JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

PERFORMANCE EVALUATION OF A PEM FUEL CELL USING CFD ANALYSIS

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Abstract : The study of the electrochemical catalyst conversion of renewable electricity and carbon oxides into chemical fuels attracts a great deal of attention by different researchers. The main role of this process is in mitigating the worldwide energy crisis through a closed technological carbon cycle, where chemical fuels, such as hydrogen, are stored and reconverted to electricity via electrochemical reaction processes in fuel cells. The scientific community focuses its efforts on the development of high-performance polymeric membranes together with nanomaterials with high catalytic activity and stability in order to reduce the platinum group metal applied as a cathode to build stacks of proton exchange membrane fuel cells (PEMFCs) to work at low and moderate temperatures. A 3-D PEM fuel cell model of size 84 cm2 active area is developed. A conventional serpentine flow field is modified and the same is considered for the supply of reactants. Computational fluid dynamics (CFD) based simulations were conducted to analyse the pressure drop, distribution of reactants (H_2 and O_2), Effect of membrane thickness, Effect of catalyst (Pt) loading, Effect of cell temperature, Effect of anode and cathode gas humidification temperature. Based on simulation results, it is observed that triple serpentine flow field performance is better than single and double serpentine flow field as it offer less pressure drop and uniform distribution of reactants.

IndexTerms **- CFD, Fuel Cell, Serpentine flow, PEM Fuel Cell.**

I. INTRODUCTION

The study of proton exchange membrane fuel cells (PEMFCs) has received intense attention due to their wide and diverse applications in chemical sensors, electrochemical devices, batteries, supercapacitors, and power generation, which has led to the design of membrane-electrode assemblies (MEAs) that operate in different fuel cell types. Fuel cells based on proton exchange membranes (PEMs) are among the most promising electrochemical-generating devices due to their high efficiency, high power density, low emissions, and energy supply.

Even when compared to devices such as Redox flow batteries (RFBs), they share practically the same configuration. Although both types of devices allow the chemical energy contained in energy vectors obtained from renewable sources to be converted into electricity, PEMFCs have advantages over RFBs, such as the absence of liquid components (which makes their use in mobile devices practical), there are no toxic components outside the cell (compared to vanadium RFB), there are no precipitation reactions that limit their energy density, they do not have electrolytes with high ohmic resistance (non-aqueous electrolytes) that can present problems of evaporation and instability, nor they present problems of dendritic growth of metals that represent safety problems, in addition to presenting a much greater long-term operating stability. These alternative energy sources provide the possibility of receiving energy from hydrogen and synthetic or bio-synthetic fuel and can operate with greater efficiency and environmental sustainability compared to thermal motors. Fuel cells are electrochemical devices used for various technological applications, such as in vehicles, mobile phones, portable electronics, and power generators.

In a typical PEMFC, the polymer electrolyte membrane is responsible for the proton conductivity that allows the transport of protons from the anode to the cathode, constituting the essential component of the electrochemical device. Among the diverse types of fuel cells, membranes based on perfluorosulfonic acid polymers, such as Nafion®, are successfully used due to their high conductivity and good chemical and mechanical properties; these are used at temperatures below 90°C and conditions of high relative humidity. Nafion® was developed by DuPont in the late 1960s and is still the state-of-the-art low-temperature PEM.

The main drawbacks of Nafion membranes for operation as low-temperature PEMFCs (LT-PEMFCs) are mainly their expensive manufacturing processes and the strong decrease in proton conductivity at temperatures above 90°C, when low hydration conditions are attained as a consequence of the loss of the ion-exchange functional groups, which takes place beginning at 130°C. These practical limitations have promoted the emergence of intermediate-temperature PEMFCs (IT-PEMFCs) and high-temperature PEMFCs (HT-PEMFCs), which operate, respectively, between 100–150°C and 120–200°C in the absence of water and are the focus in this review.

II. METHODOLOGY

Computational evaluation of PEM fuel cell performance includes three major steps. The first step is modeling the geometry of the PEMFC by means of computer-aided design software. The geometrical model forms the basis for creating a computational mesh.

The second step involves generating the mesh from the geometry. In order to solve the numerous of equations associated with a fuel cell simulation, the entire cell is split into a finite number of discrete 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. Generating a good mesh is one of the challenging steps. It needs a careful balance of generating adequate computational cells to capture the geometry without exceeding the available memory of the meshing computer. Many other factors must also be considered in order to create a computational mesh which delivers archetypal 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. The flow chart of the computational methodology can be seen in Figure 2.1.

2.1 Modeling assumptions

The developed models were assumed as 3-D, steady and isothermal. The reactants at inlet to the channel assumed as perfect gases, the flow is laminar, incompressible and the porous layers assumed as isotropic and the thermo-physical properties assumed as constant.

2.2 Governing equations

Fundamental conservation equations such as conservation of mass, momentum and charge were used to develop a mathematical model for PEMFC. Conservation of energy equation was not considered as the model was assumed as isothermal. The PEMFC was examined in four parts: flow channels, GDLs, CLs and the membrane.

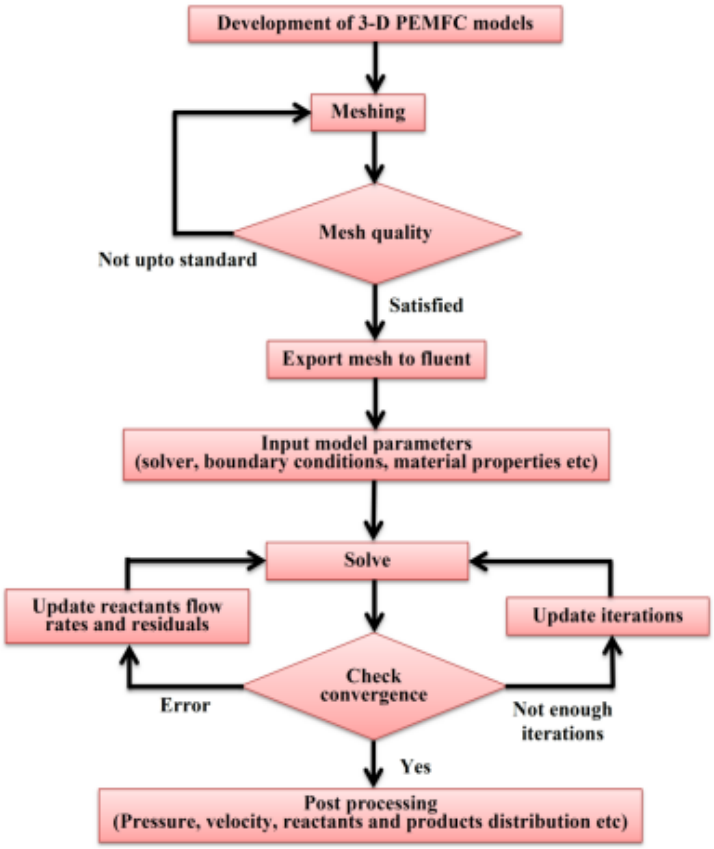

Figure 2.1 Flow chart of computational methodology

2.3 Development PEM fuel cell models

The first step in the development of FC model is modeling of individual parts of the three active area PEMFCs such as current collector, gas diffusion layer, catalyst layer (for anode and cathode) and a membrane (PEM) in SOLIDWORKS 2015. These parts have been assembled to get the complete fuel cell assembly. The geometric dimensions of these components have been given in Table 2.1. The exploded view of the PEMFC with proposed serpentine flow fields is shown in Figure. 2.2.

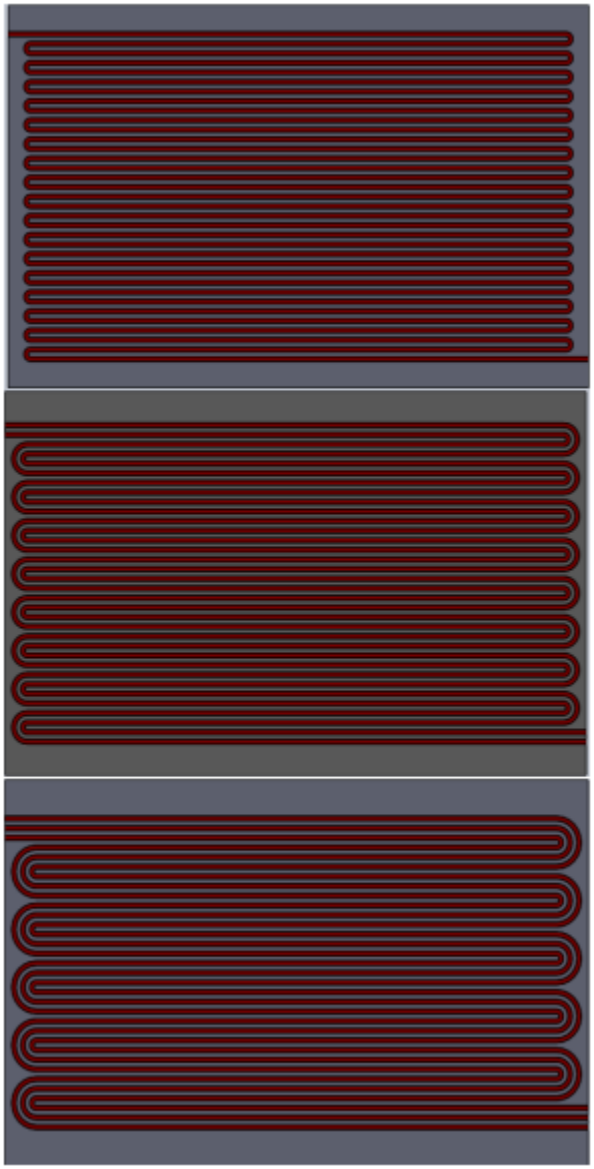

Figure 2.2 7 cm x 12 cm size single (top), double (middle) and triple (bottom) serpentine flow field designs

Table 1 Geometric dimension of three PEM fuel cells

Cell	Part	Length (cm)	Width (cm)	Height (cm)
PEMFC 2 ($7x17\ cm^2$)	Gas diffusion layers (GDL)	12	7	0.025
	Catalyst Layer (CL)	12	7	0.005
	Membrane	12	7	0.00175
	Channels	12	0.1	0.1
	Rib	12	0.1	0.1

2.4 Meshing

The second step is generating high quality mesh using ANSYS WORKBENCH MESH. The computational domain is divided into a number of elements as shown in Figure. 2. Named selections are required to define the boundary conditions of the mesh and naming conventions used are specified in Table 2. Refinement of mesh greatly influences the solution. So, the grid independency test is carried out with three different mesh sizes namely coarse, medium and fine. The current generated in the MEA is simulated with three different mesh sizes, is shown in Figure 3.5 and noticed very nominal variation of 0.3% in the results. Therefore, mesh with medium size is considered for all the simulations to save computational time and space. Now this mesh can be exported to solver.

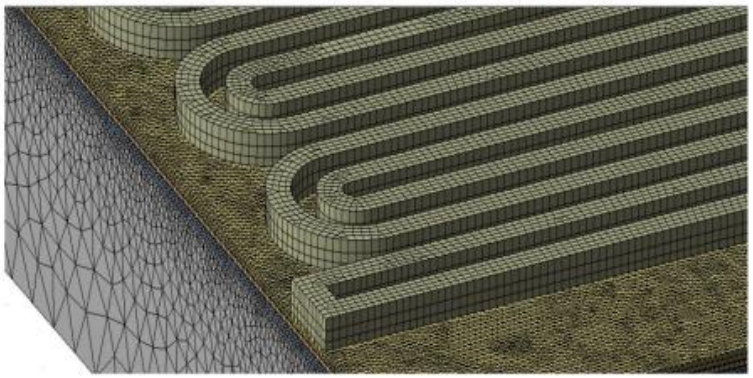

Figure 2.3 Computational mesh of 2-S PEMFC

III. Results and Discussion

Computational investigations on the performance of PEMFC using single (1-S), double (2-S) and triple (3-S) serpentine flow field configurations has been completed. Numerically predicted pressure drop, mass fraction distribution of hydrogen, oxygen, and liquid water activity along the channel at peak power performance with three flow fields presented.

3.1 Pressure drop

CFD analysis was carried out on 1-S, 2-S and 3-S flow field models to study the pressure drop from inlet to outlet. From Figures 3.1 it is observed that pressure drops are maximum at the inlets and gradually reduced towards the outlets. It is also observed that highest-pressure drops are observed in 1-S flow channels and lowest pressure drops in 3-S flow channels of PEMFC, pressure drop for 1-S, 2-S and 3-S are 25672, 13869 and 2681 Pa.

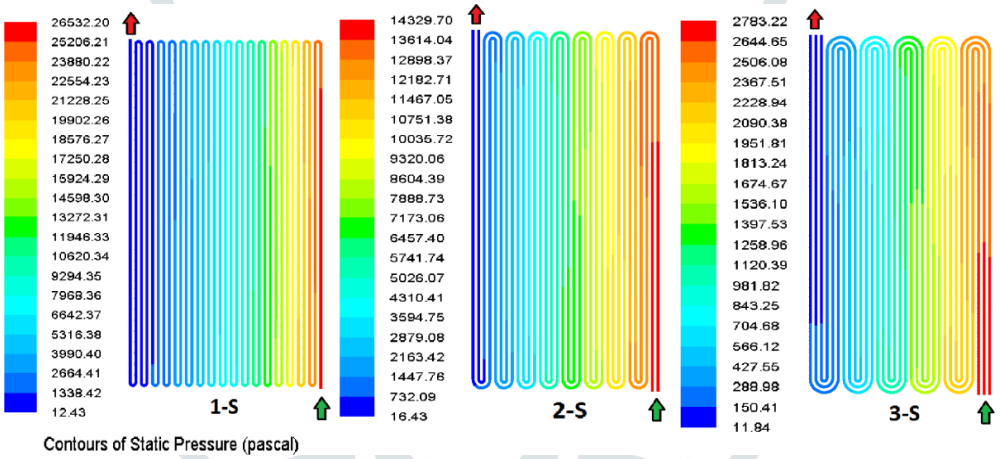

Figure 3.1 Variation of Pressure in cathode channel of PEMFC 1

3.2 Hydrogen and oxygen distribution

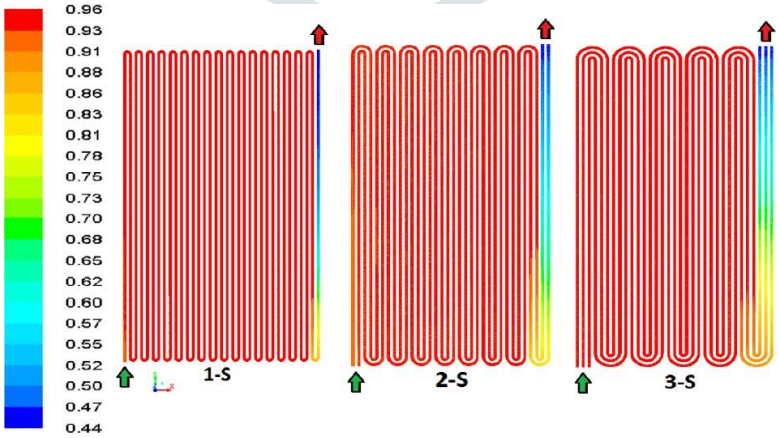

Figure 3.2 H_2 mass fraction distribution in anode channel of PEMFC at 0.5 V

Figure 3.2 shows the oxygen mass fraction distribution along the cathode flow channels (1-S, 2-S and 3-S) of PEMFC at cell potential of 0.5 V. From Figures it is observed that oxygen mass fractions are high at the channel inlets, decreased along the flow channel, and become low at the channel outlets. It is also observed that oxygen mass fraction distribution is more uniform than hydrogen mass fraction distribution. The reduction of species concentration along the channels is due to consumption of reactants in the reaction.

3.3 Effect of membrane thickness

Effect of membrane thickness on cell performance is analysed with three membranes having different thickness namely N212 (50 µm), N112 (51 µm) and N117 (178 µm). The peak power delivered by the PEMFC loaded with N112 and N117 membrane are less than PEMFC loaded with N212 membrane because the ohmic resistance of N112 and N117 is higher than N212. From these results, it is concluded that a thin membrane (N212) offers less ohmic resistance and gives high performance.

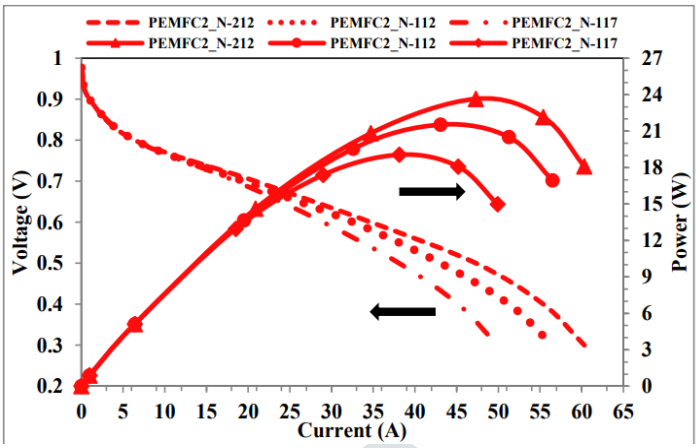

Figure 3.3 Effect of membrane thickness on performance of PEMFC

3.4 Effect of catalyst (Pt) loading

The effect of catalyst (Pt) loading on the performance of PEMFCs with an active area of 49 and 84 cm^2 were analysed by incorporating N212 membrane. The platinum loading on the cathode side is taken as 0.6, 0.8 and 1.0 mg/cm^2 and on anode side is 0.4 mg/cm^2. The catalyst loading is more critical on the cathode side due to the significant activation polarization/kinetic loss for the oxygen reduction reaction (ORR). It is observed that the cell performance has increased with increase in platinum loading. A larger catalyst loading facilitates higher surface area for electrochemical reactions, as a result, more reactant species involve in the reactions, generate more current and decrease the activation loss. It is also observed that the rate of increase in performance is more when the platinum loading increased from 0.6 to 0.8 mg/cm^2 than 0.8 to 1.0 mg/cm^2. Too high platinum loadings (more than 1 mg/cm^2) negatively influence the FC performance due to mass transport resistance caused by the thick electrode layer. In this study, all the cells delivered maximum performance with 1.0 mg/cm^2 platinum loading.

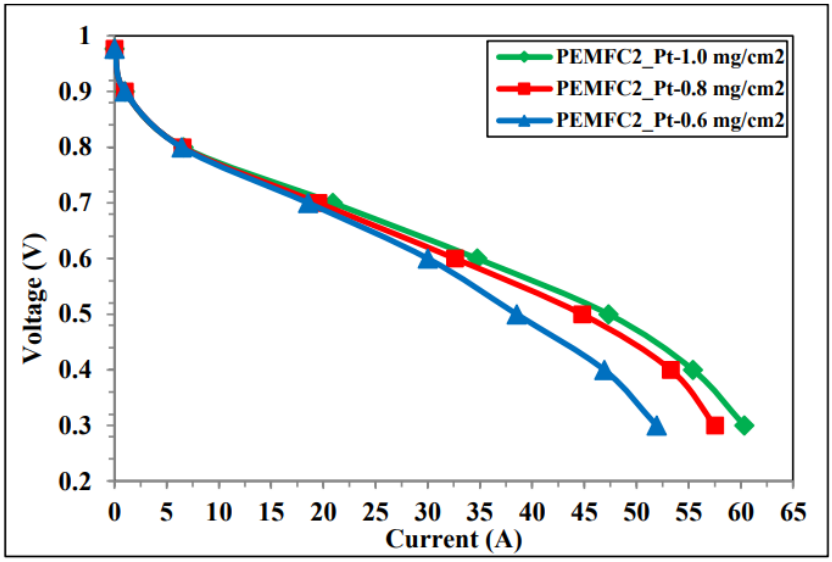

Figure 3.4 Effect of catalyst loading on performance of PEMFC

3.5 Effect of cell temperature

The effect of cell operating temperature on the performance of three PEMFCs has been studied. All the PEMFCs were assembled with 1.0 mg/cm^2 Pt loaded N212 MEA and the experiments have been carried out at different cell temperatures ranging from 40^{O}C to 80^{O}C, with an increment of 10^{O}C while the anode and cathode humidification temperatures were kept at 70^{O}C. The results are shown in Figure 3.5. It is observed that when the temperatures increased from 40^{O}C to 70^{O}C, the performance of PEMFCs is increased due to improvement in the catalytic activity, and as a result, the chemical reaction rate increases. Also increasing the cell temperature facilitates the reactant transfer in the electrodes. When the cell temperatures increase further from 70^{O}C to 80^{O}C (T_{cell}>T_{humid}) then the performance of FCs is decreased due to membrane dehydration (extreme evaporation of liquid water in the cell), which significantly increase ohmic resistance of membrane (the active catalyst surface area may also reduce). This is mostly because of increase in exchange current density with temperature. The effect of the cell temperature is more significant in the high current region. At low current region, the cell performance does not change much with the increase in the cell temperature.

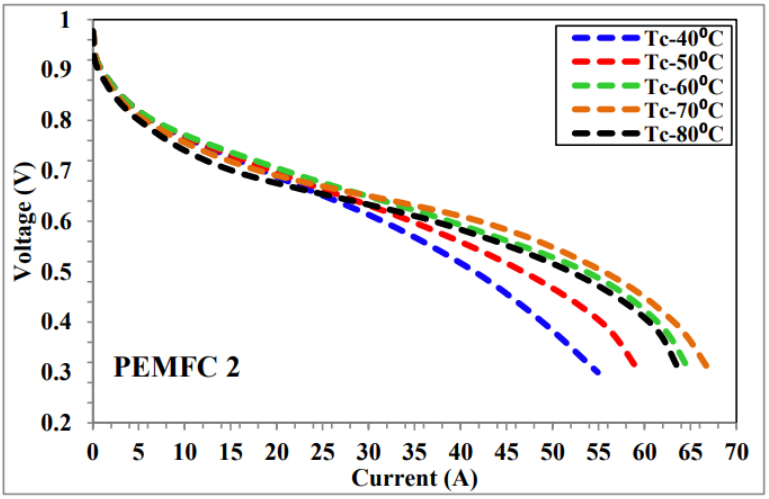

Figure 3.5 Effect of temperature on cell performance of PEMFC

3.6 Effect of anode and cathode gas humidification temperature

The effect of anode and cathode gas humidification temperature on the performance of three PEMFCs was studied with two analyses. In first set of the analysis, anode gas humidification temperatures (Th,a) are varied from 40^{O}C to 80^{O}C with an increment of 10^{O}C and the cathode humidification temperature is fixed at 70^{O}C. In the other set of analysis, cathode humidification temperatures (Th,c) are varied from 40^{O}C to 80^{O}C with an increment of 10^{O}C and anode humidification temperature fixed at 70^{O}C. For both cases, the cell temperature (Tc) is kept at 70^{O}C.

From Figure 3.6, it is observed that increase in the anode humidification temperatures indicated a positive influence on FCs performance till it reaches the cell temperature i.e. from 40^{O}C to 70^{O}C. This increase in anode humidification temperature keeps the membrane hydrated thus the ionic resistance of the membrane decreases. With further increase in the anode humidification temperature from 70^{O}C to 80^{O}C (i.e Th,a >Tc), the cells performance decreases significantly due to back diffusion.

IV. CONCLUSIONS

- PEMFCs with triple serpentine flow field performs better than PEMFCs with single and double serpentine flow fields.
- A thin membrane (N212) offers less ohmic resistance than thick membrane (N112 and N117) and results in improvement in the cell performance.
- Fuel cell performance was increased with increase in platinum loading from 0.6 to 1.0 mg/cm2. Rate of increase in performance is more when the platinum loading increased from 0.6 to 0.8 mg/cm2 than 0.8 to 1.0 mg/cm2.
- The increase in the cell temperature show positive influence on the fuel cells performance up to 70^{O}C and negative influence after 70^{O}C.
- The increase in the anode gas humidification temperature indicated positive influence on the fuel cells performance up to 70^{O}C and negative influence after 70^{O}C.
- The increase in the cathode gas humidification temperature has positive influence on the fuel cells performance up to 60^{O}C and negative influence after 60^{O}C.
- PEMFC (84 cm^{2}) developed peak power of 33.2 W at 0.5 V when the cell was operated at 70^{O}C cell temperature, 70^{O}C anode humidification temperature, 60^{O}C cathode humidification temperature, 600 ccm H_2 flow rate and 1400 ccm O_2 flow rate.

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