



Numerical Simulation of Electrochemical Processes in Polymeric Membrane Fuel Cells

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Abstract: Polymer Electrolyte Membrane Fuel Cells (PEMFCs) are identified as the most important choice to replace internal combustion engines. But there is still a long way to reach this fact, and, in order to reach such a purpose, it is necessary to carry out many optimizations on these cells. One of the methods resulting in a deeper and better understanding of physical processes within the cells is simulation of physical governing equations on fuel cells. In this article, these governing equations are introduced and a system of equations is solved for a model.

Key words: Polymeric membrane fuel cell; Electrochemical processes; Numerical simulation

INTRODUCTION

PEMFC is among the low-temperature cells, and has much potential to be a substitute to serve as a motive force in automobiles. At this time, some models of automobiles working with fuel cell power have been built and presented to the market. But there is still a long way to mass production of this kind of cells. High rate of manufacturing costs is one of the largest problems in this regard. There has been much effort in order to decrease the weight, amount of platinum used in electrodes, and optimize their control system. To keep on the trend of optimization, it is necessary to obtain a deep understanding of electrochemical and physical processes in the cell. In addition to experimental tests, one can understand deeply in this regard solving the governing equations because the results of the governing equations can determine much detail concerning condition of the cell performance.

Several regions of the cell are delineated as follows:

1. Hydrogen channel located on the left-hand side of the cell. Hydrogen enters the channel and goes out through its other side. In order to let hydrogen diffuse into the catalyst layer, the channel pressure is heightened by adjusting a pressure control valve.
2. The gas diffusion layer located beside the hydrogen channel. This region is a porous media through which hydrogen diffuses to the catalyst layer.
3. The catalyst layer is a very thin layer created by coating the platinum on the gas diffusion layer which is also a porous layer. When the hydrogen reaches the gas diffusion layer, it loses its electron and is converted to a hydrogen ion.
4. The polymer membrane located next to the catalyst layer. This membrane resists the electron movement allowing the hydrogen ion to pass, so the polymer membrane actually serves as an electrolyte in the fuel cell. It is worth noting that the membrane also diffuses into the catalyst layer, so the catalyst layer will also contain electrolyte.
5. The cathode region is located on the other side of the polymer membrane of the catalyst layer. Oxygen and hydrogen ions, along with the electron coming from the external circuit, interact with each other and consequently form water.
6. Gas diffusion layer, similar to the side of anode, is located on the left side of the catalyst layer, and causes oxygen to diffuse into the catalyst layer.

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Air or oxygen channel located beside the gas diffusion layer. Air or oxygen flows in the channel with a suitable pressure resulted by initial design.

In order to analyze the fluid flow and also to simulate electrochemical processes involved in catalyst layers, it is necessary to obtain the governing equations in such a form that all of them will be valid in all seven regions. Extensive researches have been carried out to simulate the fuel cells. For instance, Bernardi and Verbrugge [1, 2], and Sourceer et al. [3, 4] built one-dimensional models. Fuller and Newman [5], Nguyen and White [6], Gurau et al. [7], and Yi and Nguyen [8, 9] presented similar pseudo two-dimensional models which were actually the models along the fluid path. In all presented models, a certain system of equations is presented for each region of the cell, so boundary conditions are required for combining all the regions and obtaining a consistent solution for all the regions. Based on the previous model presented by Wang et al. [10], Um et al. [11] presented a consistent model in which a system of conservative equations govern all regions of the fuel cell so that there is no need for applying the boundary condition at the internal boundaries. The model is multi-dimensional, and is able to solve numerically the electrochemical equations, conservation of mass and momentum of fluid flow using Navier-Stokes equations. The obtained model is capable to simulate the fluid flow in all the porous and non-porous regions like fluid channels, diffusion layers and the membrane with one single formulation.

Although the presented system of equations is a comprehensive system, the largest problem is to solve it numerically. As noted before, to apply these equations in all regions of the fuel cell, it is necessary to write the Navier-Stokes equations in such a form through which fluid flow can be applied in both air and/or hydrogen channels and gas diffusion layers. The regions are porous ones, and the numerical solution used to solve the equations is faced with the certain types of problems. Fortunately, the process can be solved in Fluent software that is able to solve the Navier-Stokes equations in such medias. It is worth noting that the software can solve only the fluid flow and energy conservation equations, and is not able to solve the other variables needed for analyzing the fuel cell. For example, this software does not solve the electrochemical equations to obtain the potential distribution in solid and electrolyte.

In such cases, it is possible to add a new variable namely User-Defined Scalar (UDS) to the software. Actually one can introduce a new variable or UDS to the program through introducing the equation governing that UDS and then try to solve the problem. In order to define the new variables, it is necessary to write the governing equation for that variable in a general convection-diffusion form which is prescribed in Fluent.

In the present study, first general governing equations presented by Um et al. [10] are introduced and studied. Then, obtained governing equations will be converted to the general form of conservation equations applicable in Fluent software, and then the new variables or UDSs will be added to the program. Finally, these equations will be coupled to Navier-Stokes equations, and all of the fluid field along with the new variables will be solved through using coding the User-Defined Function at the software programming environment. In order to verify the present method, a numerical solution for a sample cell is also presented, and the results verify the accuracy of the present technique.

THE GOVERNING EQUATIONS

According to the Figure 1, a fuel cell is actually an electrochemical system in which several phases such as gas, liquid, and solid are interacting with each other. In such systems, fluid flows through a porous medium with a variable porosity. For instance, porosity is equal to one for open channels while several layers of the cell have different amounts of porosity. Also there are some electrochemical reactions in some parts of this space. So, from a general point of view, when analyzing a fuel cell, one would be involved inevitably in some other topics such as porous media, multi-phase environment, chemical and electrochemical reactions, and heat transfer.

In order to present a comprehensive model for such a problem, it is necessary to know the conservative equations governing the physical variables involved in the problem, and solve them. In such electrochemical systems, electrochemical reactions are generally expressed by conservation equations for mass, momentum, chemical species, and electric charge written for each phase. These equations govern bulk of the field, and are combined with each other through interface processes. There is negligible or no fluid flow in most porous electrodes,

so the equations related to mass and momentum will be removed from the system of equations. But, to generalize the formulation in the present model, effects of these factors are considered.

Principle of conservation of mass and momentum:

Fluid flows through the fuel cell by several phases, so it is necessary to develop the fluid flow equations in such a way that contains several phases. Fluid flow in phase k can be characterized using the principle of conservation of mass and momentum as follows:

Principle of conservation of mass: Mass conservation equation for a porous media is as follows:

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla \cdot (\varepsilon\rho\vec{v}) = 0 \quad (1)$$

That porosity coefficient is added to it due to existence of the porous media in the fuel cell. In the above equation, ρ is density, v is the velocity of the scalar, and ε is the porosity coefficient.

Principle of momentum conservation: Momentum conservation equation for a porous media is as follows:

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla \cdot (\varepsilon\rho\vec{v}\vec{v}) = -\varepsilon\nabla p + \nabla \cdot (\varepsilon\mu^{eff}\vec{\nabla}\vec{v}) + S_u \quad (2)$$

Similar to the previous equation, porosity coefficient is added to it due to existence of the porous media in the fuel cell. In these equations, S_u is related to source of the equation and has different amounts in several regions of the cell. S_u in the gas diffusion layer is as follows:

$$S_u = -\frac{\mu}{K} \varepsilon^2 \vec{v} \quad (3)$$

where μ is fluid viscosity, K is diffusion resistance in the gas diffusion layer, ε is the porosity of the layer, and v is the fluid velocity. In catalyst layer, S_u becomes:

$$S_u = -\frac{\mu}{k_p} \varepsilon_m \vec{v} + \frac{k_\phi}{k_p} z_f c_f F \nabla \Phi_e \quad (4)$$

where k_p is the hydraulic resistance of the membrane, ε_m and ε_c are porosity of catalyst layer and the membrane in the catalyst region, respectively. k_ϕ is electro kinetic diffusion resistance, and c_f , z_f , and F are concentration, electric charge number, and Faraday number, respectively.

Finally, the momentum in the polymer-membrane layer of the sink is as follows:

$$S_u = -\frac{\mu}{k_p} \varepsilon_m \vec{v} + \frac{k_\phi}{k_p} z_f c_f F \nabla \Phi_e \quad (5)$$

Principle of conservation of chemical species

Mass balance for a species in phase k is:

$$\frac{\partial(\varepsilon X_k)}{\partial t} + \nabla \cdot (\varepsilon v X_k) = \nabla \cdot (D_k^{eff} \nabla X_k) + S_k \quad (6)$$

where X_k is the species, S_k is the sink or source of the species, and D_k is the diffusion coefficient of the species. Since the species exist in a porous media, the amount of diffusion coefficient differs from the physical diffusion coefficient of a pure material, and it is necessary to obtain its effective amount using Bergman equation [11]:

$$D_k^{eff} = \varepsilon^{1.5} D_k \quad (7)$$

where D_k is the diffusion coefficient of pure material that is a function of temperature. This functionality can be calculated as follows:

$$D_k(T) = D_0 \left(\frac{T}{T_0}\right) \left(\frac{P_0}{P}\right) \quad (8)$$

Where D_0 is equal to the diffusion coefficient of the species in reference condition of temperature and pressure ($T=273.15$ and $P=1$ atm).

Source term is generated by electrochemical reactions in this equation, and is proper to the

amount of flow created by the fuel cell. Writing mass balance and its relation with the production or consumption amount of the material in catalyst layers, S_k is equal to:

$$S_k = \pm \frac{J}{aFc_{tot}} \quad (9)$$

where J is the source of electrical charge production and has different values considering whether that species is on the cathode or anode side. This term will be explained in detail in the section of electrical charge conservation. C_{tot} is the total amount of material input into the main channel. Each species constitutes a molar ratio of this value. Finally, a is a coefficient that is variable considering the material and its location.

Conservation of electrical charge: Electrochemical reactions happen in the interface between active material and electrolyte; therefore no charge is created in phase k nor consumed. This principle states that net flow input into a phase is equal to net flow output from that phase, so:

$$\nabla \cdot \vec{i}_k = 0 \quad (10)$$

But the flow generated on boundaries entered the phases, so the boundary condition for each phase is as follows:

$$\vec{i}_k \cdot \vec{n}_k = -\sum_j \vec{i}_{nj} \quad (11)$$

In these equations, \vec{i}_k is the current density in phase k . This electrical current is carried by electrons in solid materials, and its governing equation is explained by Ohm's principle as follows:

$$\vec{i}_n = -\sigma \nabla \phi_s \quad (12)$$

In this equation, \vec{i}_s and ϕ_s are current and potential in solid electrode, respectively, and σ is its electrical conductivity. Either in solid or in liquid phase, the charge transfer is accomplished by ions movement which happens in three ways as follows:

Ions diffusion that happens due to the existence of ions and is stated by Fick's law.

Electrolyte movement that, as noted before, is accomplished in liquid electrolytes.

Migration that is accomplished due to the existence of electrical potential gradient in battery.

In electrolyte phase, a proper form of Ohm's law should be used which consists of both effects of concentration and potential gradient. This principle is known as modified Ohm's law which can be described as follows:

$$\vec{i}_e = -k \nabla \phi_e - k_D \nabla (\ln c_e^i) \quad i = \pm \quad (13)$$

where k is effective conductivity of electrolyte, and k_D is diffusion conductivity which exists to consider the effect of ions movement and diffusion in presence of concentration gradient. The symbols $+$ and $-$ are positive and negative poles, respectively. Now, if the effects of concentration gradient are ignored, the equation of conservation of electrical charge is:

$$\nabla \cdot (\sigma_e^{eff} \nabla \Phi_e) + S_\Phi = 0 \quad (14)$$

where σ_e^{eff} is the effective conductivity of solid membrane phase which is modified by Bergman equation as follows:

$$\sigma_e^{eff} = \varepsilon^{1.5} \sigma_e \quad (15)$$

In this equation, σ_e is the conductivity coefficient of electrolyte phase or membrane that is a function of water content of the membrane and temperature as follows [3, 4]:

$$\sigma_e(T) = 100 \times \exp\left[\left(\frac{12000}{303} - \frac{12000}{T}\right)\right] \times (0.005139\lambda - 0.00326) \quad (16)$$

Where λ is the water content of the membrane, and depends on the activity of the water, a . this amount is calculated as follows [10]:

$$\lambda = \begin{cases} 0.043 + 17.18 - 39.85a^2 + a^3 & \text{for } 0 < a < 1 \\ 14 + 1.4(a - 1) & \text{for } 1 < a < 3 \end{cases} \quad (17)$$

The activity of water, a, is calculated as follows [10]:

$$a = \frac{X_{H_2O} P}{p^{sat}} \quad (18)$$

Where saturation pressure of the water vapor can be calculated as follows:

$$\begin{aligned} \log_{10} p_{sat} = & \\ & -2.1794 + 0.02953(T - 273.15) \\ & -9.1837 \times 10^{-5} (T - 273.15)^2 \\ & + 1.4454 \times 10^{-7} (T - 273.15)^3 \end{aligned} \quad (19)$$

It is worth noting that the pressure unit is represented in bar in the above equation, and X_{H_2O} and water activity (a) and λ are all defined in the membrane of the fuel cell. These equations show that the amount of electrolyte conductivity (σ) is variable depending on the water content and temperature of the membrane. The source of ion production in equation (14) is calculated as follows:

$$S_{\Phi} = J \quad (20)$$

Which are calculated using electrochemical reactions on the sides of anode and cathode respectively as follows:

$$I_a = a j_{0,a}^{ref} \left(\frac{X_{H_2}}{X_{H_2,ref}} \right)^{0.5} \left(\frac{\alpha_a + \alpha_c}{RT} F \eta \right) \quad (21)$$

for anode and:

$$J_c = -a j_{0,c}^{ref} \left(\frac{X_{O_2}}{X_{O_2,ref}} \right) \exp\left(-\frac{\alpha_c F}{RT} \eta\right) \quad (22)$$

for cathode.

In these two equations $a j_{0,c}^{ref}$ and $a j_{0,a}^{ref}$ are the amount of reference electrical current multiply by the active area of cathode and anode, respectively. Also

α_a and α_c are the charge transfer coefficient of anode and cathode, respectively. In these two equations, η is the overpotential which is described as follows:

$$= \Phi_s - \Phi_e - V_{oc} \quad (23)$$

More details regarding these equations can be found in several references.

SIMULATION OF THE GOVERNING EQUATIONS

For solving these equations, it is necessary to use the CFD numerical methods. As it was mentioned in this study, these equations were solved using fluent software. But the major problem is that this software is capable to solve the momentum and energy equation to obtain the velocity field and pressure and temperature gradient in the cell but it does not have any equation for the conservation of species (equation (6)) and conservation of electrical charge (equation (14)). Moreover, the source and sink terms which are in momentum equation (equation (2)) are not prescribed in the software. Therefore, we need a way to include these unknowns into the original system of equations.

Hopefully, this software includes two different capabilities that make it possible to introduce these unknowns into the code. Specifically, these capabilities are User-Defined Function or UDF and User-Defined Scalar (UDS). UDF make it possible to add extra sources or sinks into the momentum equation while UDS can be used to add a new unknown to the software. The general form of a UDS for a new unknown, A_k , is as follows:

$$\underbrace{\frac{\partial \rho A_k}{\partial t}}_{\text{unsteady}} + \frac{\partial}{\partial x_i} \left(\underbrace{F_i A_k}_{\text{convection}} - \underbrace{\Gamma_k \frac{\partial A_k}{\partial x_i}}_{\text{diffusion}} \right) = S_{A_k} \quad (24)$$

where Γ , F_i and ρ are diffusion coefficient, flux and density of that variable.

To add a new unknown to Fluent, the variable should be expressed in the form of equation (24). For our simulation, the new unknowns are:

ϕ_e : Electrical potential of electrolyte phase, equation (14).

X_{H_2} : Molar concentration of Hydrogen, equation (6).

X_{O_2} : Molar Concentration of Oxygen, equation (6).

A closer look to the above equations reveals that these equations are in the form of the general UDS (24) and are completely consistent with it. Therefore, these unknowns can easily be introduced to Fluent.

An electric charge conservation equation is in stable condition and independent to the velocity distribution so first and second term of left hand in the equation (24) becomes zero. It is seen in the relation that Γ_k equals to σ and A_k equals to Φ_e . For the equation of chemical species conservation, ρA_k also equals εX_k and Γ_k equals F_t , D equals εv . Applying these variations, all chemical species will be solvable by fluent software.

Applying momentum equation: Despite oxygen and hydrogen channels, other areas such as catalyst, gas diffusion layer, and polymer membrane all are porous media. Therefore, it would be necessary to add extra sources terms to the momentum equation, as is described in equation (2). The extra sources are related to the drag force which is induced by the porous medium. This source term is as follows:

$$S_i = -\left(\sum_{j=1}^3 D_{ij} \mu v_j + \sum_{j=1}^3 C_{ij} \frac{1}{2} \rho |v| v_j\right) \quad (25)$$

where S_i is a representation of the sink in the momentum equation, i is a direction of (x, y, z) coordinate axis, μ is viscosity and v_i is velocity in the desired direction. Also, D_{ij} and C_{ij} are predetermined matrixes.

In a homogenous porous medium in which the drag force is independent of direction, equation (25)

is simplified as follows:

$$S_i = \left(\frac{\mu}{\alpha} v_i + C_2 \rho |v| v_i\right) \quad (26)$$

where α is a material permeability and C_2 is an internal resistance.

Darcy's law in the porous environment: For laminar flow in a porous region, coefficient C_2 is zero and pressure drop is proportional to fluid velocity, permeability rate, and viscosity which is as following for a homogenous network:

$$\nabla P = -\frac{\mu}{\alpha} v \quad (27)$$

Now regarding the fact that flow in a fuel cell stack is totally laminar, it would be enough to use equation (27) instead of equation (26).

There are two ways to simulate a porous medium in Fluent:

This software is capable to simulate porous media. Hence one can use this facility and directly develop a porous area and include a $\varepsilon \nabla P$ term in a momentum conservation equation.

Another way is to use the normal equations for non-porous media but including extra sink to the momentum equation using UDF.

In the present study, we have used the second strategy for simulating the porous media.

Conservation of Electrical Charge: As mentioned before, to introduce a new variable as a UDS, it should follow equation (24). To add a new variable for accounting the potential distribution in different layers, we need to add an equation for the conservation of electrical charge. This equation is in the form of equation (14). Comparing equation (14) with the general form of a UDS (equation (24)) it can be seen that the former is in the form of the latter. Namely, it does not include the transient and convective term. Therefore, equation (14) can be easily applied to the software.

Conservation of Chemical Species: In the present study, we need to calculate the concentration of H_2

and O_2 in all regions. Hence we need to add these new variables to the software. The conservation of any chemical species is described by equation (6) which is consistent with equation (24). Hence, these new variables can be added to the software via UDS capability without any difficulty.

Table 1: Thickness of different areas of fuel cell

Region	Value (cm)
Entrance channel	0.0029
Gas diffusion layer	0.0254
Catalyst	0.0762
Polymer membrane	0.023

RESULTS AND DISCUSSION

As aforementioned, hydrogen is used in fuel cell as a fuel and it is converted to hydrogen ions in catalyst Layers. These ions, move toward the cathode. Mathematically speaking, hydrogen is consumed and hence it has a sink term in anode side as described by equations (9) and (21). After that, in the cathode side, oxygen combines with hydrogen ions and produces water. According to equation (14), the amount of the generated current in each numerical grid can be obtained as:

$$\vec{i} = -\sigma \nabla \Phi_e \quad (28)$$

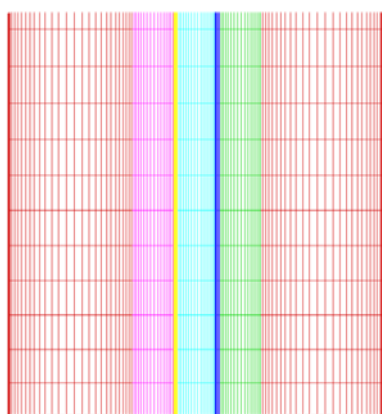


Figure 2: meshing method

Therefore, for calculating the total generated current, this quantity should be integrated all over the interface between the catalyst layer and the polymer membrane:

$$I = - \int_{y_{\min}}^{y_{\max}} \sigma \nabla \Phi_e \quad (29)$$

To validate the model, we have simulated a sample cell from reference [10]. The thickness of different regions of the fuel cell is shown in Table 1. The channel height in the present study is equals to 7.112 cm. Comparing the height of the channels to its thickness, we see that it is a very long and slender channel.

Figure 2 shows the grid generation for the lower part of the cell (since the numerical domain is very slender, the whole domain is not shown here). As it can be seen a very fine grid is used for simulation. Moreover, we have clustered the numerical grid near the boundaries to accurately capture the variable gradients.

The studied cell works in a constant temperature condition at 353 K. In oxygen channel (cathode direction), an air flows in which it is assumed $X_{O_2} = 0.21$ for its entrance regarding the molar ratio of oxygen in the air. At the anode side, the molar ratio of hydrogen is assumed to be $X_{H_2} = 0.8$ since the production of pure hydrogen is almost very expensive.

Figure 3(a) shows the velocity vectors obtained from the simulation. As it can be seen, the fluid flows almost in both channels and the velocity field in porous layers are very small. Figure 3(b) shows the velocity filed in different layers with different scales to show that although very small but porous layers have also velocity field.

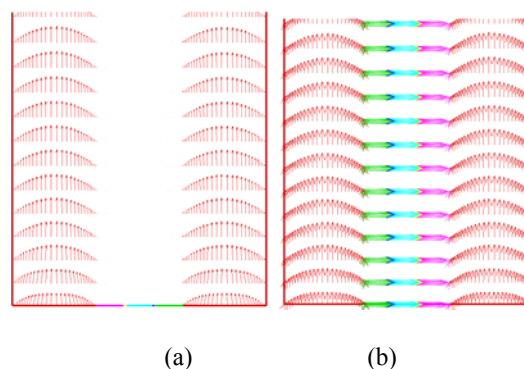


Figure 3: (a): Velocity profile in a fuel cell mesh
(b): Velocity vector along x and y direction

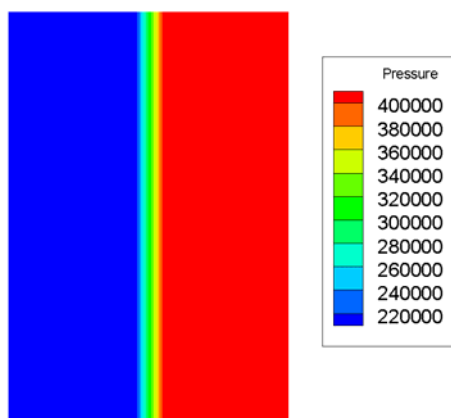


Figure 4: Pressure cantor on PEM cell

Figure 4 shows the pressure contours in the whole domain. As it can be seen, pressure is almost uniform all along the channels and varies only from left to right. This is because the velocity amplitude of the fuel and oxidant gases are very small resulting into a negligible pressure drop along the channels. Figure 5 shows the variation of pressure at a cross section located at the middle height of the cell. From the figure, it can be seen that the pressure drop from the anode to the cathode is linear. Figure 6(a) shows the potential distribution contours in the polymer membrane. It should be noted that in the present study, the conservation of charge is solved on the entire cell sandwich, including the fluid channels. At the anode and cathode channels, the potential distribution is calculated and the value zero obtained. From the figure, one sees that the potential at the cathode is -0.6 V reaching to 0 when moving toward the anode. Figure 6(b) shows the potential distribution at the middle cross section along the x axis. One can divide the obtained profile into three regions:

1. Potential distribution at the cathode side where the potential distribution has a positive curvature.
2. Potential distribution at the membrane which has a linear shape.

Potential distribution at the anode side where the potential distribution has a negative curvature. The linear part of this profile shows that in the membrane, we do not have any sources of electrical charge. However, the slope of the curve is an indicator for the generated current.

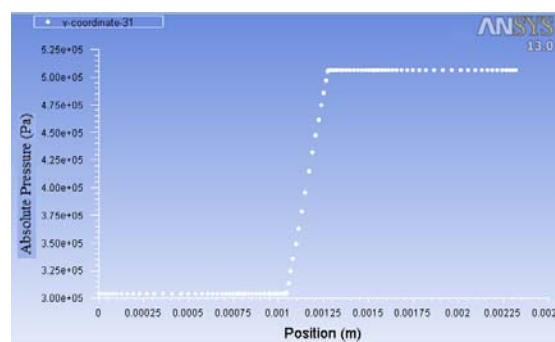


Figure 5: Pressure profile along X axis

The more slope means the higher the current density. The positive and negative curvature at the catalyst layers means that in those areas, we have sources and sinks for generation of electrons. This is completely consistent with the operation of a fuel cell.

The slope of the potential profile (Figure 6(b)) at both ends has become zero. This means that there is no current flow to the gas diffusion layers.

Figure 7(a) is the contour plot of the molar fraction of oxygen. From the figure one sees that the oxygen enters the cell with $X_{O_2} = 0.21$, is consumed along the channel and leaves it with $X_{O_2} = 0.2$.

While the concentration of oxygen varies along the channel, this figure shows that the oxygen concentration at the catalyst layer is almost uniform. This is one of the main roles of GDL which is providing a uniform distribution of oxidant at the reaction site. A uniform distribution of oxidant at the reaction site greatly affects the performance of the fuel cell.

We can observe a similar manner for hydrogen molar fraction which is plotted in Figure 7(b). As it can be seen, hydrogen enters the channel with $X_{H_2} = 0.8$ and leave it with $X_{H_2} = 0.75$. Again we can see that although the hydrogen concentration is not uniformly distributed at the gas channel, but its concentration is almost uniform at the anode catalyst layer.

Finally the characteristic curve of the fuel cell is shown in Figure 8. In this figure, the results of the present study are compared with the numerical results of the reference [10]. This figure shows that the present simulation method is quite accurate.

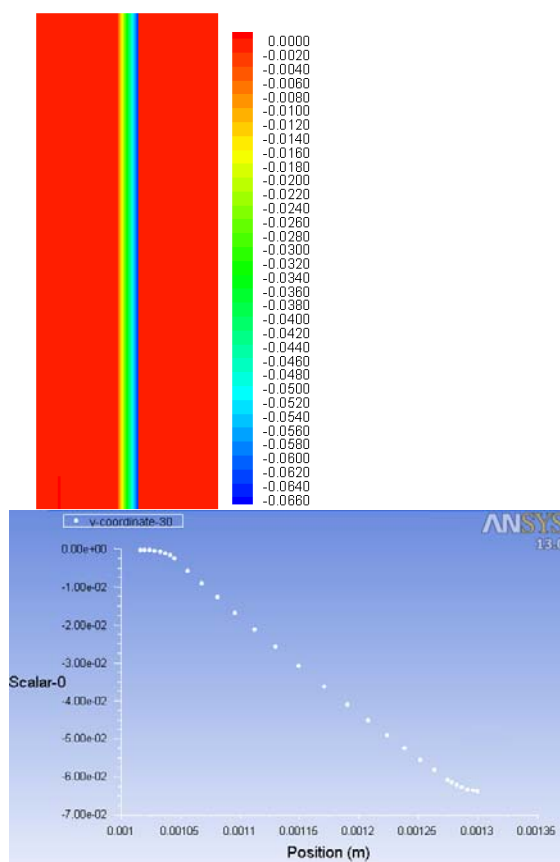


Figure 6: (a): Leveling lines of electric potential (b): electric potentials profile at the middle section

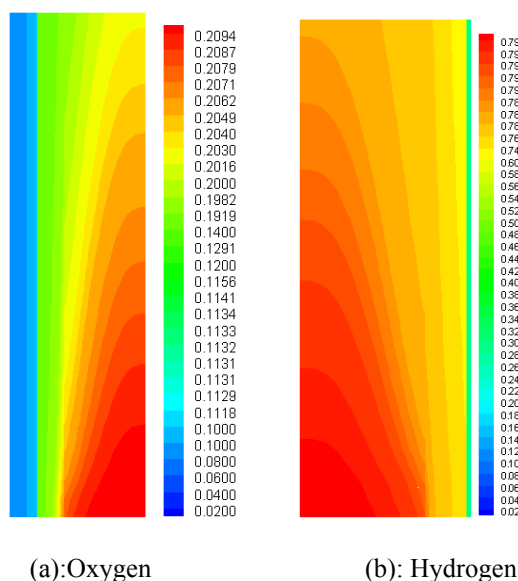


Figure 7: Mass fraction of chemical species

Table 2 : physical parameters and properties at 353k

Quantity	Value at 353K	
Gas channel length, L	7.112	cm
Gas channel height, H	0.2286	cm
Gas channel width	0.0762	cm
Backing layer width	0.0254	cm
Catalyst layer width	0.00287	cm
Membrane width	0.023	cm
Current Collector dimensions in x and z direction	0.0762 x	cmx cm
Fixed charge concentration, c_f	1.2×10^3	mol/cm ³
Oxygen diffusivity in gas	5.2197×10	cm ² /s
Hydrogen diffusivity in gas	2.63×10^2	cm ² /s
Dissolved hydrogen diffusivity in active layer and membrane	1.22×10^6	cm ² /s
Dissolved hydrogen diffusivity in active layer and membrane	2.59×10^6	cm ² /s
Faraday constant, F	96487	C/mol
Hydraulic permeability of membrane, k_p	1.8×10^{14}	cm ²
Permeability of backing layer, K	1.76×10^7	cm ²
Electrokinetic permeability, K_ϕ	7.18×10	cm ²
Universal gas constant, R	8.314	J/mol.K
Fixed site charge, Z_f	-1	
Cathodic transfer coeff, α	2	
Anodic transfer coeff, α_a	2	
Backing layer porosity, ϵ	0.4	
Membrane water porosity, ϵ_m	0.28	
Volume fraction membrane in catalyst layer, ϵ_{mc}	0.4	
Inlet nitrogen-oxygen mole ration, X_{N_2}/X_{O_2}	0.79/0.21	
Air-side inlet pressure/fuel-side inlet pressure	5/3	Atm
O ₂ stoichiometric flow ratio, ζ	3.0	
H ₂ stoichiometric flow ratio, ζ	2.8	
Relative humidity of inlet air/fuel (anode/cathode)	100/0 %	
Ref.exch current density x area of anode, $_{ref}^-$	5.0×10^2	A/cm ³
Ref.exch current density x area of anode, $_{ref}^+$	1.0×10^4	A/cm ³
Total mole concentration at the anode side, c_{tota}	66.817×10^6	mol/cm ³
Total mole concentration at the cathode side, c_{totc}	17.808×10^6	mol/cm ³

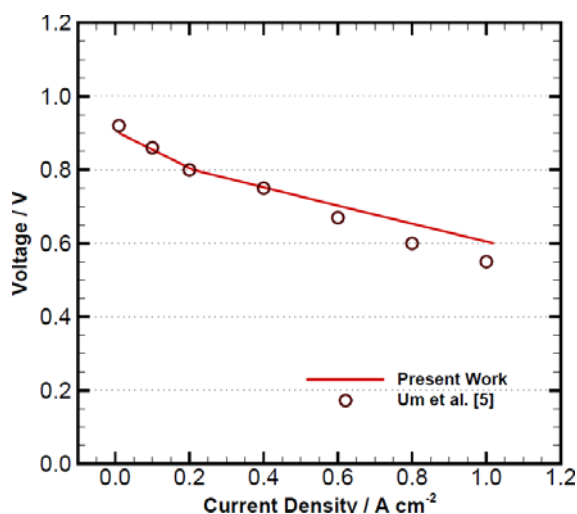


Figure 8: Changes in electrical potential on the solid

CONCLUSION

The governing equations of PEMFC were solved using Fluent software. It is evident that this software does not have intrinsic equations for solving all the required physical variables but it has a facility called UDS which enables one to add extra user-defined scalars to the program. In the present study it was shown that the governing equations of the PEMFC can be casted into the general format of UDS provided by Fluent. Then the whole equations were

solved numerically and the results were compared and verified.

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