Improved PEMFC performance using zig-zag path of flow channel

In the work presented here, we have attempted to improve the flow channel configuration of the Proton Exchange Membrane Fuel Cell (PEMFC).

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Abstract
The proposed configuration incorporates the features of the straight channel and the serpentine channel. The channel offers zig-zag flow path for reactants. This research examines the overall performance efficiency of the modelled fuel cell configuration. Initial findings with straight channel geometry indicate close agreement with experimental results. Numerical simulation was conducted for the design of the zig-zag path channel, and the results were compared with the PEMFC straight flow single channel. This investigation demonstrates significant improvement in polarization curve due to the uniform distribution of pressure over the flow path. Modification in flow path also increases the power density by almost 30 percent compared to the straight flow single channel PEMFC.

Introduction
Fuel cell technology is today seen as one of the solutions to the energy and climate change crisis. With all available fuel cell configurations, the Polymer Electrolyte Membrane Fuel Cells (PEMFCs) attracted more attention due to their suitability for different applications [1]. The construction of PEMFCs is simple (Figure 1). The anode channel, cathode channel and Membrane Electrode Assembly (MEA) which is composed of three reigns. MEA is sandwiched between cathode channels and anode [1]. It consists of the Gas Diffusion Layer (GDL) on cathode & anode side and electrolyte catalyst layer, which is the central component of the assembly. It separates the cathode side and the anode side.

PEMFCs use hydrogen as fuel and oxygen from the air as an oxidizer. The reaction produces water and heat as biproducts and pass electrons into external circuits that can either be used to store electrical energy or transform it into mechanical energy. In order to ensure the healthy operating condition of the membrane, the reactants are humidified before entering the channel. The humidity level in the membrane affects the proton conductivity. Water deficiency in the membrane can result in declination of proton conductivity and may cause permanent damage. Hydrogen and air flow through the anode and cathode, respectively. Part of the main stream of these reactants diffuses and reaches the catalyst from either side through anode and cathode GDL. Electrochemical reactions occurring at the catalyst are:

Anode: $H_2 \rightarrow 2H^+ + 2e^-$

Cathode: $\frac{1}{2} O_2 + 2H^+ + 2e^- \rightarrow H_2O + HEAT$

The water produced due to the above electrochemical reaction is largely evaporated through the gas channels. Water produced at higher rates at higher current densities may cause water flooding issues. Bhambure and Vaze [2] have recently conducted Computational Fluid Dynamics (CFD) investigations to quickly flush out water flooded in the anode and cathode flow channels within two minutes.

Research over the past decades has concentrated on the creation of PEMFC cell structure, catalytic and membrane materials, operating parameters, flow field configuration, thermal and water control in PEMFCs [3]. Hashemi et. al [4] investigated the PEMFC performance for straight and serpentine flow channels using CFD. Numerical simulation studies are very helpful in understanding the fuel cell, but CFD simulations are complex and require several assumptions [5]. Theoretical 1D research and other studies have focused on electrochemical kinetics and transport phenomena. For the first time, Springer et. al [6] developed a 1D steady state isothermal model to evaluate PEMFC efficiency. Bernardi and Verbrugge [7] have developed a 1D model based on GDL reactant transport. For their study, they assumed steady state, isothermal and ideal gas behaviour conditions and determined electrochemical and transport phenomena in MEA. GDL gas diffusion was modelled as porous media transport phenomena. Bruggmen's equation was used to calculate the diffusivities and to pass the proton through the membrane of the Nernst-Plank equation. Electrode kinetic modelling was based on the Butler-Volmer equation. The pressure drop in the channel has not been considered. These studies have drawbacks, such as that 1D analysis does not capture full physics, as real phenomena are not isothermal by nature.

For the PEMFC analysis, 2D approaches have also been established [8, 9, 10]. Research with isothermal conditions was carried out in a study conducted by Nguyen and White [9]. The modelling method considered thermal transfer between solid walls, and reactant and membrane water transport by electro-osmatic drag. But for modelling, GDL was not considered. Membrane drying based on electro-osmic forces was studied by Fuller and Newman [8]. The model uses diffusive mass transfer equations. The convective mass transfer of gases in a model was considered by Gurau et. al [10].

CFD methods have been used recently to analyse PEM fuel cells. The knowledge provided by CFD methods contributed to a more detailed understanding of PEMFC physics. These methods have made it simpler to investigate the transportation of PEMFC phenomena and electrochemical kinetics. The first 3D PEMFC model developed by Dutta et al. [11] determined velocity, density and pressure variation in GDL. Its findings revealed current directional dependence on GDL and membrane mass transmission phenomena. Few researchers have attempted FEM. Futerko and Hsing [12] used FEM to solve transport and potential equations in GDL and channel and demonstrated that with Mole fraction of reactants, water content in membrane, current density depends on the pressure distribution in channel and GDL. With a 3D isothermal model, Kumar and Reddy [13] have optimised serpentine flow field dimensioning. For the channel height, ground width and channel width, 1.5 mm, 0.5 mm and 1.5 mm were the optimum dimensions in their investigation.

In the present study, new channel geometry was developed and compared with straight channel geometry. For the straight channel modelling, geometrical and experimental data from literature was used.

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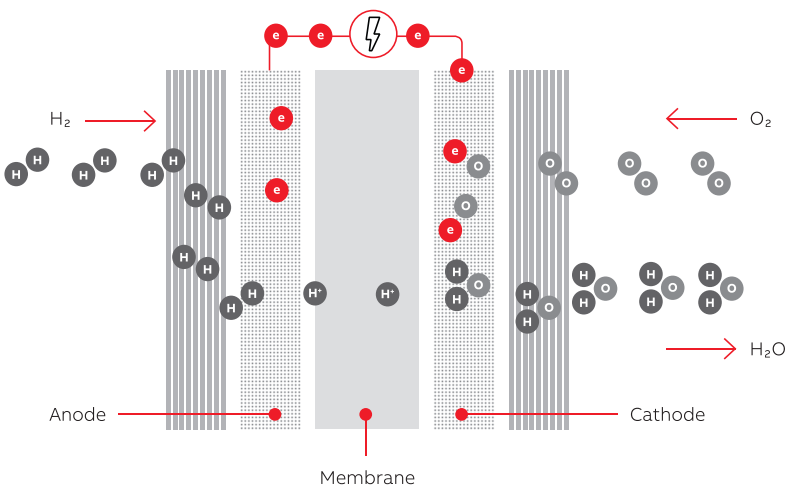
Figure 1: Schematic diagram of PEMFC



Computational Methods

The present study considers transport equations in channels, gas diffusion layers, and membrane [14]. Numerical simulations considered following assumptions throughout the study:

- Isothermal conditions
- Steady state operation
- Reactant gases are considered to behave like ideal gas
- GDLs and membrane are isotropic and homogeneous
- Proton conductivity of membrane is constant
- Negligible contact resistance of current collector and MEA
- Incompressible flow

Boundary conditions and parameters used in the simulation are tabulated in Table 1 and Table 2, respectively.

Reign	Boundary condition
Anode plate collector terminal	$\emptyset_{sol} = 0$ $\frac{\partial \emptyset_{mem}}{\partial y} = 0$
Cathode plate collector terminal	$\emptyset_{sol} = V_{cell}$ $\frac{\partial \emptyset_{mem}}{\partial y} = 0$
Other wall boundaries	$\frac{\partial \emptyset_{mem}}{\partial x} = 0$ $\frac{\partial \emptyset_{mem}}{\partial y} = 0$ $\frac{\partial \emptyset_{mem}}{\partial z} = 0$
Anode channel inlet	$y_{H_2} = y_{H_2,in}$ $y_{H_2O} = y_{H_2O,in}$ $T_{in,an} = T_{H_2,an}$ $m = m_{in,cat}$
Cathode channel inlet	$y_{O_2} = y_{O_2,in}$ $y_{H_2O} = y_{H_2O,in}$ $T_{in,cat} = T_{O_2 cat}$ $m = m_{in,cat}$

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Table 1: Boundary conditions

Parameter	Value Anode Cathode
Reference current density	1,000 20 (A/m²)
Reference concentration	1 (kmol/m³)
Concentration exponent	1
Exchange Coefficient (a)	1
Open circuit voltage	1.07 V
GDL Porosity	0.6
Viscous Resistance (GDL and Catalyst)	1×10^{11} (1/m²)
Porosity (Catalyst)	0.112
Membrane equivalent weight	1,100 (kg/kmol)
Protonic conduction coefficient	1
Protonic conduction exponent	1
Surface to volume ratio	2×10^5 (1/m)

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Table 2: Parameters used for simulations

The operating conditions used are listed in Table 3.

Temperature	323 K
Pressure	1 Atmosphere
Anode inlet velocity	2 m/s
Cathode inlet velocity	2 m/s
H_2 Mass fraction (Anode)	0.3
H_2O mass fraction (Anode)	0.7
O_2 mass fraction (Cathode)	0.14
H_2O mass fraction (Cathode)	0.079

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Table 3: Operating conditions

Material properties used in simulation are listed in Table 4 below:

Electrolyte thermal conductivity	1.3 (W/m-K)
Electrolyte electrical conductivity	17.1223 (S/m)
Catalyst, GDL thermal conductivity	10 (W/m-K)
Catalyst, GDL electrical conductivity	300 (S/m)
Collector thermal conductivity	100 (W/m-k)
Collector electrical conductivity	4,000 (S/m)

Table 4: Material properties used for simulation

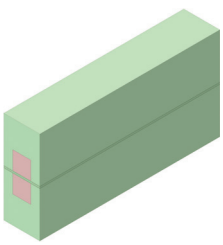

Figure 2: Single channel geometry

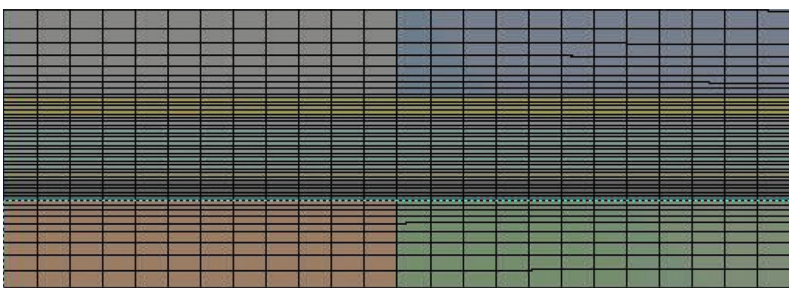

Figure 3: Meshing in MEA reign

SIMPLE algorithm with least square cell based spatial and second order discretization schemes were used in this CFD based PEMFC model. The CFD solution is said to be converged when residue for all the equation reached 1 × 10-4.

Single Channel PEMFC Model

Geometric data of the single channel PEMFC model and other required simulation data were obtained from Awan et. al [15]. Figure 2 shows the geometry of a single straight channel PEMFC. The structured grid as shown in Figure 3 has been constructed. Cells in membrane, catalyst and GDL reign were divided into four to six divisions in the Y direction (through plane). Drastic jumps in cell size from GDL to channel have been prevented. In order to avoid numerical error, analysis of grid sensitivity has been carried out. Figure 4 displays the outcome of grid independence analysis. Current density and temperature are considered to be a grid independent parameter. The grid marked with the red box has been selected for further validation of CFD model with experimental results. For single channel geometry, the mesh with 36,480 elements was selected for further simulations following a grid independence study.

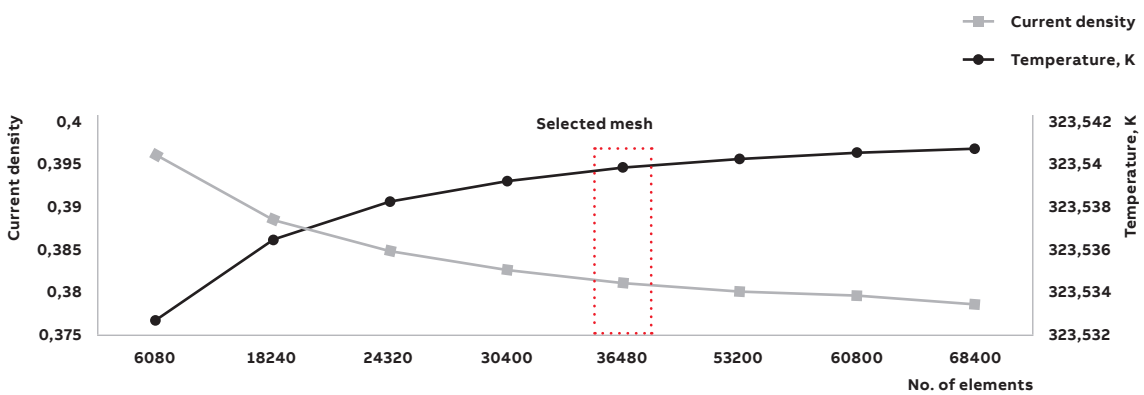

Figure 4: Grid independence study

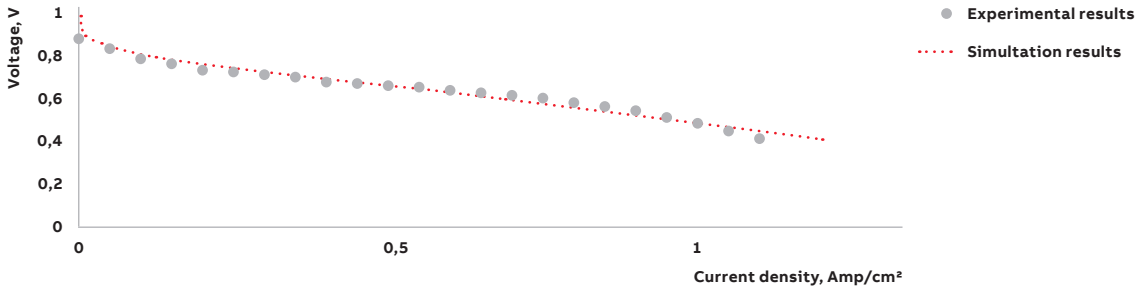

Figure 5: Comparison of experimental and present simulation results for single straight channel geometry

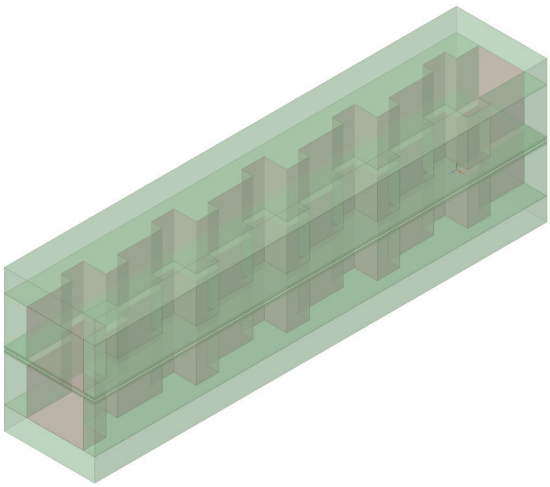

Figure 6: Zig-zag channel geometry

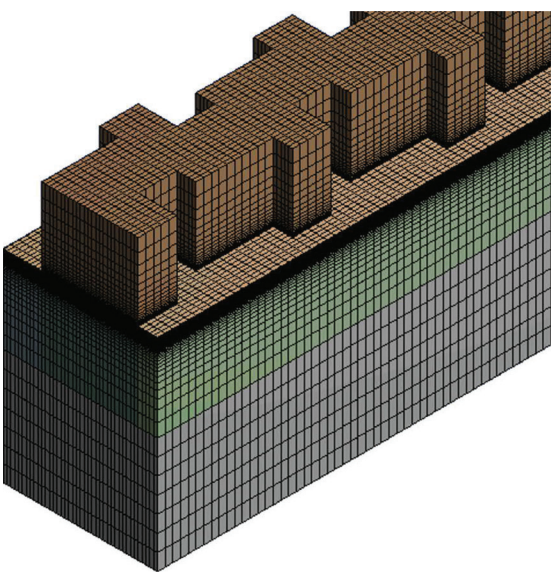

Figure 7: Mesh for zig-zag channel

In order to verify the CFD model, simulation results are compared with experimental results reported by Wang et al. [16]. Figure 5 represents the comparison between numerical simulation and experimental results of the polarization curve. It was observed that the CFD model follows the experiments exactly. Further comparison of the new flow channel configuration is currently being conducted with this model to demonstrate effectiveness and performance improvement.

Zig-zag channel PEMFC model

Numerous efforts were made by researchers to increase the power density of the fuel cell. Various designs with parallel flow, counter flow, serpentine flow, interdigitated designs, bio-inspired designs etc. were suggested to improve the power density of PEMFC. In the present study, we have attempted to improve the design by utilizing the back pressure and increasing the resting time of the reactants in the flow channels. This new channel, called the zig-zag flow channel, is designed to increase local back pressure. Due to the extruded sections and grooves in channels, pressure near obstacles increases, which increases the reactant diffusion in porous GDL. Increased diffusion increases the reaction rate as a result of the improved fuel cell performance. The zig-zag flow channel is as described in Figure 6. This new design was checked for the grid sensitivity to prevent numerical errors. The grid independence study was carried out with three different sets of mesh elements. The optimized grid was found to be with 316,000 elements (Figure 7) and further simulations carried out using this grid. The fine grid size used in MEA and the coarse grid was created in the collector domain. Numerical simulation was carried out taking into account the above grid and boundary conditions of the PEMFC single-channel flow.

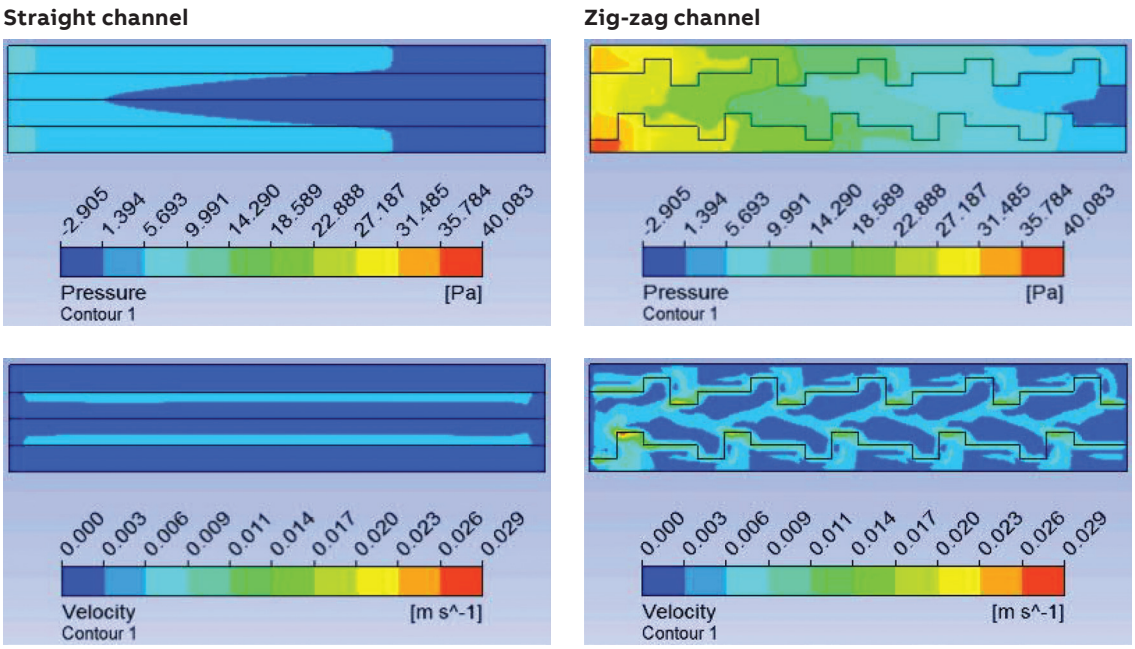

Figure 8: Contour maps (a) Pressure (b) Velocity in GDL

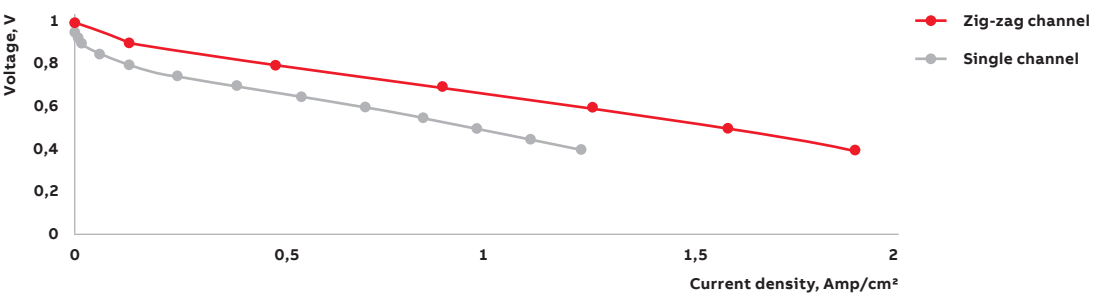

Figure 9: Polarization curve comparison

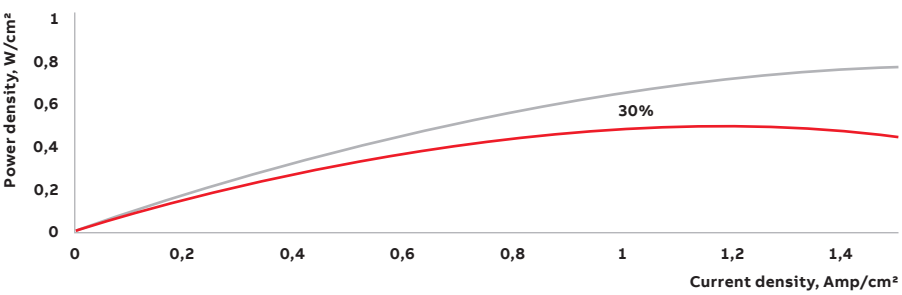

Figure 10: Power density curve comparison

Figure 8 (a) indicates distribution of the pressure in the gas diffusion layer. Pressure in zig-zag channel configuration is higher due to the extruded barriers in the flow channel. It has also been observed that pressure is evenly distributed from inlet to outlet. This has helped to increase the use of the reactant for electrochemical reactions, which results in more power output from the zig-zag channel. Figure 8 (b) shows the velocity distribution in GDL. Velocity in GDL for zig-zag channel configuration is more than for the straight channel case. Better velocity distribution ensures more reactant penetration in GDL, but less for straight channel.

Figure 9 provides a comparison of the polarization curve between the single straight channel and the zig-zag channel. The latest design indicates a major change of the polarization curve. Typical PEMFC power density is 0.4 to 0.8 W/cm2. When the power density of the zig-zag channel is compared to the single channel as shown in Figure 10, there is a significant increase. The new

zig-zag channel design reveals a 30 percent increase in power density compared to the PEMFC single-channel flow configuration for the same type of boundary conditions.

Conclusions

The three-dimensional PEMFC model for single straight channel geometry was developed and successfully validated with experimental results from the literature. This validation showed a perfect match with experiment results. We also developed a new design for the configuration of the flow channel on the cathode and anode sides that carries the reactant. The validated CFD model is then used to examine the new design. It has been found from the CFD investigation that the new zig-zag channel configuration uniformly distributes the reactant, which contributes to the proper use of the reactant. It also increases the receptive time of residence for the successful use of reactants. The polarization curve of the new zig-zag flow channel design showed promising improvements over the single PEMFC channel. The conclusion is that the power density of the new design showed an increase of 30 percent compared to the PEMFC single channel. The improved performance of the new design was due to an improvement in back pressure due to the extruded obstacles in the flow channel.

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