EFFECT OF INDENTATIONS ON THE PERFORMANCE OF PEM FUEL CELL

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ABSTRACT

Proton Exchange Membrane Fuel Cell (PEMFC) is an electrochemical device that converts H_2 and O_2 to electricity. The performance of a fuel cell is influenced by the flow field of gas reactants and product distribution. In this work, the performance of a single channel PEMFC is numerically investigated through Computational Fluid Dynamics (CFD). The performance of a fuel cell is investigated for a wide range of operating conditions such as operating voltage, temperature, relative humidity, and geometric parameters such as membrane thickness. The predicted polarization, power density, contours of temperature, and fuel utilization are analysed to identify an optimum condition for the operation of PEMFC. To improve the performance of PEMFC, indentations (rectangular and shark fin) are proposed in the flow channel. This supports significantly enhancing the performance of PEMFC without using any conventional H_2 recirculation system.

Keywords: *PEMFC, polarization curve, relative humidity, membrane thickness, flow channel indentations, CFD.*

INTRODUCTION

A fuel cell is an energy conversion device where H_2 is used as fuel and produces electrical energy. A fuel cell can be classified based on operating temperature such as high temperature (600°C or higher); medium-temperature (100°C to 300°C) and low-temperature (less than 100°C) fuel cells. The low-temperature fuel cell is called a proton exchange membrane (PEM) fuel cell.

The performance of PEMFC depends upon channel geometries, stack design, operating parameters (temperature, humidity, pressure, mass flow rate of gaseous stream), and characteristics of the gas diffusion layer, membrane, and catalyst layer [1].

Wang et al. found that the performance of PEMFC is influenced by operating temperature, pressure, and humidification of the gaseous reactant streams [2]. Liu et al. characterized the performance of a fuel cell using various Nafion membranes in a direct methanol fuel cell (DMFC). The performance of DMFC had improved significantly at low methanol concentrations [3]. Rismanchi and Akbari analysed the predicted flow field, current distribution, and cell voltage to characterize the behaviour of straight-channel PEMFC. At low current density regions, the current distribution was found to be uniform [4].

Rismanchi et al. analysed the performance of single-channel fuel cell using CFD. The model predictions are in good agreement with experimental observations in low current density regions and underpredict in high current density regions. The liquid water effects are not considered in their modelling [4].

Thomas et al. reported that water management is a critical and important parameter in characterising performance of PEMFC [5]. Ghanbarian and Kermani found that transport rates across the PEMFC are influenced by the extent of gases reactant and products. This supports the consumption rate of O_2 in the catalyst layer [6].

Jourdani et al. found that the thickness of the membrane supports the enhancement of the performance of PEMFC [7]. Asifa et al. found that water content and

temperature significantly influenced the electrochemical performance of PEMFC. They observed that the conductivity of the membrane increases with an increase in temperature and it enhances the diffusion of protons within the membrane [1]. Vuppala et al. showed that membrane thickness and its protonic conductivity are the important parameters that influence the performance of a fuel cell [8].

The performance of PEMFC is influenced by a complex interaction between hydrodynamics, transport mechanisms and electrochemical reactions in the gas channels. Therefore, finding an optimum condition for the operation of a fuel cell is very complicated. In most of the literature, the performance of a fuel cell has been improved by varying operating, design parameters, membrane modifications, catalyst layer design, hydrogen recirculation and by designing stack systems [9 - 15]. In the present work, various baffle configurations are proposed to enhance the performance of single-channel PEMFC without using hydrogen recirculation and stack design. The behaviour of PEMFC is predicted using transient 3D computational fluid dynamics (CFD) simulations.

The manuscript is organized by describing the geometry of single channel fuel cell at first. Then transport equations and simulation methodology are presented. Subsequently, CFD predictions are discussed in the results and discussion section. The findings are presented in the summary and conclusions.

Schematic of Proton Exchange Membrane Fuel Cell (PEMFC)

The schematic of a single straight channel PEMFC with a length of 10mm is shown in Fig. 1. It has a *current collector,* gas channel (GC), gas diffusion layer (GDL), catalyst layer (CL) and membrane. The corresponding dimensions of PEMFC are shown in Fig. 1. This is obtained from Asifa et al. [1].

CFD modelling

The flow field in PEMFC is numerically investigated using commercial CFD software (Ansys Fluent V2019 V1). CFD model was developed with the assumption of (i) constant cell temperature (isothermal); (ii) laminar flow (everywhere); (iii) impermeable membrane for reactant gas; (iv) gases follow ideal gas law; (v) porous GDL layer; (vi) membrane, gas diffusion and catalyst layer: isotropic materials; (vii) incompressible fluids.

The flow field is predicted by solving transport equations such as continuity, Navier Stokes (momentum), species, energy and charge equations. The summarized form of these transport equations are:

Continuity equation:

$$\nabla.(\rho\vec{u}) = S_m \quad (1)$$

Navier Stokes equation:

$$\frac{1}{\varepsilon}\nabla.(\rho\vec{u}\vec{u}) = -\nabla p + \frac{1}{\varepsilon}\nabla.(\mu\nabla\vec{u}) - S_u \quad (2)$$

Energy equation:

$$\nabla(\rho C_p\vec{u}T) = \nabla(k^{eff}\nabla T) + S_T \quad (3)$$

Species transport equations,

$$\nabla . (\rho\vec{u}\omega_i) = \nabla \cdot (\rho D_{i,eff}\nabla\omega_i) + S_i \quad (4)$$

where $\vec{u}$ is the superficial velocity vector, ρ is the density (gas phase), ε is the membrane porosity, p is the absolute pressure, μ is the viscosity (gas phase), C_p is the heat capacity of gaseous reactants, k^{eff} is the thermal conductivity (effective), T is the temperature, S_T is source term for energy equation, S_m is source

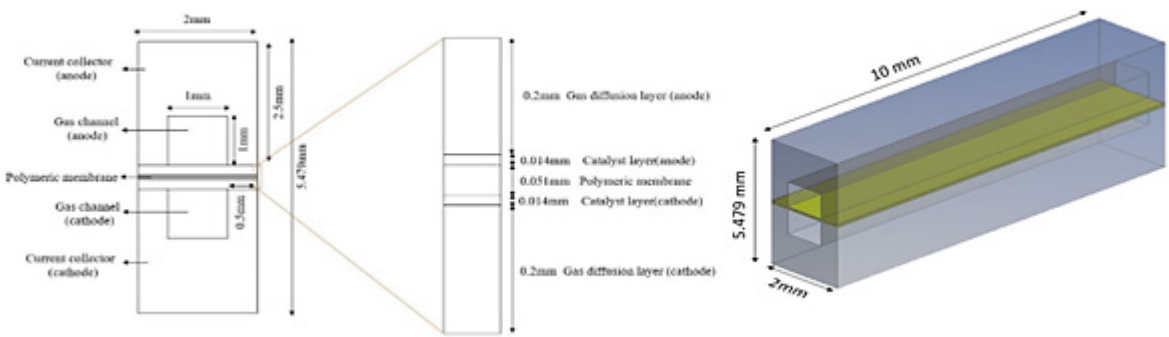

Fig. 1. Scheme of PEM fuel cell: (a) - front view; (b) - top view.

term due to electrochemical reaction; S_u is source term due to Darcy's drag force imposed on the fluid by the pore walls, The basic transport equations along with electrochemical model [16] for single cell PEMFC are solved to characterize the performance of PEM fuel cell. The transport equation details and others are obtained from the literature [17].

Simulation methodology

To characterize the flow field in single channel PEMFC, 3D CFD simulations are performed using commercial software Ansys 2019 R1. The Geometry of PEMFC is developed (Hexagonal elements) through Ansys Workbench V19.0. CFD predictions are checked for grid independence and 1,47,800 is found to be optimum in terms of accuracy and computational errors. The QUICK scheme is used to discretize convective and diffusive terms in Navier-Stokes equations. The phase coupled SIMPLE algorithm is used to couple pressure and velocity fields. CFD simulations were performed with optimum time step size ($\Delta t = 0.01$s). The operational and boundary conditions (BCs) are specified for CFD simulations. The velocity inlet BC is imposed at the anode and cathode inlet channels with appropriate values for a mass fraction [Hydrogen (H_2), Oxygen (O_2), water (H_2O)]. The pressure outlet BC is specified at the anode and cathode outlet channels of PEMFC. The electrical BCs are imposed at the anode and cathode terminal [0 V (anode); 0.4 - 0.9V (cathode)]. PEMFC is operated at a constant temperature (323 K) and reference pressure (1 atm) with appropriate physicochemical parameter values. The convergence criterion for residuals (10^{-6}) is set for all the transported variables.

RESULTS AND DISCUSSION

To characterize the performance of single channel PEMFC, 3D CFD simulations are performed using commercial CFD software (Ansys 2019 R1). The predicted velocity vectors for H_2 ion (protons) and O_2 ion across the membrane is depicted in Fig. 2. The counter-current mode of operation is maintained during the flow of H_2 and O_2 ions across the membrane. The predicted velocity gradient is observed to be fairly constant over the length of PEMFC.

To characterize the performance of a fuel cell, a predicted polarisation curve (voltage loss or over

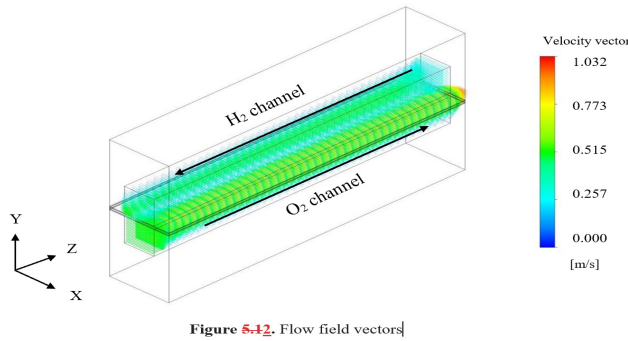

Fig. 2. Contours of vectors across the membrane in single channel PEMFC.

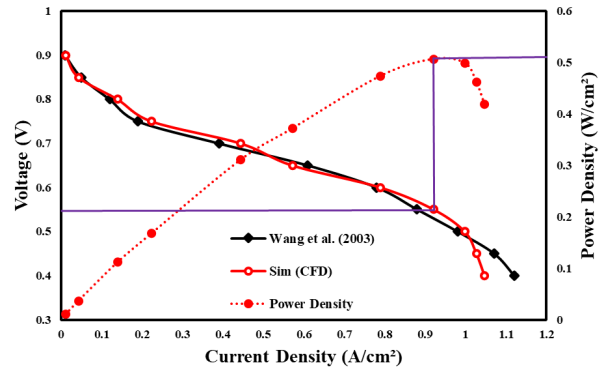

Fig. 3. Single channel PEM fuel cell polarization curve.

potential) is analysed. This is obtained by varying voltage at the cathode and it is shown in Fig. 3. Three distinct regions are observed such as low, moderate and high current density regions. A significant drop in voltage (cell potential) is observed at low current density regions due to activation loss. The linear decrease in voltage is being observed in moderate current density regions due to ohmic losses and once again significant voltage drop is observed at high current density regions. The CFD predictions are validated with experimental observations by Wang et al. [2]. The variation of power density (power per unit active area) with current density profiles is also depicted in Fig. 3. The power density for single channel PEMFC is found to be maximum (0.5 W cm^{-2}) when 0.55 volts is used. The magnitude of current and power density was obtained for 323K (input temperature) and 1 atm (pressure).

Further, predicted contours of temperature for various operating voltages of PEMFC are shown in Fig. 4. It is observed that the temperature of PEMFC increases as the reaction is exothermic. The magnitude of temperature increases across the cell layers as voltage

decreases and it is found to be high when 0.4 V is used. This is attributed to the extent of reaction at a lower voltage (high current density).

To find an optimum temperature for the single channel PEMFC, it is being operated with wide operating temperature ranges (293 K - 363 K). Accordingly, the predicted polarisation curve is analysed. This is depicted in Fig. 5 and voltage is observed to decrease as the operating temperature of PEMFC increases. The voltage drop is found to be significant in the high current density region and hence the efficiency of a PEM fuel cell decreases. The voltage drop is minimum when 323 K (optimum) is used. This is attributed to water formation which decreases the conductivity of membrane.

To overcome the problem of the drop in voltage at high current density regions, various thickness of the membrane is considered in the present investigations. The predicted current density is analysed by varying voltage across the PEMFC. This is shown in Fig. 6. Once again, the voltage drop is found to be significant at higher current densities. It is insignificant at lower and medium current densities. Also, a voltage drop is high when a thicker membrane (0.125 mm) is used and its magnitude is low when a thinner membrane (0.015 mm) is used. A thinner membrane offers maximum power density. This is attributed to an increase in conductivity value when the thickness of the membrane decreases. Hence to optimize the performance of single channel PEMFC, the membrane thickness should be made as thin (0.015 mm, optimum) as possible. However, care must be taken durability of the fuel cell membrane during fabrication. Thus, membrane thickness plays a critical role in characterizing the performance of PEMFC.

Further, the effect of membrane thickness on the flow of hydrogen ions is analysed by quantifying predicted protonic potential values (Fig. 7(a)). Its value is observed to be low (decrease in the flow of hydrogen ions) when a thinner membrane (0.015 mm) is used.

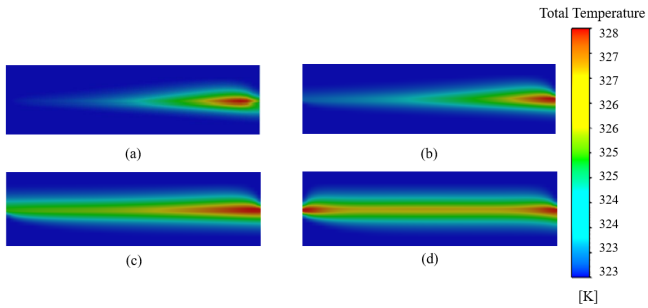

Fig. 4. Contours of temperature for (a) 0.9 V; (b) 0.7 V; (c) 0.5 V; (d) 0.4 V.

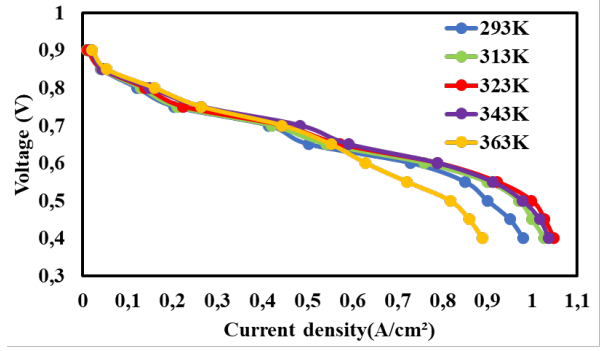

Fig. 5. Effect of operating temperature on polarisation curve.

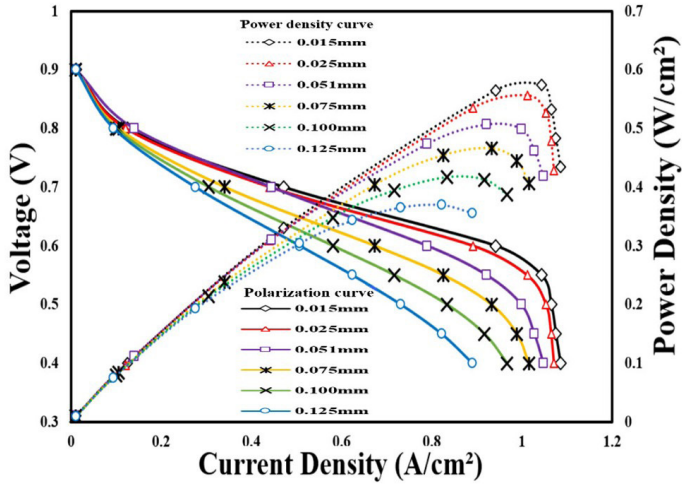

Fig. 6. Effect of membrane thickness on polarization curve and power density.

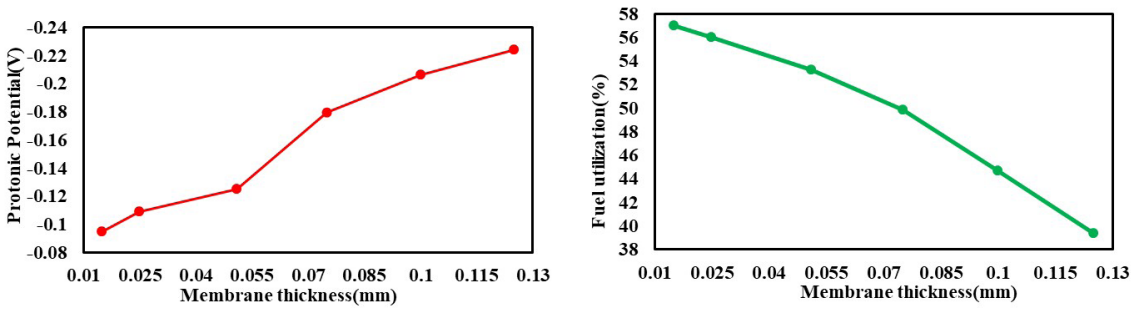

Fig. 7. Effect of membrane thickness on: (a) protonic potential; (b) Fuel utilization.

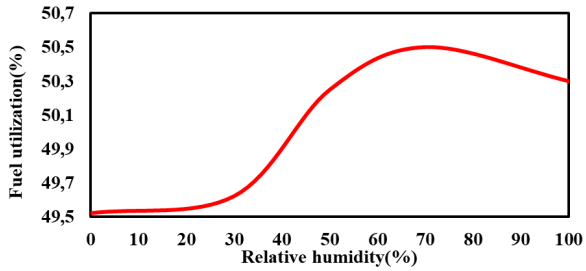

Fig. 8. Effect of relative humidity on fuel utilization efficiency.

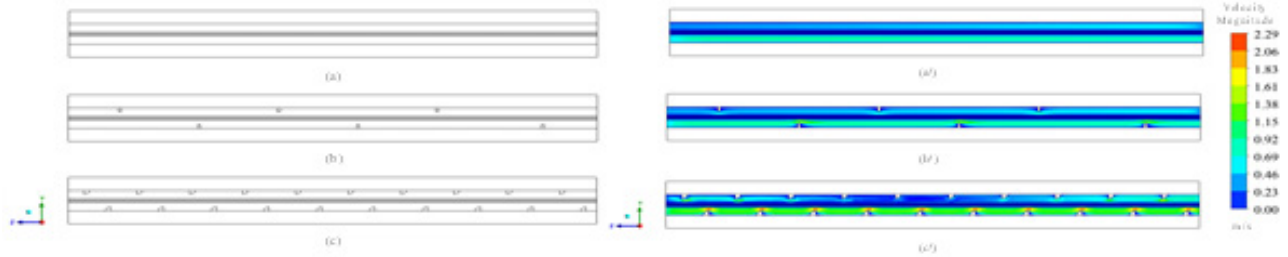

Fig. 9. Scheme of proposed indentations and contours of velocity magnitude (a-a^{l}) no modification, (b-b^{l}) rectangular, (c-c^{l}) shark fin.

This supports water formation (decrease) during fuel cell operation. Thus, a thinner membrane shows advantages in characterizing the performance of PEMFC by limiting protonic migration between the anode and cathode interface.

To characterize PEMFC, the extent of fuel utilization is calculated in terms of membrane thickness and it is defined in terms of H_2 mole balance [18].

$$\beta_H = \frac{Q^{in}_{bulk,A} P^{in}_{H,A} - Q^{out}_{bulk,A} P^{out}_{H,A}}{Q^{in}_{bulk,A} P^{in}_{H,A}} \quad (5)$$

where, $Q^{in}_{bulk,A}$ is a volumetric flow rate at the inlet (anode); $Q^{out}_{bulk,A}$ is a volumetric flow rate at the outlet (anode); $P^{in}_{H,A}$ is the partial pressure at the anode (inlet); $P^{out}_{H,A}$ is the partial pressure at the anode (outlet).

The fuel utilization efficiency is calculated for a wide range of membrane thicknesses (thinner to thicker). This is shown in Fig. (Fig 7(b)). It is observed that the efficiency of fuel utilization decreases with an increase in membrane thickness and a thinner membrane (0.015 mm) supports higher fuel utilization. Thus, the thickness of the membrane (permeation) plays a limiting factor in the design and scale-up fuel cell.

Since the extent of reactant relative humidity (RH) adversely affects the performance of PEMFC, RH at the cathode is varied from 0 to 100 % (100 % humidified H_2 at the anode, accordingly fuel utilization efficiency is calculated. This is shown in Fig 8. The observed fuel utilization efficiency is maximum at high RH (or nearly saturated humidity). At lower RH, the fuel utilization efficiency is low due to a decrease in protonic conductivity (H_2O content). The fuel utilization efficiency decreases at high RH (> 90 %). This is attributed to increased water concentration (not shown) at the cathode side of fuel cell due to the electrochemical reaction. Thus, the performance of PEMFC reduces at a

higher value of RH. Hence, the RH value (optimum, 70 %) must be controlled to prevent flooding in PEMFC.

To enhance the performance of PEMFC further, indentations (rectangular; shark-fin) are proposed along the flow channel of PEMFC. The schematic proposed indentations are shown in Fig. 9. The distance between the two rectangular indentations is maintained as 4mm (height, 0.4 mm; width, 1 mm) whereas the shark-fin indentation is 3.5 mm (height, 0.5 mm; 1 mm). The predicted flow field (contours of velocity) for the corresponding indentations are depicted in Fig. 9.

To characterize flow channel indentations, predicted contours of velocity along PEMFC length are depicted in Fig. 9. It is observed that gradual changes in flow channel area on the addition of indentations. This results in variation in local current density. To quantify this, the polarization curve is analysed. This is shown in Fig. 10.

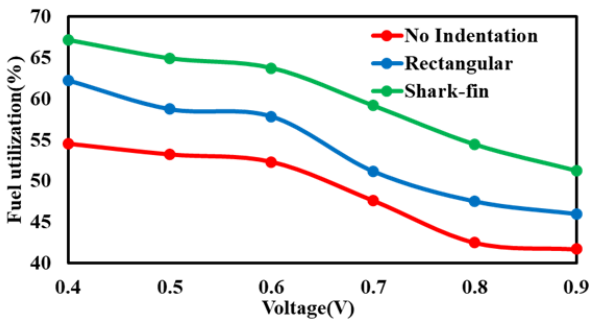

Fig. 10. Effect of indentation on power density and polarization curves.

It is observed that voltage drop and produced electric current are insignificant at lower current densities and significant at higher current densities. The extent of electric current produced by the shark fin indentation is relatively high at high current regions and results in enhancement in the performance of PEMFC. This is attributed to an increase in the velocity of gaseous reactants over the indentation as it changes the cross-section of the flow channel.

Further, fuel utilization efficiency is calculated for various flow channel indentations and it is shown in Fig. 11. It is observed that flow channel indentations significantly enhance fuel utilization efficiency and its value is found to be maximum when shark fin indentation is used. This flow channel indentation directs the flow of gases towards membrane assemblies and hence higher protonic conductivity is observed. Thus, the flow channel indentations support improving the performance of PEMFC without using the conventional method (H_2 recirculation devices).

CONCLUSIONS

The performance of single channel PEMFC is characterized numerically using computational fluid dynamics (CFD). This is quantified by analysing predicted polarization curve for a wide range of operating voltages (0.9 - 0.4 V). The predicted power density is found to be high (0.5 W/cm^2) when 0.55 V is used. Further, an optimum temperature (323 K) for

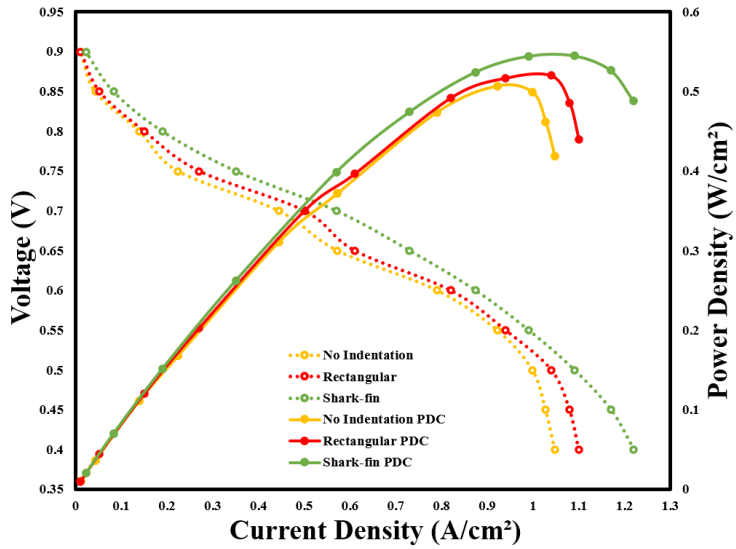

Fig. 11. Effect of indentation on fuel utilization efficiency.

the operation of PEMFC is identified. The performance of PEMFC is investigated for a wide range of membrane thicknesses and it is found that the extent of power density produced by PEMFC is maximum for thinner membrane (0.015 mm). The effect of relative humidity (RH) on fuel utilization efficiency is calculated and it is found to be maximum at 70 % (RH). To improve the performance of a PEMFC, indentations (rectangular and shark fin) are proposed in the flow channels. The indentations (shark fin) were found to increase the electric current produced by the PEMFC and fuel utilization efficiency. Thus, flow channel indentations help to increase the gaseous reactants in the gas diffusion layer and support in improving the performance of PEMFC.

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