance region of channel is dried while other regions are saturated. Hence output voltages have smaller values in comparison to case 4 (100% inlet humidity).

At low current densities, the output voltage is almost independent of operating temperature except at the 25% inlet humidity in which output voltage is reduced with the increasing of temperature. However, the pressure drop shows a different behavior when operating temperature increases at low current density. It is observed that temperature increment leads to reduction in pressure drop in all cases except case 4 (100% inlet humidity).

As mentioned earlier, some researchers tried to diagnose drying/flooding in PEMFC by measuring pressure drop [32]. Water accumulation in PEMFC channels will affect pressure

drop. Hence, it is expected to be a linkage between output voltage and pressure drop. Increasing and decreasing of pressure drop indicate flooding and drying respectively; resulting in voltage drop. According to the present results, pressure drop and voltage variation have different trends at different inlet humidities. Inconsistency in the results implies that two phase multiplier isn't always a suitable criterion to predict the cell condition. Since the pressure drop and the cell voltage are bulk quantities, they don't present any information on the condition within the cell. Therefore, variations of others parameters such as current distribution and two phase flow regime inside channels have to be investigated in addition to the cell voltage and pressure drop in order to better estimation of cell performance and lifetime.

Current distribution

One of the most important factors in the lifetime of polymer fuel cells is the formation of hot spots on the membrane which is a result of non-uniform current distribution on membrane [33,34]. Therefore, in order to understand the fuel cell condition properly, the current distribution is very

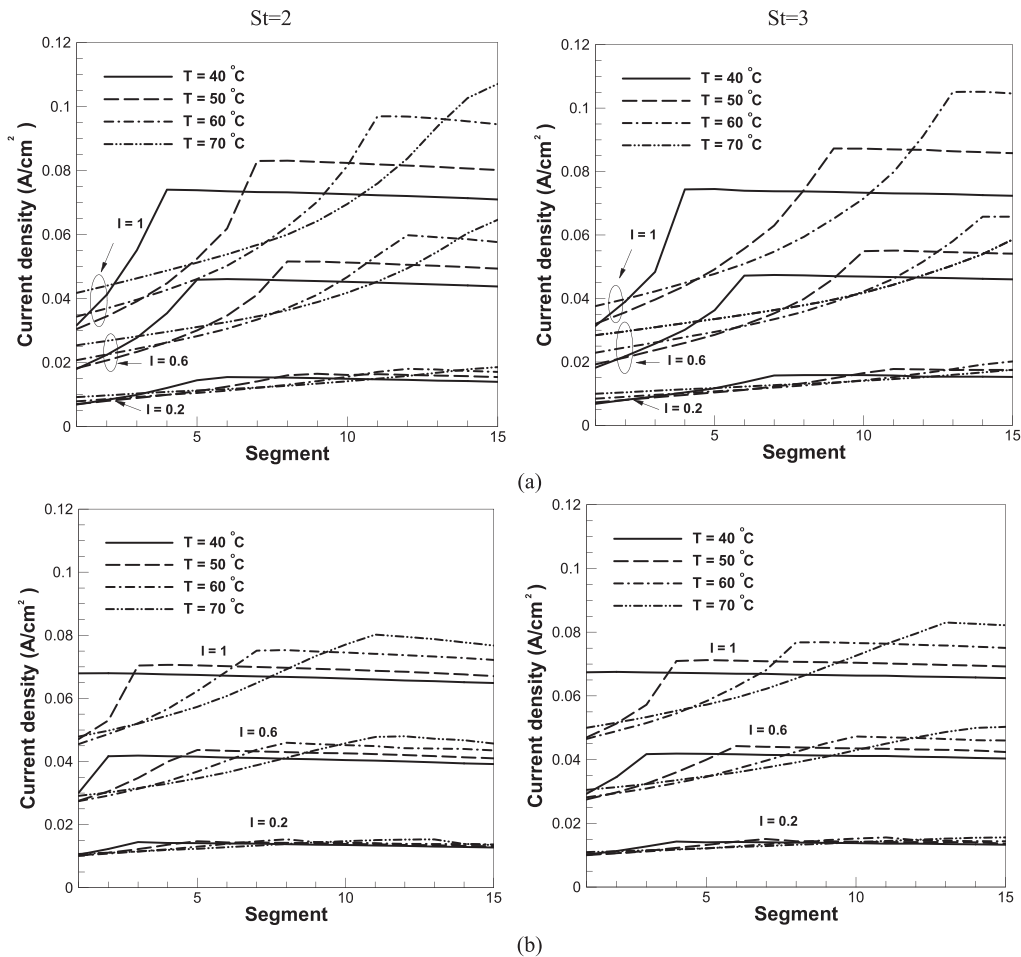


Fig. 5 – Current density distribution for inlet humidity (a) 25%, (b) 50%, (c) 75 and (d) 100%, (left column St = 2, right column St = 3).

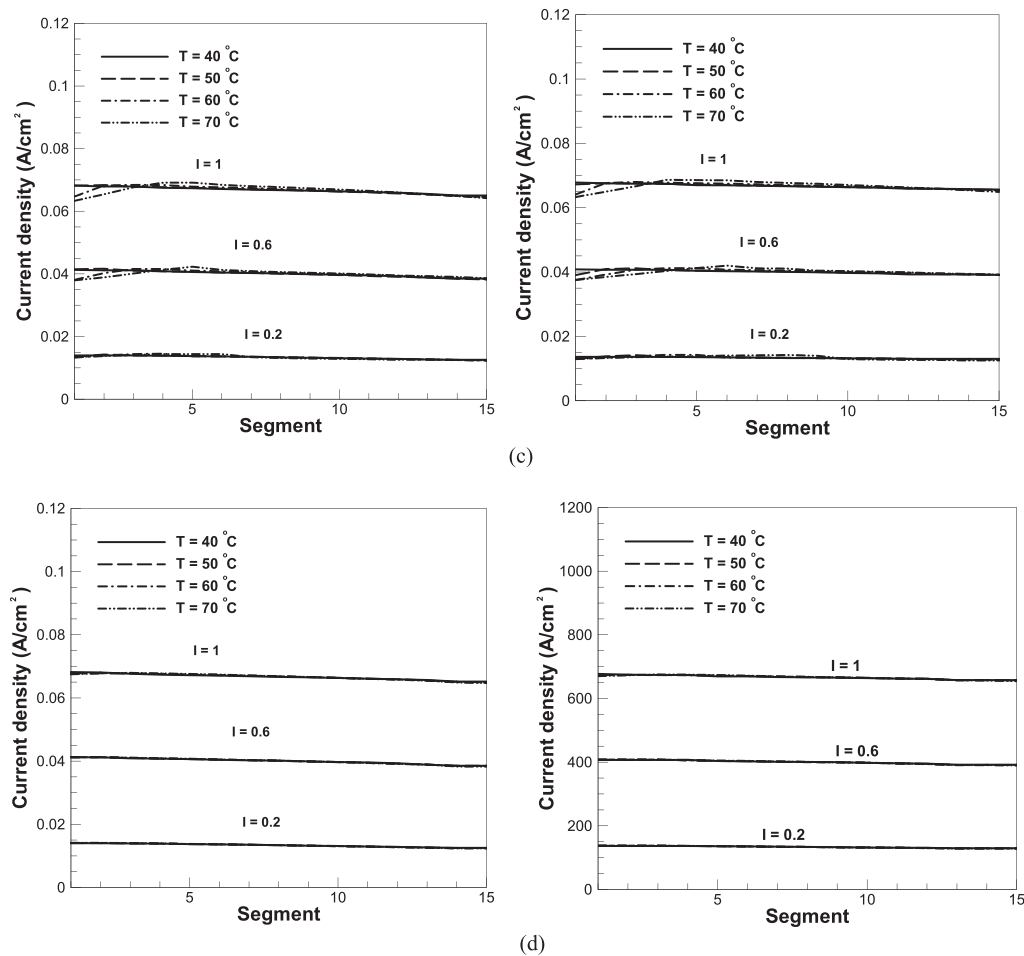


Fig. 5 – (continued).

important. Thus development of a model with the capability of forecasting the current distribution is so valuable.

Both membrane drying and two-phase flow pressure drop can affect current distribution. In Fig. 5, current distribution is depicted in different operating conditions. For moderate and high current densities at all inlet humidity except 100%, non-uniformity is observed in current distribution, especially at high temperatures. It occurs as a result of variations of membrane humidity at different segments. The variation of current density in segments is more intense at high temperatures owing to more humidity reduction in membrane that is a result of an increase in electro osmosis drag and consequently lower humidity at the anode side. As far as, at $\phi_{in} = 25\%$, $T = 70\text{ °C}$ and $I = 1\text{ A/cm}^2$, local current density increases from 0.03 at the first segment up to 0.1 A/cm^2 at the last segment.

Increase of inlet humidity to 100% results in more uniform current distribution, as shown in Fig. 5d. In this case, temperature variation has negligible effect on fluctuations of local current density at different segments. Therefore, according to the present results, the best way of current distribution control at high current density is the increase of inlet humidity and then a reduction in operating temperature. Uneven current distribution can be attributed to the membrane dehydration as reported in Ref. [5,35]. At high current density and low inlet humidity, the lowest local current density can be

observed near inlet regions followed by a steep gradient and then it is reduced gradually. Similar trend for co-flow arrangement was reported by Ref. [22]. In fact, higher current density enhances water transfer by the osmosis effect augmentation; accompanied with lower local current density near channel inlet. Then, Membrane will be hydrated along the channel due to produced water at the cathode side. Hence, local current density increases quickly and reaches to the maximum value. After that, as a result of flooding in GDL, a decreasing trend is observed in local current density, as shown in Fig. 5. Increasing cell temperature will augment water evaporation. Hence, the peak location of current density distribution will be shifted toward the outlet. Therefore, increasing of temperature intensifies current density gradient. Thus, decreasing cell temperature, despite the lower output, result in smoother distribution of local current density. Although inlet gas humidification shows better current distribution (Fig. 5c and d), higher water content maybe display negative effect when flooding occurs in PEMFC in which both current distribution and output voltage will be worse [35], hence idea of self-humidification has been implemented to use excess water for humidifying of dry regions [6].

Formation of high liquid water content causes GDL porous media blockage and also coverage of the channel with water that leads to non-uniform current distribution on membrane

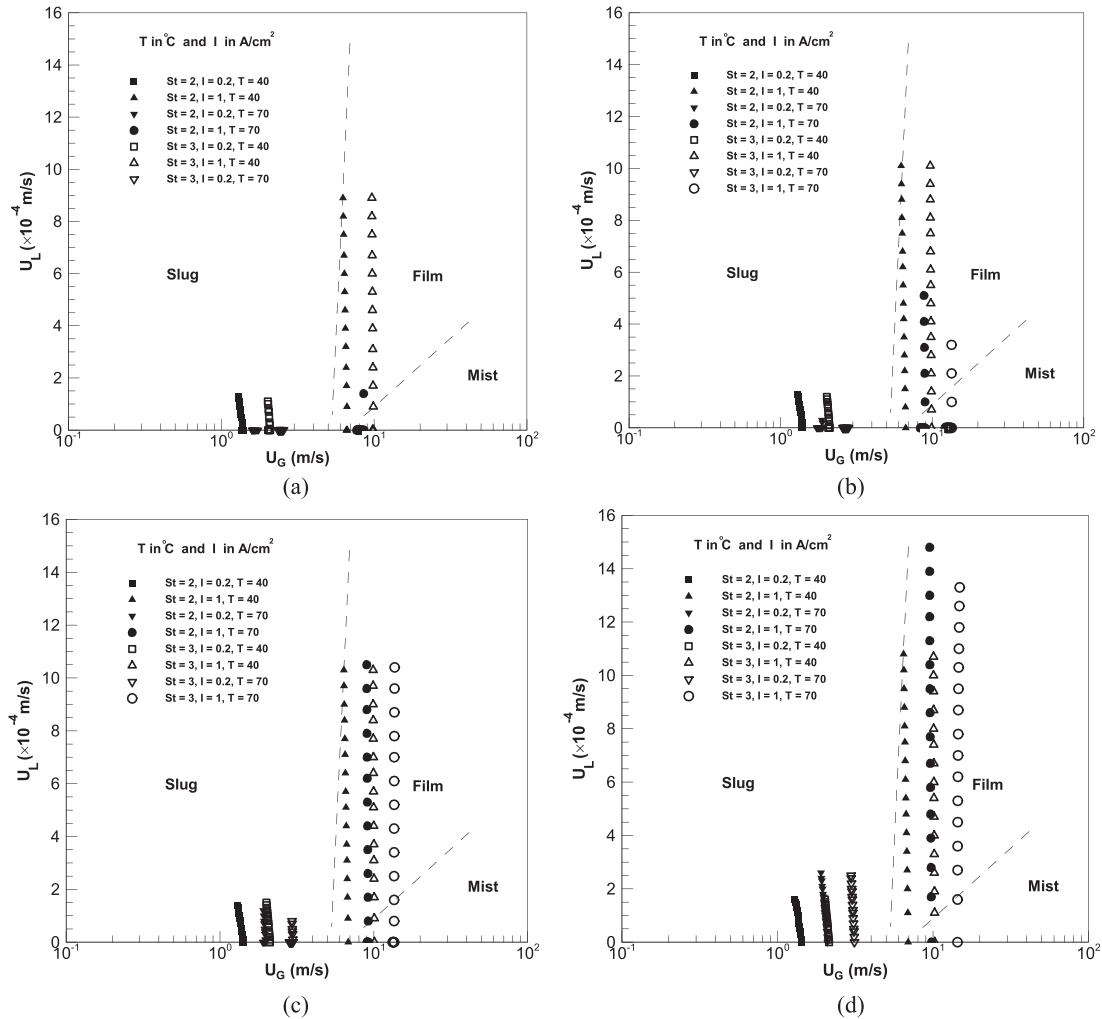


Fig. 6 – Flow regime map variations in cathode side channel at different operating conditions for inlet humidity of (a) 25%, (b) 50%, (c) 75% and (d) 100%.

surface. Since a constant value of saturation (nearly zero) at GDL/channel interface has been considered in the present simulation, same as Refs. [25,36], the cell flooding would not be predicted with high level of accuracy. In order to rectify this deficiency of the model used in the present study, two phase flow map is used in the following.

Two phase flow pattern

Two-phase flow formation inside the fuel cell causes the blocking of porous media pores and consequently an increase in resistance against mass transfer resulting in high voltage drop especially at high current densities. Also, water accumulation in the channel increases the possibility of porous media surface flooding. Therefore, in this condition, a high level of non-uniformity in current density leads to a reduction in fuel cell lifetime. Previous experimental studies showed that two phase flow in a fuel cell exists in three regimes [6]: slug, film and mist flow. Experimental observations prove that in the slug regime, porous media surface is flooded in water that results in a major drop in the performance of fuel cell [37].

Calculation of velocities of water and gas at each segment, individually, is a capability of the present simulations. Therefore, it is possible to determine the type of two-phase flow regime using a two-phase flow pattern obtaining from velocities. The two-phase flow pattern inside the fuel cell channels extracted from experimental data by Kandlikar et al. [37] is used to evaluate the flow regime in the present study. Fig. 6 shows the results for different segments at different operating conditions. In each case, produced water is added along the channel and therefore, the water velocity increases in later segment, as shown in Fig. 6. The flow pattern indicates that at low inlet gas velocity, the water flow regime in the channel is always slug. But by increasing the inlet gas velocity, flow regime transits from slug to film and finally mist regime. Due to high gas velocity, the possibility of slug flow formation is reduced, even at low temperatures and low stoichiometries, as shown in Fig. 6. In these cases, flow regime is film flow in the major part of the channel.

In low current density corresponding to low inlet gas velocity, appearance of liquid water in channels will be followed by slug flow. Hence, in order to prevent slug flow formation,

three approaches can be applied: increasing inlet stoichiometry, increasing cell temperature and decreasing inlet humidity. Two later approaches will reduce water content in cell whereas increasing inlet stoichiometry will change flow regime from slug toward film or mist flow.

At high current density, because of higher inlet gas velocity, flow pattern is almost always mist or film regime. In last segments, flow regime transits from film towards slug, by accumulation of produced water (higher superficial liquid velocity), as shown in Fig. 6.

There is a dynamic load in fuel cell vehicles. Changing of fuel cell load between high and low current density should change flow pattern as mentioned above and as a consequent, local starvation can occur which is main factor fuel cell decay [35].

Conclusion

Water control is a crucial parameter on the performance and lifetime of PEM fuel cell. In the present study, a modified segmented model is conducted to predict performance, current distribution and flow regime in PEM fuel cell at various operating conditions. Hence, it is useful tool to diagnose water management in order to set the best cell temperature, inlet humidity and reactant stoichiometry at different current densities. Also, two phase pressure drop is calculated to investigate its relation with water management diagnosis. Based on simulation results, main achievements are as follows:

In low current density:

- Output voltage has a little variation with inlet conditions. Also, current distribution shows smooth behavior. Thus, flow regime is the main factor that must be considered in water management.
- The flow map results show that liquid formation in the channel is followed by slug flow and therefore, in this situation, water management strategy should be focused on prevention of forming two phase flow.
- Higher cell temperature and reduction of inlet humidity as well as higher inlet stoichiometry can be recommended to prevent the liquid formation in channel. For this purpose, a higher cell temperature is the best approach, since it can control slug flow formation and increase cell voltage too. Although lower inlet humidity is the simplest way, inlet humidity less than 50% leads to a non-uniform current distribution. Higher stoichiometry helps to control water production but it has less effect in comparison to cell temperature. Also, fuel consumption efficiency will be reduced by increasing stoichiometry.
- In association with two phase pressure drop, any formation of liquid in channel changes pressure drop and hence, it can be used as a signal for identifying liquid formation.

In high current density:

- Although higher cell temperature enhances output voltage, it leads to higher non-uniformity at current distribution, even at fully saturated inlet condition.

- In fully saturated inlet gas condition, the results show almost a uniform distribution of current density especially at low cell temperature. Therefore, it is suggested that a fully saturated condition is applied at high current density. In this way, smoother current distribution will be followed by higher output voltage unless the slug flow regime takes place.
- As a result, output voltage and flow regime are two main factors in fuel cell performance. Therefore, cell voltage and flow regime in the channel can be expected to be related together. As shown in results, both two phase pressure drop and voltage have the same trend and the maximum output voltage will be limited by mass transport limitation in GDL due to covering of its interface with the channel by water. Hence, it can be deduced that two phase pressure drop can be the indicator of cell performance if the membrane is in fully saturated condition. Otherwise, when some parts of the membrane are in dry condition, two phase pressure drop and voltage have different trend at various temperatures. In fact, higher pressure drop means regions in membrane are in saturated condition and output voltage is a tradeoff between flooded and dried regions.

Generally, pressure drop and output voltage due to simplicity in their measurement are two common parameters used to diagnose water management in PEMFC. For experimental conditions, current density distribution as well as flow pattern visualization is much more difficult and cost compared with output voltage and pressure drop, hence modeling is a powerful tool in this way. The results of the present modified model show that inlet humidity has less effect on current distribution and output voltage at low current density. Therefore, membrane humidification is a good approach. However flooding in channel is a main issue that must be considered in water management diagnosis which pressure drop measurement is a simple and inexpensive tool in this way. At high current density with humidified inlet gas, output voltage and pressure drop have similar trend and flooding or drying condition can be predicted by pressure drop.

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