Analysis of Parameters Influencing the Performance of PEM Fuel Cell by ANSYS

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Abstract: **Proton exchange membrane (PEM) fuel cells are promising power generation sources for mobile and stationary applications. However, there are several technical problems to be solved in order to achieve practicability and popularization. Especially, water management inside a PEMFC is essential for high performance operation. "Water flooding" and "dry out" is a critical barrier for high efficiency and high power density. To alleviate these issues, it is necessary to analysis the Proton Exchange Membrane Fuel Cell for different gas flow parameters and serpentine model is chosen with the area of 25 cm² by varying the temperature and pressure are analyses and the optimum temperature and pressure are chosen from ANSYS 14.5 software.**

Keywords: **PEM, water management, flooding, dry out, flow parameters.**

1. Introduction

Fuel cell is the device in which electro chemical reaction takes place where chemical energy in the fuels is directly converted into electrical energy. The fuel cells can be operated for energy conversion with higher efficiency; they are not limited by the thermodynamic restrictions of conventional power systems, like Carnot efficiency. Additionally they have low environment impact as combustion process and no pollutants are generated. The fuel cells are currently under rapid development and promise to become an economically viable commercial power source in many areas, especially for transportation, stationary, portable and automobile applications, because of their high energy density at low operating temperatures and zero emissions.

A typical fuel cell power system consists of different components:

 Single cells, where electrochemical reactions occur. Single unit cells are the core of a fuel cell. They convert chemical energy into electrical energy.

• Stacks, consisting of the necessary number of cells and they are connected to provide the required power capacity.

In a PEM fuel cell, hydrogen is continuously supplied to the anode or negative electrode, and an oxidant, often oxygen or air, is also continuously supplied to the cathode or positive electrode. Electrochemical reactions occur at the electrodes, generating an electric current through the electrolyte thus driving the corresponding electric current that performs the electric work on the load.

At the anode, hydrogen is fed to the cell and a reaction takes place at the catalyst layer:

$$
H_2 \longrightarrow 2H^+ + 2e^-
$$

The protons migrate through the polymeric membrane and react with the oxygen and the electrons at the cathode catalyst layer:

$$
1/2O_2 + 2H^+ + 2e^- \longrightarrow H_2O
$$

Therefore, the overall reaction taking place in the cell is:

$$
H_2+1/2O_2 \longrightarrow H_2O
$$

Fuel cells are modular, so that unit cells can be combined into a stack to achieve the voltage and power required for the specific application. This involves connecting multiple unit cells in series via electrically conductive materials.

2. Literature Review

AtillaBiyiokoglu [1] presented complete computational model for fuel cell including its all phenomena together, This would be very useful to conduct analytical/numerical studies on fuel cells. In his study governing equations and assumptions were briefly reviewed and presented.

Aysu [2] discussed in his study about the water formation in a fuel cell when using parallel and serpentine type flow channels in the fuel cell. In his study parameters like rate of water injected rate, flow field type, electrode size, velocity and temperature of humidified gas and temperature of the model were considered. As per his study the serpentine flow filed type showed better performance than normal parallel flow type.

Biao Zhou wenbohuang and Andrzejsobiesisk [3] developed a steady state two-dimensional mathematical model with pressure and phase change effects and illustrated inlet humidification and pressure effects on PEM fuel cell performance using this model. This was used to predict the following parameters along the fuel cell channels: mole no of liquid model and water vapour, pressure, temperature, density, viscosity, vapor mole fraction, volume flow rate, required pumping power and current density.

Ferng et al. [4] described in their study the effects of operating temperature and pressure on fuel cell performance. The predicted performance at elevated temperature.

GalipH.Guvelioglu and Harvey G.Stenger [5] analyzed the performance at various hydrogen flow rates, air flow rates and humidification levels. They showed that hydrogen and air flow rates and their relative humidity were crucial to current density, membrane dry out and electrode flooding. Uniform current densities along the channels are known to be crucial for thermal management and fuel cell life.

Grujicic.M, K.M. Chittajallu [6] The performance of polymer electrolyte membrane (PEM) fuel cells is studied using a single-phase two-dimensional electrochemical model. The model is coupled with a nonlinear constrained optimization algorithm to determine an optimum design of the fuel cell with respect to the operation and the geometrical parameters of cathode such as the air inlet pressure, the cathode thickness and length and the width of shoulders in the interdigitated air distributor. The results obtained are rationalized in terms of the effect of the fuel-cell design on the air flow fields and the competition between the rate of species transport to and from the cathode active layer and the kinetics of the oxygen reduction half-reaction.

Henriques.T et al. [7] developed a three dimensional model of the original PEM fuel cell with parallel plus a transversal floe channel design using Comsol Multi physics. Using this model the effects of different channel geometries and respective cathode flow rates on the fuel cell's performance were studied. This model gives improvement in fuel cell efficiency up to 26.4%.

Mengbo Ji and Zidong Wei [8] The major issue impacting the performance and durability of PEM fuel cells, namely the water management, has been methodically reviewed.Water management strategies must be addressed with due consideration to the overall system design, to maintain the overall system simplicity and minimize the system parasitic power loss, thereby decreasing the costs and increasing reliability. Of all strategies against water flooding, materials and structures of the MEA should be given more attention because the first drop of water is produced therein, and there is almost no any significant parasitic power loss and on assistant equipment is needed by adjusting materials and structures of the MEA. The separate channels for water and reactant gases transport, specifically, in a porous electrode would be a promising way for the final solution of water flooding harassing PEMFCs.

Ruy Sousa Jr and Ernesto R.gonzalez [9] discussed the possibilities of methanol in fuel cell instead of Hydrogen. They had developed mathematical modeling of polymer electrolyte fuel cells for discussing electro catalysis of the reactions and water management schemes to cope with membrane dehydration.

Shawn Litster et al. [10] Proton exchange membrane PEM fuel cells require humidified gases to maintain proper membrane humidification, but this often results in a problematic accumulation of liquid water. Typically, excessive air flow rates and serpentine channel designs are used to mitigate flooding at the cost of system efficiency. The system also employs an external electro-osmotic _EO_ pump that actively removes excess water from the channels and gas diffusion layer. For a 25 cm2 fuel cell with 23 parallel air channels, we demonstrate a 60% increase in maximum power density over a standard graphite plate with a low air stoichiometry of 1.3. Experimental and modeling results show that simple passive water transport through the porous carbon alone can prevent flooding at certain operating conditions and flow field dimensions.

3. Problem Identification

3.1 Water Management

Water plays an important role in PEM Fuel cells.

- Water is required for humidification and stack cooling and it is produced by the fuel cell during power generation.
- PEM Fuel membrane conductivity depends on membrane humidity, hence water has to be fed into the stack for good fuel cell good performance. – gas humidification by bubbling through water, or using membrane gas humidification is adopted usually- new methods to be explored.

Fig.1 Water Management

- Excess water has to be removed to avoid flooding of the electrode pores, for good performance.
- Maintaining optimum water balance in the fuel cell stack and entire system requires proper design, control strategies.

3.2 Objective

The main objective of this work is to analyse the better performance of a 2x2 serpentine flow channel by varying flow parameters like temperature and pressure along with the bend angles will be chosen to have better improvement in the fuel cell technologies.

4. Ansys Fluent 14.5

4.1 Introduction

Ansys Fluent was chosen as the fuel cell modeling software because it is currently the most complete three-dimensional modeling software commercially available. Their implementation of a fuel cell model is fairly complete and includes a straight forward graphical user interface which simplifies the modeling and simulation effort. The software is also capable of being run in parallel so that larger and more computationally demanding simulations can be completed in reasonable time frames.

The workflow involves three major steps. The first step is modeling the geometry of the fuel cell using PRO - E software. The geometrical model forms the basis for creating a computational mesh. The second step involves creating the mesh from the geometry. In order to solve the myriad of equations associated with a fuel cell simulation, the entire cell is divided into a finite number of discreet volume elements or computational cells. The relevant equations are then solved in each individual cell and integrated over the computational domain to give a solution for the entire domain. Many other factors must also be taken into account in order to generate a computational mesh provides representative results when simulated. The third and final step involves inputting the various physical and operating parameters of the simulation. Some of these include thermal and electrical properties of the various materials, operating temperatures and pressures, inlet gas flow rates, open circuit voltage, porosity, and humidification among many others.

4.2 Modeling And Simulation

In Ansys Fluent 14.5, the modeling and simulation of a PEM fuel cell involves three basic steps. The first step is to create the geometry of the fuel cell using PRO - E software. It is found that the best software for this purpose is a combination of Creo Elements and Ansys Design Modeler, which is part of the Ansys Fluent software package.

The second step involves decomposing the geometry into a computational mesh. Ii explored in two options for performing this task. The first involves using Ansys Meshing, which is part of the workbench. It is found that using the workbench meshing is more straight forward and easier to use, but suffers from limited applicability to more complex geometries. ANSYS 14.5 is a powerful program with several idiosyncrasies which must be worked around in order to generate a good mesh.

The third and final step in the process is to generate a simulation based on the computational mesh. This step requires the careful monitoring of input variables. There are at least 100 different variables to input, some directly related to model and material properties, and others that are related to the solver methodology. The simulation process includes creating automated scripts to generate data and setting up the simulation for parallel processing. Examples are given for basic commands for running

jobs on the Linux based computer cluster at Arizona State University, but these commands are applicable to many cluster computers employing a Moab-Terascale Open-Source Resource and QUEue manager / Portable Batch System (TORQUE/PBS) to manage the scheduling of batch jobs.

Importing the external geometry

File \rightarrow import \rightarrow parasolid file \rightarrow open

The Design Modeler should show an import under the tree outline with a lightning bolt next to it. Press the generate button and the geometry should show up in the graphics window.

Generating a face on channel openings

Creating a lines from points for channel boundary

Fig.3 Creating lines from points

Under details view, change the operation to "add frozen" by clicking on the field and using the pull down menu that appears.

Once the line has been generated, a surface can be defined by the created line and the three other edges of the channel wall. To do this,

```
\longrightarrow Surfaces from edges \longrightarrow Apply
Generate
```
(Repeat this process for all other channel openings until they have all been covered by surfaces.)

After the surfaces are created the channels can be filled in using the fill tool.

 $tools \longrightarrow Fill \longrightarrow Generate$

(The geometry should now have 13 parts in it.)

Rename the 9 fuel cell parts using the following naming convention depicted in figure 6.5. The part names should include Current a, channel a, gdl a, catalyst_a, membrane, catalyst_ ϕ , gdl_c, channel_c, current_c.

4.3 Blocking

The purpose of blocking is to designate different areas of the mesh that should be meshed differently. Blocking is a way to control which areas of the mesh are finer and which areas are left coarser. An initial block is created and then split into several individual blocks, with each new split block corresponding to a different region of the fuel cell. Many fuel cell designs have very simple geometries which are relatively simple to block.

Fig.5 Spliting of Parts

4.4 Meshing Parameters

Once the blocks have been created it is possible to change the number of nodes at each edge of the block. Changing the edging parameters is one of the fastest and easiest ways. Begin by first turning on edging by expanding the blocking section of the model tree and right clicking on edges and selecting counts from the context menu.

Fig.6 Meshing Parameters

Fig.4 Setting of Blocking

Once the initial block is generated, it can then be split by using the split block tool. Splitting works by choosing an edge, and then designating where along that edge the split should be placed. Change the split method to prescribed point and press the select edge button to activate select mode. Then, select the left vertical wall edge of the fuel cell geometry

4.5 Generating Mesh With Solution Controls

Select the compute mesh tool. The volume mesh should be selected by default. Change the mesh type to Cartesian, change the enforce split to final, which will cause the Cartesian file box to appear, and select your Cartesian grid file. This file should have the same name as your project with a .crt file extension. Then click compute and mesh generation will begin.

The default solver settings are not sufficient to obtain a converged solution. Therefore, the following modifications must be made.

- 1. Set the under-relaxation factor for Pressure to 0.7, Momentum to 0.3, Protonic Potential to 0.95, and Water Content to 0.95.
- $Solve \longrightarrow$ Controls \longrightarrow Solution
- 2. Modify the multigrid settings.
	- Solve \longrightarrow Controls \longrightarrow Multigrid (a) Select F-Cycle from the Cycle Type drop-down lists for all equations.
	- (b) Enter 0.001 for Termination Restriction
	- for h2, o2, h2o, and Water Saturation.
	- (c) Select BCGSTAB from the Stabilization Method drop-down list for h2, o2, h2o, Water Saturation, Electric Potential and Protonic Potential.
	- (d) Enter 0.0001 for Termination Restriction
	- for Electric Potential and Protonic Potential.
	- (e) Increase the value of Max Cycles to 50 in the Algebraic Multigrid Controls group box.
	- (f) Click OK to close the Multigrid Controls

Fig.7 Advanced solution controls

 0.77777777

3. Enable the plotting of residuals.

 $Solve \longrightarrow$ Monitors $Residual$

- 4. Initialize the solution.
	- $Solve \longrightarrow \text{Initialize} \longrightarrow \text{Initialize}$
	- (a) Set Temperature to **353 K.**
	- (b) Click Apply.

(c) Click Initialize and close the Solution Initialization panel.

5. Save the case and data files as pem-singlechannel.cas.gz and pem-single-channel.dat.gz.

- File **Write Case & Data...**
- 6. Request 200 iterations.

The solution residuals will drop to acceptable values.

Fig.8 Iteration process ends with Solution is Converged

5. Results And Discussions

 (2x2) Serpentine Flow Channel

Fig.9 Polarization curve

The serpentine flow channel $2x290^0$ bend is analyses by varying the voltage at constant operating temperature of PEM fuel cell and from the solution, the current density are calculated and this chart shows that at 0.75V, the power density will be maximum.

(2) On Comparing With Different Operating Temperature

Current

Table 4 Power density obtained for 303 K

(2x2) Serpentine Flow Channel

Table 5 Various parameters involved for analyzing 90⁰ bend at 313 K

Table 6 Power density obtained for 313 K

Fig.11 Polarization curve for 313 K

The serpentine flow channel $2x290^0$ bend has better performance compared with the U bend and hence the 90° bend is analyses by varying the operating temperature of fuel cell at 313K it shows 0.755463 W/cm² at 0.75V.

(2x2) Serpentine Flow Channel

Fig.10 Polarization curve for 303 K

The serpentine flow channel 2x2 has better performance compared with the U bend and hence the is analyses by varying the operating temperature of fuel cell at $303K$ it shows 0.7439795 W/cm² at 0.75V.

S.No.	Parameters		Values		
1	Area		25 cm^2		
2	Temperature		323 K		
3	Pressure		2 bar		
4	Mass flow rate		Anode		Cathode
			6.9X10 7kg/s		$1.3X10^{-6}$ kg/s
Current density $(A/cm2)$		Voltage(V)	Power density $(W/cm2)$		
1.045392		0.05	0.0522696		
1.046144		0.15	0.1569216		
1.04644		0.25	0.26161		
1.046134		0.35	0.3661469		
1.04594		0.45	0.470673		
1.045441		0.55	0.57499255		
1.045563		0.65	0.67961595		
1.015186		0.75	0.7913895		
0.724988		0.85	0.6162398		
0.054176		0.9	0.0487584		

analyzing 323 K

Table 8 Power density obtained for 323 K

Fig.12 Polarization curve for 323 K

The serpentine flow channel 2x2 has better performance compared with the U bend and hence the is analyses by varying the operating temperature of fuel cell at $323K$ it shows 0.7913895 W/cm² at 0.75V.

(2x2) Serpentine Flow Channel

Table 9 Various parameters involved for analyzing 353 K

Table 10 Power density obtained for 353 K

Fig.13 Polarization curve for 353 K

The serpentine flow channel 2x2 has better performance compared with the U bend and hence the analyses by varying the operating temperature of fuel cell at $353K$ it shows 0.754005 W/cm² at 0.75V.

(2) On Comparing With Different Operating Pressure)

Table 11 Various parameters involved for alyzing 0.5 bar

Current density $(A/cm2)$	Voltage(V)	Power density $(W/cm2)$	
2.912831	0.15	0.43692465	
2.43965	0.25	0.6099125	
1.983132	0.35	0.6940962	
1.545939	0.45	0.69567255	
1.131207	0.55	0.62216385	
0.743075	0.65	0.48299875	
0.38924	0.75	0.29193	
0.097289	0.85	0.08269565	
0	0.95		

Table 12 Power density obtained for 0.5 bar

Fig.14 Polarization curve for 0.5 bar

The serpentine flow channel $2x^2$ 90^0 bend are analyses at 0.5 bar pressure which is below the atmospheric pressure. It shows higher performance but it is not a suitable level because, a single unit cell produces maximum of 1 W/cm².

(2x2) Serpentine Flow Channel

Table 13 Various parameters involved for analyzing 1 bar

Fig.15 Polarization curve for 1 bar

The serpentine flow channel 2x2 are analyses at 1 bar pressure which is below the atmospheric pressure. It shows higher performance but it is not a suitable level because, a single unit cell produces maximum of 1 $W/cm²$.

(2x2) Serpentine Flow Channel

Table 14 Power density obtained for 1 bar

S.No.	Parameters	Values		
	Area	25 cm^2		
$\overline{2}$	Temperature	353 K		
3	Pressure	2 bar		
4	Mass flow rate	Anode $1.3x10^{-6}$ kg/s	Cathode $4.3x10^{-5}$ kg/s	

Table 16 Power density obtained for 1.5 bar

Fig.16 Polarization curve for 1.5 bar

The serpentine flow channel $2x^2$ 90^0 bend are analyses at 1.5 bar pressure which is above the atmospheric pressure. It shows higher performance but it is not a suitable level because, a single unit cell produces maximum of W/cm²

(2x2) Serpentine Flow Channel

Table 17 Various parameters involved for analyzing 2 bar

Table 18 Power density obtained for 2 bar

Fig.17 Polarization curve for 2 bar

The serpentine flow channel 2x2 are analyses at 2 bar pressure which is above the atmospheric pressure, and it shows performance but it is suitable level because, a single unit cell produces maximum of 1 W/cm² and hence 2 bar provides better performance.

6. Conclusion

To alleviate the water management issues, we are creating serpentine flow channels with varying temperature of 303 K, 313 K, 323K, 353K and Pressure of 0.5 bar, 1 bar, 1.5 bar, 2 bar ratio for analyzing to get numerical validation using ANSYS FLUENT software and the optimum design channels

On comparing the temperature of fuel cell, it will be operating from 30^0C-150^0C , the low temperature fuel cell is choosen i.e., 30^{0} C- 80^{0} C and their corresponding performances are individually evaluated. Among those temperatures 323 K has better performance and it is choosen for further pressure analysis.

The main flow parameter of pressure are varied by keeping constant temperature and mass flow inlet (anode & cathode), the performance are analyst at 0.5, 1, 1.5, 2 bar. Since 0.5&1 bar are below atmospheric pressure, it will not choosen even though it shows better performance. The result of the 1.5 bar provides more than 0.9 W/cm², which is not a optimum range of a single fuel cell and hence it is concluded that at 2 bar, it shows good performance.

At 323 K, 2 bar, with $1.3 \text{X} 10^{-6}$ kg/s for anode & $4.3X10^{-6}$ kg/s for cathode as mass flow inlet for serpentine flow channel (2x2) shows good performance improvement than other combinations.

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