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FLOW GEOMETRY OPTIMIZATION OF PROTON EXCHANGE MEMBRANE FUEL CELLS FOR REDUCING CATHODE FLOODING AND PERFORMANCE IMPROVEMENT

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ABSTRACT

This analysis is a three-pronged approach towards optimization of flow geometry, reducing cathode flooding and improving the performance in Proton Exchange Membrane Fuel Cell (PEMFC). The design of the flow geometry is highly responsible for the performance of the PEMFC hence, it is essential to optimize the flow geometry for each flow rate. This exertion numerically analyses three different variants of flow geometry in PEMFC i.e., a 25 cm^2 PEM fuel cell with rib to channel ratio of 2:2, a 25 cm^2 PEM fuel cell with slope of 1:50 & rib to channel ratio of 2:2, and finally a 36 cm^2 PEM fuel cell with slope of 1:20 & rib to channel ratio of 1:1, using tools of Computational Fluid Dynamics (CFD). This study uses hexahedral meshing of the geometry which will be more realistic when compared to those obtained by using tetrahedral meshing. Although there are infinite variants, the arbitrarily selected aforesaid three fuel cell variants are designed and analyzed to find the optimum design of the PEM fuel cell. This primary step was carried out to enhance the performance of PEMFC within the ideal operating voltage range (0.4-0.6 V) such that the fuel cell can function in interference with the battery. The secondary step aims at reducing liquid flooding in the interface between the rib and Gas Diffusion Layer (GDL). In general a stoichiometric ratio of 2.5 is used in experimentation and analysis thus; the tertiary step is to achieve a near stoichiometric reaction by precise optimization of flow geometry, thereby improving the fuel usage. This trident numerical approach is done using FLUENT fuel cell module. The knowledge gained by this analysis will tend towards commercialization and enhanced versatility of fuel cells.

Keywords: cathode flooding, numerically analyses, rib to channel ratio, slopes, hexahedral, stoichiometric

INTRODUCTION

Fuel cells are energy conversion devices which convert the chemical energy of the fuel into electrical energy without conventional conversion step. Fuel cells have advantages of relatively high conversion efficiency compared with conventional power sources, almost no pollution emission during operation, less moving parts (considering fuel cell as a part of the system), multiple choices of potential fuel sources and nearly instantaneous recharge capability compared to batteries [1]. Different fuels are used in fuel cells depending upon the type. Fuel cells are generally classified according to the electrolyte used. Out of many types of fuel cells, Proton Exchange Membrane fuel cells also known as Polymer Electrolyte Membrane fuel cells, hereafter referred as PEM fuel cells, are the most commonly used fuel cells in automotive applications like cars, buses, submarines and airplanes. They are used as primary power source and also as auxiliary power source. The advantages of PEM fuel cells are that they operate at low temperatures, start quickly, have more power to volume ratio and are flexible in orientation as compared to other types of fuel cells [2].

Typically a single PEM fuel cell consists of 9 layers: Anode current collector with grooved gas channels for flow of hydrogen, Anode Gas Diffusion Layer (GDL), Anode

catalyst layer, Electrolyte membrane, Cathode catalyst layer, Cathode Gas Diffusion Layer and Cathode current collector with grooved gas channels for flow of oxygen / air. The same is shown schematically as Figure 1.

Humidified fuel and oxidant are supplied in the gas channels, first these diffuse through gas diffusion layers and then reach the catalyst layers. At the interface of the membrane and the catalyst layer, the half-cell reaction takes place at both electrodes, one is named anode where oxidation is taking place, whereas reduction is taking place at the cathode. The half reactions at anode and cathode are shown in equation (1) and equation (2) respectively. At the anode the hydrogen gas splits into protons and electrons, this specific membrane acting as an electrolyte only allows protons to pass through while the electrons go around the external circuit. At the cathode, electrons and protons combine with oxygen to form water. The overall reaction is depicted in equation (3). This is the way by which we will be able to harness the chemical energy of hydrogen directly into electrical energy [3].

Anode Reaction $H_{2(g)} \rightarrow 2H^+ + 2e^-$ .....(1)

Cathode Reaction $\frac{1}{2}O_{2(g)} + 2H^+ + 2e^- \rightarrow H_2O_{(l)}$ .....(2)

Overall Reaction $H_{2(g)} + \frac{1}{2}O_{2(g)} \rightarrow H_2O_{(l)}$ .....(3)

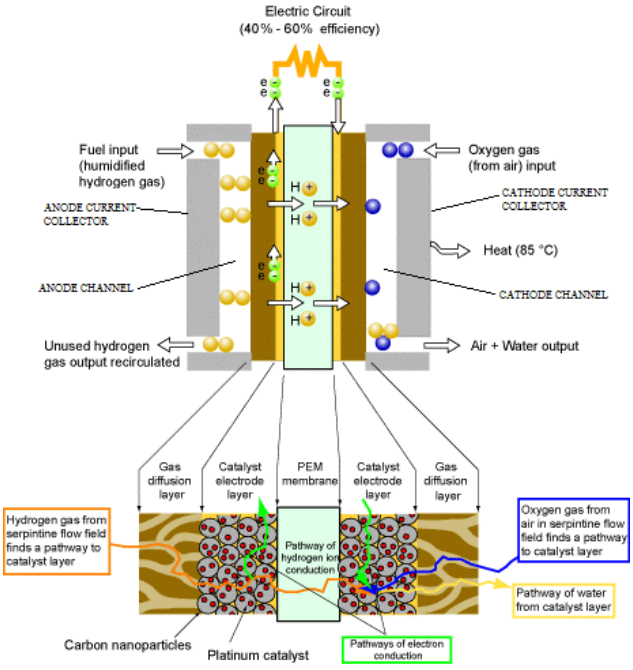

Figure 1. Schematic of Fuel Cell [19]

I. PROJECT OBJECTIVE

The main objective of this work is to reduce cathode flooding and improving the performance in PEM Fuel cell.

The cathode flooding is one of the major problem in PEM fuel cell. Water or moisture plays a key role in the performance analysis of PEM fuel cell. The membrane needs moisture for ionic conductivity and structural integrity. A decrease in water content leads to poor performance of fuel cell membrane whereas an increase in the water content can lead to water flooding of the GDL and catalyst layers and also coverage of the reaction sites with water. Thus a proper water balance is a very critical design parameter of PEM Fuel cell.

In PEM fuel cell, there are different types of flow channel designs available. In which, Serpentine flow channel design have high power output but also high cathode flooding rate and Parallel flow channel design have lower cathode flooding rate but low power output. So a fuel cell model of anode with serpentine flow channel design and cathode with parallel flow channel design is made to reduce the cathode flooding. Further, a slope is added to cathode parallel flow channel design to further reduce the cathode flooding which is likely to increase the PEM fuel cell performance.

To further improve the performance (power) of the PEM fuel cell, we can increase the active area of the fuel cell and decrease the rib thickness.

II. MODELING PROCEDURE

The following three fuel cell models are analyzed.

Model 1 : A 25 cm^2 PEM fuel cell model, with both anode and cathode have serpentine flow channel and rib to channel ratio of 2:2, herein referred as Model 1, as shown in figure 2.

Model 2 : A 25 cm^2 PEM fuel cell, with anode having serpentine flow channel and cathode having parallel flow channel with slope of 1:50 and rib to channel ratio of 2:2, herein referred as Model 2, as shown in figure 3.

Model 3 : A 36 cm^2 PEM fuel cell, with anode having serpentine flow channel and cathode having parallel flow channel with slope of 1:20 and rib to channel ratio of 1:1, herein referred as Model 3, as shown in figure 4.

A. Design Phase

Design of above mentioned Fuel cell models are done using SOLIDWORKS 2012.

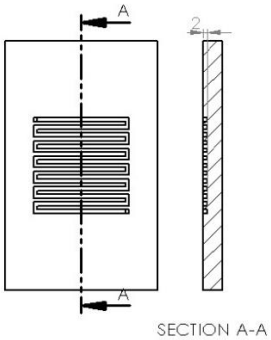

Figure 2. Serpentine flow channel design of graphite plate of Model 1 Fuel cell.

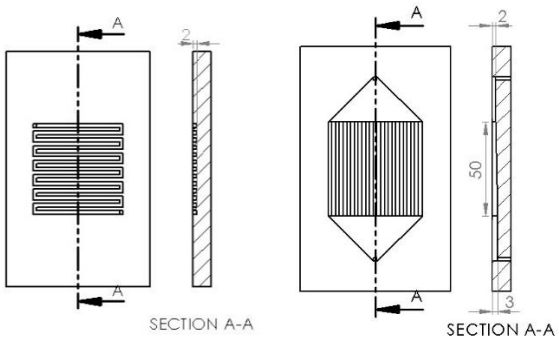

Figure 3. Anode (left) and Cathode (right) graphite plate of Model 2 Fuel cell.

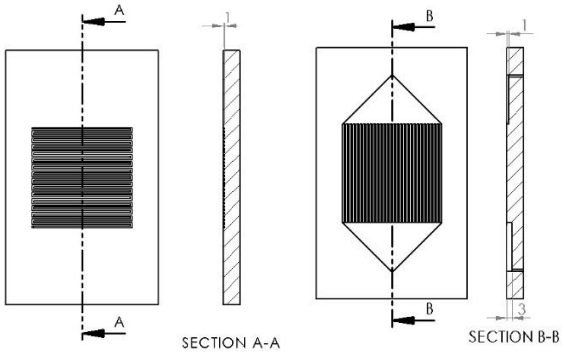

Figure 4. Anode (left) and Cathode (right) graphite plate of Model 3 Fuel cell.

The dimensions of the Membrane Electrode Assembly (MEA) are shown in Table I.

TABLE I
MEMBRANE ELECTRODE ASSEMBLY DIMENSIONS [17]

Components	Thickness
Catalyst Layer (Anode)	25 µm
Catalyst Layer (cathode)	50 µm
Gas Diffusion Layers	360 µm
Membrane	50.8 µm

B. Meshing and Simulation Phase

Meshing of above designed fuel cell models are done using ICEM CFD.

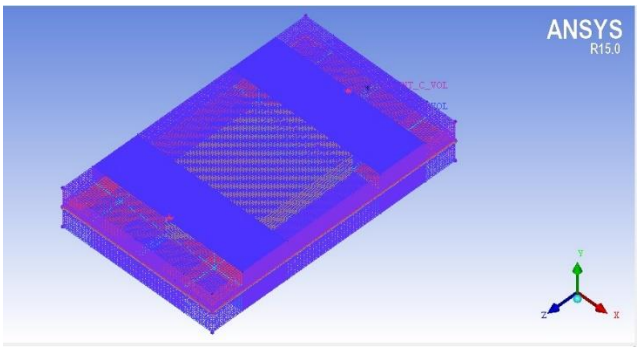

Figure 5. Meshing diagram of Fuel cell.

Tetrahedral cells are preferred for complex geometry because of ease of fitting in the volume but for relatively simple geometries of fuel cell, hexahedral elements are preferred because of their ability to generate a uniform and conformal mesh with lesser number of elements therefore in this study hexahedral elements were used. The details of the mesh are shown in Figure 5 and Figure 6.

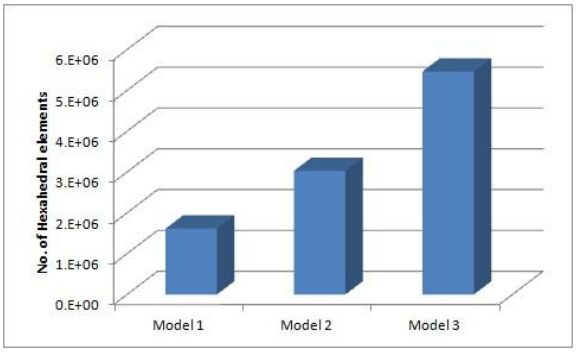

Figure 6. Meshing details of all three Fuel cell Models.

Once the mesh was created and zones and surfaces are identified in ANSYS ICEM CFD, it was imported in the ANSYS FLUENT software. Material properties boundary conditions, initial conditions, operational conditions and modelling parameters were defined. The software computes the results of coupled non-linear equations, the details of which are given in [9][12].

Table II gives the material properties used for the fuel cell model and Table III gives the boundary conditions applied for the fuel cell models respectively. The boundary conditions were selected and flow rates and mass fractions were calculated so as to match the experimental conditions.

This study was carried out using fuel cell module were activated [12] which leads to the assumptions of steady state, non-isothermal, multiphase flow in the GDL using mixture model and isotropic properties of the GDL and considers the following.

Joule heating: It takes the heat generated by charge transport in energy source term.

Electrochemistry Sources: It accounts for the electrochemistry effects in the model.

Reaction heating: It takes the heat generated by chemical reaction in energy source term.

Butler-Volmer Rate: It takes account of transfer currents inside the catalyst layers. Transfer currents are approximated by Tafel approximation when this option is not used.

Membrane Water Transport: It takes account of movement of water inside the membrane.

TABLE II
MATERIAL PROPERTIES [18]

Com ponents	Property	Units	Current Studv
Bipolar plates	Electrical conductivity	S/m	7500
	Thermal conductivity	W/m K	31.5
Catalyst layers	Active surface area per unit volume	m^{-1}	2×10^5
	Electrical conductivity	S/m	1800
	Permeability	m^2	1.45×10^{-11}
	Thermal conductivity	W/m K	12
	Porosity		0.112
Gas diffusion layers	Electrical conductivity,	S/m	1800
	Permeability	m^2	1.45×10^{-11}
	Thermal conductivity	W/m K	12
	Porosity		0.4
	Density	kg/m^3	2719
Electrolyte	Equivalent weight	kg/kmol	1100
	Thermal conductivity	W/m K	0.36
	Electronic conductivity	S/m	1×10^{-16}
	Density	kg/m^3	1980

TABLE III
BOUNDARY CONDITIONS [17]

		Units	Current Study	Reference
Fuel cell Temperature		°C	60	[17]
Anode humidification temperature		°C	60	[17]
Cathode humidification temperature		°C	60	[17]
Anode pressure		bar	4	[17]
Cathode pressure		bar	4	[17]
Anode flow rate		kg/s	2×10^{-6}	calculated
Cathode flow rate		kg/s	6.08×10^{-6}	calculated
Inlet mass fraction Anode	H_2	%	34	calculated
	H_2O	%	3	calculated
Inlet mass fraction Cathode	O_2	%	89.09	calculated
	H_2O	%	0.5	calculated
	N_2	%	10.41	calculated

Multiphase: It computes the approximate liquid water transport inside the Gas Diffusion Layer.

The solution controls are done by F-Cycle with BCGSTAB (bi- conjugate gradient stabilized method) was selected for the solution of the three species equations, electrical and potential equations and saturation equations. The termination criteria were lowered from default 0.01 to 0.001 for species and saturation equations whereas the termination criteria for two potential equations are reduced further to 0.0001, as recommended by the ANSYS Inc. fuel cell module.

Another important parameter in numerical simulation is under-relaxation factor. In pressure-based solver, under-relaxation factor soothes the convergence behaviour of outer nonlinear iterations with the help of an additional multiple of the computed change in the quantity [13] . Lower values of under-relaxation factor results in slow convergence whereas high values of under relaxation factors can result in divergence or an oscillating value of the solution. The most favourable value of under relation factor depends upon the how and is required to be sought for each case differently [14]. In this study the under relation factor were fixed according to the recommendations of ANSYS FLUENT for fuel cell simulations initially and then tailored according to diverging or converging results in first few simulation runs. The under relaxation factors were set finally as in Table IV.

TABLE IV
UNDER RELAXATION FACTORS [18]

Quantity	Under Relaxation Factor
Energy	1.0
Electric potential	1.0
Protonic potential	0.95
Water saturation	0.5
Water content	0.95
Pressure	0.7
Density	1.0
Momentum	0.3
H_2	1.0
O_2	1.0
H_2O	1.0

An important indicator or solution convergence is the residual between two consecutive calculations. A declining graph of' residuals means that solution is progressing towards convergence whereas the increasing values of residuals indicate divergence. In this study, the solution was taken as converged when the mass continuity residual was in the order of 10^{-3} and the difference between anode and cathode currents was less than 0.0001 A/cm^2.

III. RESULTS AND DISCUSSION

Design and Simulation of all three Fuel cell Models are completed and their results are discussed below.

A. Validation of Simulation Results of Model 1 with the Experimental data

Validation of simulation results with the experimental data is required when pursuing a Numerical simulation.

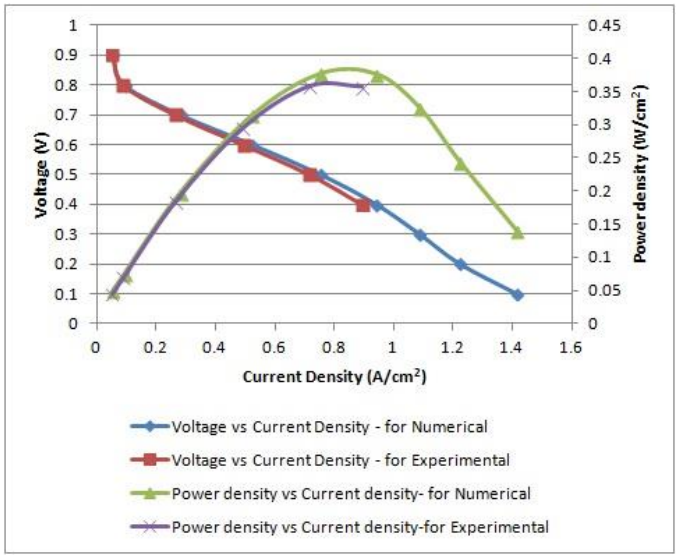

Figure 7. Comparison of Polarization and Performance Curve of Experimental data and Numerical results of Model 1.

It is clear from Figure 7, the polarization curve (voltage vs current density) and performance curve (power density vs current density) for numerical simulation of Model 1 matches with experimental results [17]. The average error percentage between them is around 5%.

B. Comparison of Numerical results of Model 1 and Model 2

Both the Numerical Results of Model 1 and Model 2 are compared below.

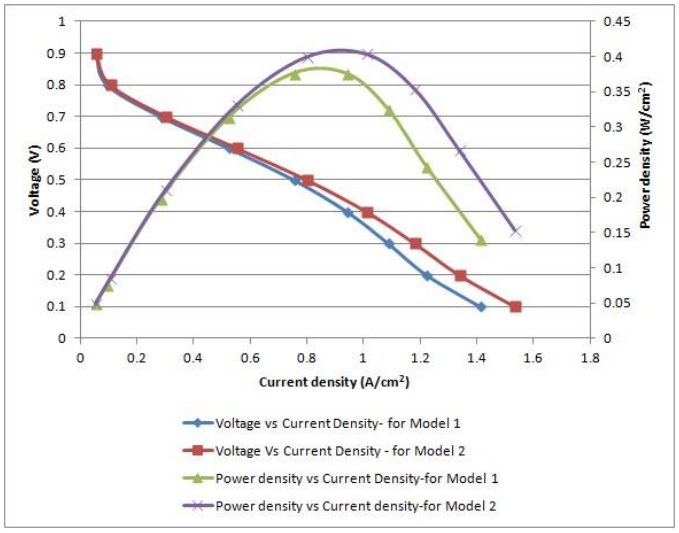

Figure 8. Comparison of Polarization and Performance Curve of Model 1 and Model 2.

Figure 8 shows the polarization curve and performance curve of model 1 and model 2. The polarization curve and performance curve of model 2 shows better results than that of model 1. So from that, we can say, increase in the slope of cathode channel, increases the performance of the fuel cell.

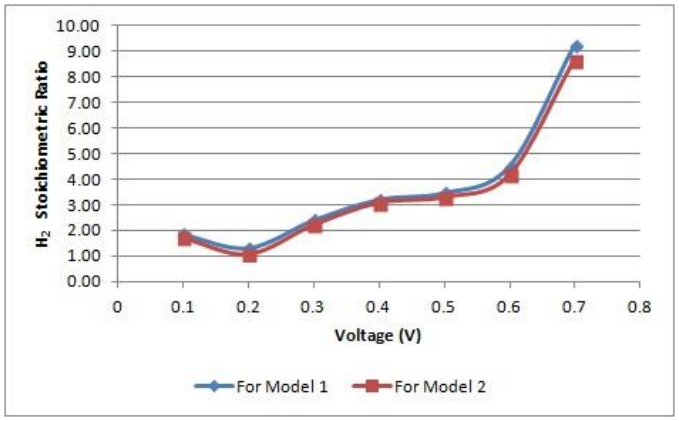

Figure 9. Comparison of H_2 stoichiometric ratio of Model 1 and Model 2 for different voltage.

Figure 9 shows the stoichiometric curve of model 1 and model 2 for different voltage. The fuel (H_2 gas) wastage of model 2 is lesser when compared to that of model 1. So from that we can say, increase in the slope of cathode channel, decreases fuel wastage.

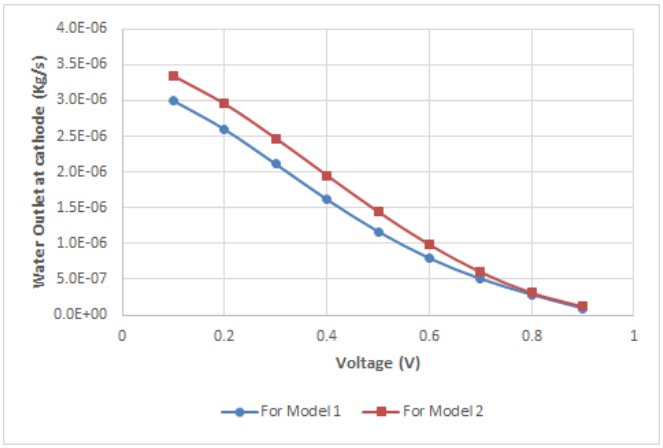

Figure 10. Comparison of Cathode channel water outlet of Model 1 and Model 2 for different voltage.

Figure 10 shows the water removal rate at cathode of model 1 and model 2 for different voltage. The water removal at cathode of model 2 is more when compared to that of model 1. So from that we can say, increase in the slope of cathode channel, will increase cathode water removal.

C. Comparison of Numerical results of Model 2 and Model 3

Both the Numerical Results of Model 2 and Model 3 are compared below.

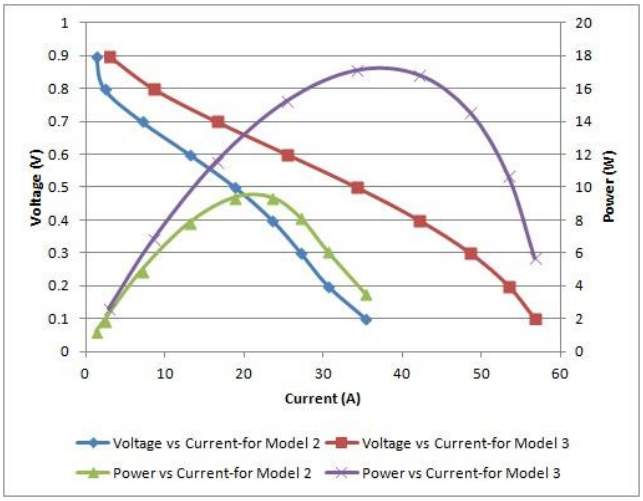

Figure 11. Comparison of Polarization and Performance Curve of Model 2 and Model 3.

Figure 11 shows the polarization curve and performance curve of model 2 and model 3. The polarization and performance curve of model 3 shows better results than that of model 2. So from that we can say, increase in the slope of cathode channel, decrease in rib thickness, increase in cell active area will increases the performance of the fuel cell.

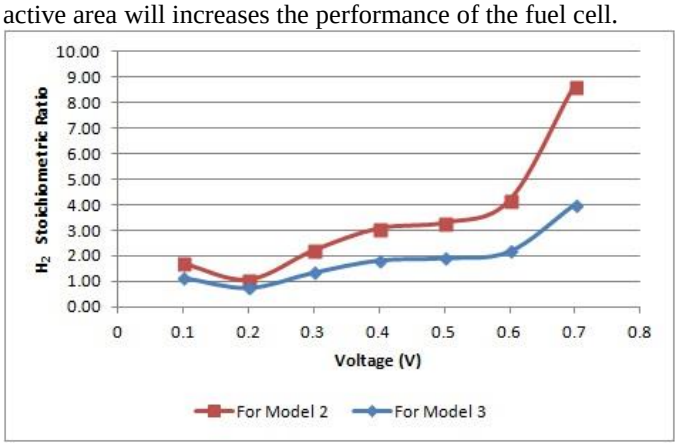

Figure 12. Comparison of H_2 stoichiometric ratio of Model 2 and Model 3 for different voltage.

Figure 12 shows the stoichiometric curve of model 2 and model 3 for different voltage. The fuel (H_2 gas) wastage of model 3 is lesser when compared to that of model 2. So from that we can say, increase in the slope of cathode channel, decrease in rib thickness, increase in cell active area will decreases fuel wastage.

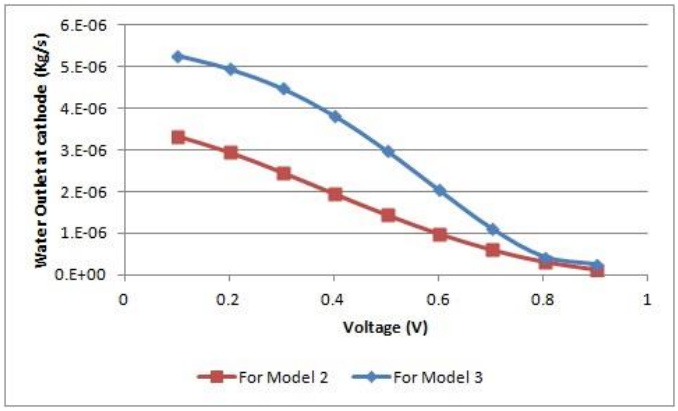

Figure 13. Comparison of Cathode channel water outlet of Model 2 and Model 3 for different voltage.

Figure 13 shows the water removal rate at cathode of model 2 and model 3 for different voltage. The water removal at cathode of model 3 is more when compared to that of model 2. So from that we can say, increase in the slope of cathode channel, decrease in the rib thickness, increase in cell active area, will increase cathode water removal.

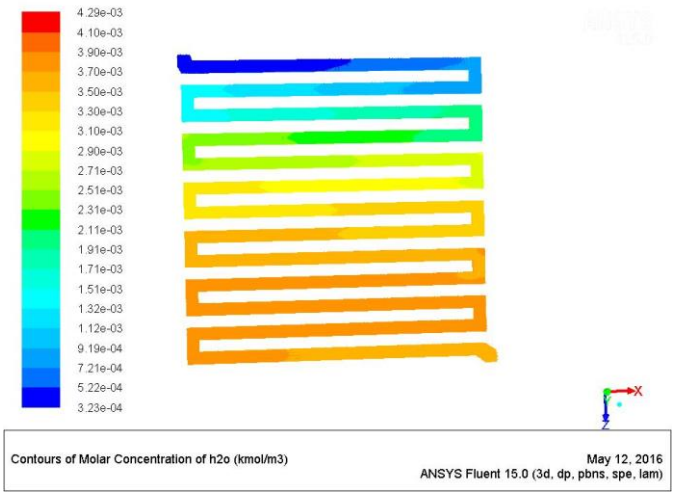

Figure 14(A).Molar concentration of H_2O in cathode channel in model 1.

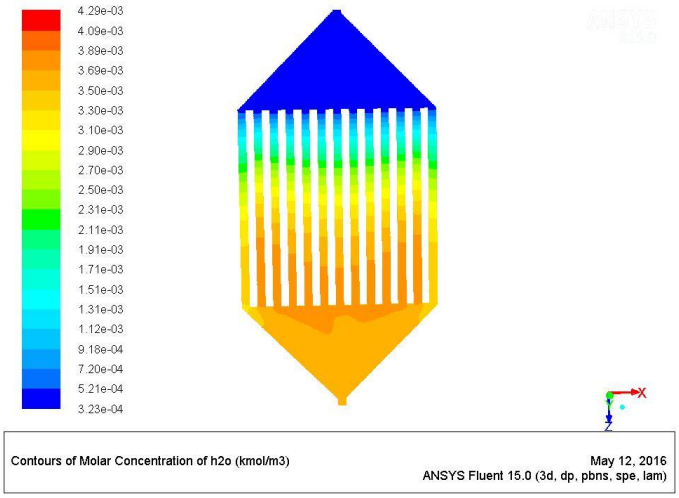

Figure 14(B).Molar concentration of H_2O in cathode channel in model 2.

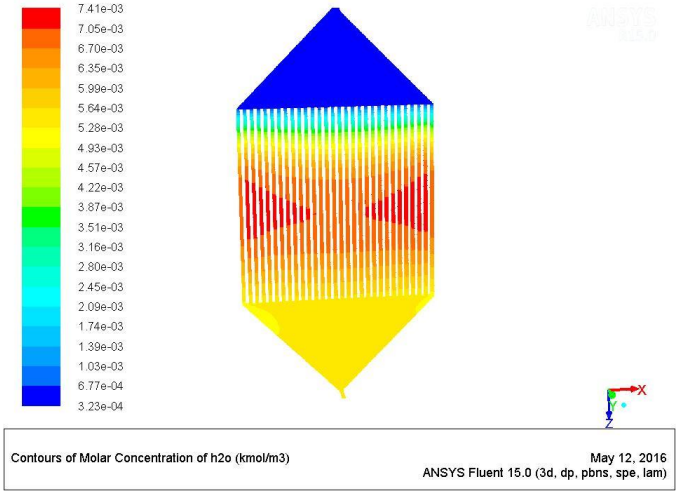

Figure 14(C).Molar concentration of H_2O in cathode channel in model 3.

Figure 14 (A), 14(B) and 14(C) are the graphic plot of molar concentration of H_2O in cathode channel for models 1, 2 and 3.

From which we can say that, among the models considered cathode flooding rate is lesser for model 2 when compared to model 1, and least for model 3.

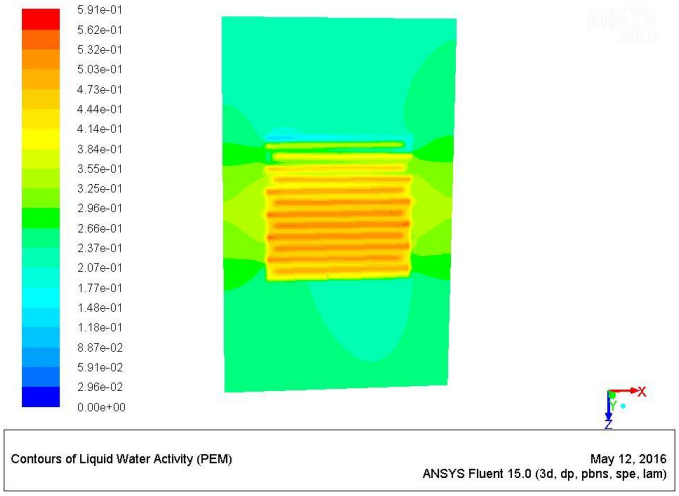

Figure 15(A).Membrane liquid water activity for model 1.

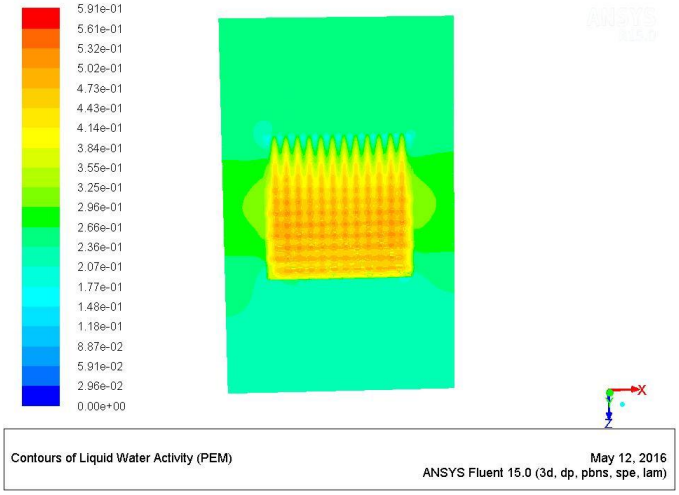

Figure 15(B).Membrane liquid water activity for model 2.

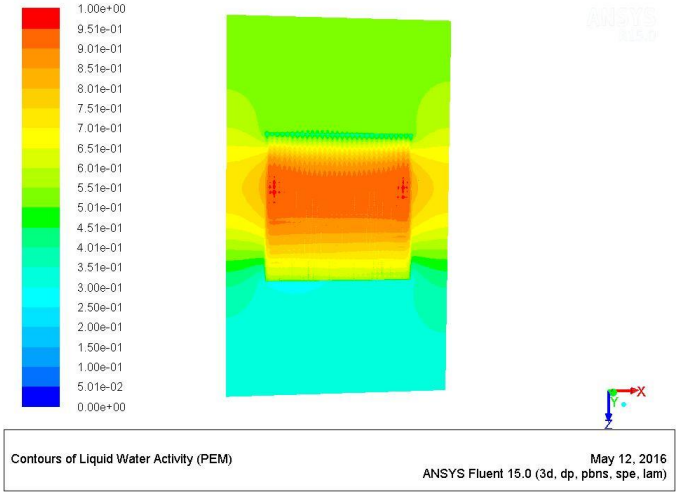

Figure 15(C).Membrane liquid water activity for model 3.

Figure 15(A), 15(B) and 15(C) shows liquid water activity in membrane for model 1, 2 & 3. Liquid water activity in membrane for model 2 is more when compared to that of model 1. Also liquid water activity in membrane for model 3 is more when compared to that of model 2 and model 3.

IV. CONCLUSION

From above results, we can conclude that using parallel flow channel with slope will improve the fuel cell performance and also reduce the rate of cathode flooding. On further investigation, increase in the slope of parallel cathode channel & increase in cell active area or decrease in graphite plate rib thickness is also proven to increase fuel cell performance drastically and huge drop in the cathode flooding rate.

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