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Science of the total environment <u>ARTICLE</u>

Numerical Modelling and CFD Simulation of a Polymer Electrolyte Membrane (PEM) Fuel Cell Flow Channel Using an Open Pore Cellular Foam Material

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12 ABSTRACT

Fuel cell performances varies with different structural configurations and materials. However, the 13 14 two main areas that determine this performance metric are the membrane electrode assembly (MEA) and the bipolar plates. The MEA provides the platform for the electrochemical reaction to 15 occur and the bipolar plate serves as a medium between the reactants (hydrogen and air) and the 16 catalyst layer. The bipolar plate is the first point of contact for the reactants inside the fuel cell, so 17 a badly designed item with a high pressure drop will have a negative impact on fuel cell 18 performance. Numerical modelling and simulation tools like ANSYS have a huge impact on 19 engineering industry as they help designs to be validated and analysed before any physical 20 construction. 21

This investigation considers five suitable flow plate designs for PEM fuel cell, each completely different from the readily available, traditional serpentine designs on the market. The work explored the possibility of replacing these flow channels with an aluminium cellular foam with different inlet and outlet orientations. The designs were further optimised and modelled in ANSYS. The results obtained were compared with other designs in the literature. Compared to the serpentine flow design, the open pore cellular foam material showed a very small pressure drop in the range of 30-40 Pa. This indicates a possibility of replacing the traditional flow plate designs with the proposed ones.

30 Key words: Computational Fluid Dynamics (CFD), Optimization, Fuel cell, Serpentine, Design
31 of Experiment (DOE)

32 INTRODUCTION

Fuel cells are electrochemical devices that transform the chemical energy of reactants into 33 electrical energy with a very high efficiency. Fuel cells produce waste heat and generate water as 34 a reaction product. The fuel (hydrogen) is supplied to the negative electrode (anode) while the 35 36 oxygen from air being the oxidant is supplied to the positive electrode (cathode) as seen in Proton Exchange Membrane fuel cells, among others. The chemical reaction at the anode produces 37 electrons for an electric current. All fuel cells have very high efficiencies which are often 38 independent on the size of the system. Their design is also scalable and they produce zero or 39 40 almost zero greenhouse gas emissions. As they have no moving parts, their operation is highly reliable as a result of their being vibration-free and less susceptible to wear and tear [1]. Fig. 1 41 shows a 3D view of a five stack fuel cell. 42

Though the advantages of fuel cells are enormous, their disadvantages cannot be overlooked. Cost remains a major challenge to the fuel cell industry, which has impaired their commercial success for general use. Storage of pure hydrogen is also a major issue. In situations where fuel that is not pure is used, additional fuel reformation technology has to be taken into account. Fuel cell performance also decreases when impure hydrogen gas is used. Traditional power generation

48 largely depends on fossil fuels which are now being discouraged around the world because of their high impact on the environment. Fuel cells are used for a number of portable applications, in the 49 transportation sector and even the stationary sector. Most scientists believe that portable devices 50 like mobile telephones and laptop computers will soon demand high power to keep them running 51 52 for longer. As fuel cells are scalable with very simple recharging capabilities compared to batteries, they are a suitable option for portable devices in the near future. The limitations of fossil fuels and 53 the high demand for them by the transport industry contribute to fluctuations in prices, 54 necessitating an alternative energy source. In its defence, the transport industry has undergone 55 significant recent improvement as there is a growing number of hydrogen fuel cell cars on today's 56 roads, with researchers still conducting investigations to improve the current automobile 57 58 technology to develop a product that is cheaper and more reliable. The unreliability of the power 59 supply in some parts of the world affects most companies negatively [2]; an improvement in 60 current fuel cell technology will do much to alleviate this. In order to generate more electricity and heat for living space, the stationary fuel cell is usually preferred. There are currently eight types of 61 fuel cells available: Alkaline Fuel cells (AFCs), Phosphorous Acid Fuel cell (PAFCs), Solid Oxide 62 63 Fuel Cells (SOFCs), Molten Carbonate Fuel cells (MCFCs), Zinc-air fuel cells (ZAFCs), Protonic Ceramic Fuel cells (PCFCs), Biological fuel cells (BFCs) and Proton Exchange Membrane fuel 64 cell (PEMFCs)[2,3]. The PEMFC, also called the polymer electrolyte cell, generates a high power 65 density at low weight, cost, and volume. PEMFCs are normally made up of an anode, cathode and 66 an electrolyte membrane as shown in Fig. 2. 67

Oxidation of hydrogen occurs at the anode while reduction of oxygen occurs at the cathode. The
electrons are transported from one to the other through an electric circuit, hence the fuel cell is
used as a DC source. The fuel cell has a carbon paper, mainly for covering the electrolyte on both

71 anode and cathode sides of the fuel cell. The porosity of this backing layer is normally in the range 0.3 to 0.8. It plays a vital role in the transfer of the reactants as well as the reaction product to the 72 flow plate of the reactive sites [3]. While the electrons produced at the anode are drawn away into 73 the electric circuit, the ions that also result from the electrochemical reaction travel through the 74 75 electrolyte to cathode. At the cathode, an electrochemical reduction occurs due to the electrons returning from the external load. One actively used electrolyte material, Fluorinated Teflon by 76 Dupont, is mostly used in PEM fuel cells and referred to as a "Nafion membrane", as shown in 77 Fig. 3. 78

Nafion membranes provide a high chemical reaction and thermal stability. The electrodes are thin 79 80 films that are well attached to the membrane. Electrodes with a low platinum loading perform well compared to those with a high platinum loading. Adding the polymer in a soluble state into the 81 82 pores of the support structure (carbon) is one of the approaches taken to improve the usage of the platinum. The interface between the electrocatalyst and solid polymer electrolyte is increased by 83 adapting this approach. Water management in the fuel cell is very crucial, as less or more water 84 could damage the fuel cell. Therefore fuel cell design must carefully consider flooding and its 85 prevention. The electrochemical reaction produces water which is expected to leave the cell after 86 the electrochemical process but poor cell design means it is produced faster than its rate of escape. 87 This flooding prevents the MEA from functioning at its full potential hence nearly one-third of the 88 MEA surface is utilised. [4-6]. The bipolar plates and the membrane electrode assembly are the 89 90 two most important parts of the fuel cell. The transport of the reactants to the reactive site occurs 91 through the bipolar plate. The membrane electrode assembly, having the platinum catalyst layer 92 on its surface, functions as the platform where the electrochemical reaction occurs. Supplying 93 reactant at high concentrations to the catalyst layer with less obstruction will therefore significantly

94 improve fuel cell performance. The design of the bipolar plate is also important as it determines the water management through the cell and creates a platform where the generated current can be 95 collected [7]. The membrane electrode assembly is often located between two flow plates. It is 96 composed of a proton exchange membrane and a gas diffusion layer which is porous in nature but 97 98 conductive electrically. Bipolar plates in the fuel cell are normally made of graphite with a metallic housing but this design is gradually falling out of practice. Most newly developed PEM fuel cells 99 100 are made of a polymer called acetyl to reduce the weight of the fuel cell, which in effect reduces its overall cost [8-10]. Fig. 4 shows some new types of fuel cell on the market that use acetyl. 101

Though graphite has some good electrical properties, it has some major setbacks that have prompted the paradigm shift by researchers around the world from relying on it as the sole material for the bipolar plate. The tensile strength of graphite is very low and it is also very brittle. It is also very expensive to machine. With the bipolar plate accounting for almost 70% of the weight of the entire cell according to Lawlor et 2009, Dong *et al.*, 2007 [11, 12], it is recommended that the material for the bipolar plate be made lighter as nearly 40% of the cost of a fuel cell depends on the bipolar plate.

109 Metals have recently become more popular as the material of choice for bipolar plates as their 110 advantages include low cost, ease of processing, high mechanical strength, high electrical conductivity and high thermal conductivity. The normal practice is for the flow channels to be 111 machined on the bipolar plate. This is done to achieve uniform distribution of the reactants and 112 thus helps make better use of the MEA. The flow channel can be straight, parallel and even 113 serpentine [11 - 15]. Other investigations concluded that the performance of any fuel cell is highly 114 dependent on the bipolar design [13 - 20]. This is simply because a poorly designed bipolar plate, 115 116 as mentioned earlier, often leads to problems with water removal and obstructs reactant transport.

117 Another researcher undertook a detailed study of the various types of flow plates in a fuel cell and also recommended that, for effective fuel distribution, the bipolar plate must be carefully designed 118 [21]. It therefore confirms that an improperly designed bipolar plate will lead to uneven 119 distribution of the electrochemical reactant in the fuel cell, which reduces the utilisation of the 120 121 catalyst layer [22]. Open pore cellular foam (OPCF) material has recently been used by a number of researchers around the world as an alternative to the traditional flow field design. This is simply 122 because the gas distribution through the OPCF material is fairly even, overcoming the poor 123 distribution in other set-ups. Again, the pressure drop between the inlet and outlet through the open 124 125 pore cellular foam material (OPCFM) is subject to the size of the pores of the foam [23 - 25]. Fig. 5 shows an OPCFM with a porosity of 90% obtained from Goodfellow, UK. 126

Carbon foam has been utilised as the gas flow field was first proposed by Marice et al. [26]. Other 127 128 researchers, like Tsai et al/ [27], also confirmed that flow plate material made of metal foam contributed significantly to the efficiency of the fuel cell. They critically explored the effect that 129 flow plate design had on the efficiency of PEM fuel cells. Their investigation brought to light that 130 flow plate designs play an active role when building a fuel cell using foam material or even the 131 132 traditional fuel cell designs. Kumar and Reddy [28, 29] used foam material in place of channels of conventional flow plates. This modification is not considered appropriate as the full benefit of the 133 134 OPCFM was not explored. With all these advantages of using the OPCF, researchers are still facing challenges in relation to the housing unit where the foam will be placed. The present work is an 135 extension to earlier work [2] where in this investigation a newer approach to the designs have been 136 137 carried to optimise the use of Open Pore cellular foam materials. This paper seeks to investigate a 138 new housing unit for the OPCF material, where the results are analysed on the pressure, flow 139 regimes and velocity profiles.

140 There has been a big increase in the precision of engineering designs as scientists are better able to predict the success or failure of their designs by simulation, thus saving time and money 141 Computational fluid dynamics (CFD) simulation software is one such example, as it can predict 142 and analyse the various flow regimes in a fuel cell design and, in some cases, compute the stresses 143 144 as well. Research into the development and optimisation of flow plates has been studied using CFD simulations [30-37]. Apart from many uses, CFD is also capable of providing information 145 about the distribution of pressure through the flow channel, the pattern of the pressure and the drop 146 in pressure. The velocity at which material enters and leaves the PEM fuel cell can all be predicted 147 148 using the CFD tool. With this information obtained from the CFD simulation, designers can easily create or modify their designs without wasting energy in the workshop on ideas that are not feasible 149 150 or practical. One of the important factors considered in a fuel cell is the even distribution of the 151 oxidant (air/oxygen) and fuel (hydrogen) on the Gas diffusion layer. The pressure of these reactants 152 must be distributed evenly over the Gas Diffusion Layer. This is very important as it determines the amount of catalyst being utilised during the electrochemical process. These are the parameters 153 that define fuel cell performance. The flow channels on the bipolar plates serve as the medium to 154 155 supply and uniformly distribute the oxidant and fuel to the catalyst layer. CFD analysis to help predict the flow distribution across the channels and check the pressure and velocity through the 156 157 bipolar plate channels was performed by Kumar and Reddy, 2003, [33], Lozano et al., 2008 [36] and Barreras et al. 2011 [37]. This research work intends to explore other suitable flow plate 158 159 designs using OPCF material. The designs were optimised and varied across selected velocities in 160 literature (1, 3, 6, 9, 12 m/s). Different types of manifold designs were considered and their flow regimes were checked through CFD simulation analysis. 161

162 NUMERICAL MODELLING, OPTIMISATION AND SIMULATION

163 As explained earlier, pressure distribution on the gas diffusion layer and the membrane electrode assembly are important parameters when designing a fuel cell. Other factors, like temperature 164 distribution and even the speed at which the reactive gases travel to the reactive site are all very 165 important as they influence the output or efficiency of the cell. The outcome of the simulation can 166 167 also clearly show areas in the design where there could be the possibility of dead zones. Dead zones are areas around the fluid domain where the gas is static. It could also be described as the 168 169 area around the fluid domain that may not be in contact with the reactive gas. This leads to accumulation and retention of water in the cell. A vital function of the gas is to be able to carry 170 171 any water along the channels as it flows towards the outlet of the channel. Accumulation of water prevents some areas on the MEA from being utilised, hence reduces fuel cell performance. 172 173 Excessive water in the fuel cell could cause flooding of the cell which will also create serious 174 problems in the functionality of the PEM fuel cell. This clearly stipulates that the design of bipolar 175 plate even affect the water management in the cell.

176 FUEL CELL DESIGN

177 ANSYS software was used to determine the flow regimes for the bipolar plate of a fuel cell with an active reaction area of 25 cm². A number of designs were suggested for the bipolar plate to aid 178 179 in the channelling of hydrogen to the reactive sites of the MEA. Manifolds were created in order to channel the hydrogen towards the foam material. CFX in ANSYS was used as the CFD 180 181 technique to analyse housing designs for both the anode and cathode regions of the fuel cell. The 182 electrochemical reaction in a PEM Fuel cell operates under moderate conditions when compared to the other types of fuel cell. The rate at which the various reactive gases travel through the bipolar 183 184 flow plate design may be low but the fuel cell will still produce some current. Theoretically, it is 185 possible to calculate the pressure drop in the fluid domain but the type of flow must first be

determined. The flow could be laminar or turbulent. This is determined through the calculation of 186 187 the Reynolds number. For the purpose of this investigation, the flow was considered laminar since it has been well established that the reactants inside the fuel cell are in laminar flow, with a 188 Reynolds number Re < 2300. The flow was also kept as a single phase. The laminar flow design 189 190 was also utilized by Ramos - Alvarado et al. [38]. Various designs were then simulated with 191 specific boundary conditions clearly depicted in Table 1. The final model contained 290,000 -316,853 elements. Fig. 6 shows the anode housing designs with their respective CFD mesh using 192 ANSYS CFX. 193

194

Table 1: Boundary conditions used in running the simulations.

| Design Modeller | CFX |
|-----------------|-------------------------|
| Mesh | Mixed Tet and Quad |
| Sizing | Proximity and Curvature |
| Smoothing | Fine |
| Transition | Fast |
| Elements | 316,853 |
| Solver | CFX |
| Model flow | Laminar |
| Fluid | Hydrogen |
| Solid walls | Aluminum |
| Porosity | 0.93 |
| | |

Parameter Response

| 1951 | Inlet Velocity | 1m/s |
|-----------|---------------------------|-----------------------------------|
| 9 5 | Temperature | 320 |
| 1961 | Monitors | Mass flow Continuity |
| 9 6 | Interfacial area density | 0.50 |
| | Heat transfer coefficient | 0.01 |
| 1971 9 | iteration | 100 |
| 7 | Solver type | Pressure based – Double precision |
| 1981 | | F |
| 9 | | |

From Table 1, the meshing was kept as Mixed Tet and Quad and a fine mesh was generated. The number of elements was also 316,853. The fluid domain for the gas was kept as being porous and the porosity of the aluminium foam used was 0.93. The speed of the gas entering the fuel cell was also maintained at 1 m/s and the flow kept as laminar. The number of iterations was also kept at 100 for convergence to occur during the simulation. The sizing of the mesh was also maintained at proximity and curvature but during the simulation for design 5, which is the serpentine flow channel, the fluid domain was maintained in settings since the channel was not porous.

206 NUMERICAL MODEL

Extensive research in the design of metal foams have been undertaken, where key characteristics that determine the performance of the foam has been established both experimentally and theoretically [38-45]. One of the performances measured is the pressure drop in the foam material and different mathematical models have been developed. Flow in a porous media can be determined by the well known Darcy's Law [45]:

212212

Δ*P v* 10

213213
$$\frac{1}{L} = (-) V$$

(1)

Where, ΔP is the pressure drop over length L (m), v is the fluid viscosity (m²/s), V is the fluid 215 velocity (m/s) and γ (m²) describes the permeability of a porous media. However, Darcy's law can 216 217 be used only for low Reynolds numbers (Re < 0.1). In instances where there are high flow velocities (>0.1 m/s), the drag induced by the ligaments of the foam material becomes important. 218 There is also a major influence of both turbulence and inertia and the pressure drop therefore 219 220 displays a parabolic trend with the increasing velocity [46]. Therefore to consider this, a modified form of D'Arcy model, that describes the pressure drop in the porous medium at these velocities 221 222 also known as the Hazen Dupuit-Darcy model is used,

223223

224
$$\frac{\Delta P}{L} = \frac{v}{\gamma} V + \rho C V^2$$
(2)

225

226 Where, ρ is the density of the gas in the medium (kg/m³), and, $C = f/\sqrt{\gamma}$ is the coefficient related 227 to the structure of the permeable medium, with *f* being the coefficient of inertia. The permeability 228 γ (m²) of porous media is related to the porosity and the mean pore radius, is given by [38], 229229

230230
$$\gamma = \frac{\zeta^3}{180(1-\zeta)^2} d_p^2$$
 (3)

231231

Where, ζ is the porosity of the foam material and d_p is the pore diameter. For the traditional hollow (serpentine) channels, since the flow is laminar in a functional PEMFC, one can define permeability, γ for the channel through the well-known Hagen–Poiseuille equation [38],

235235
$$\gamma = H \frac{d_h^2}{32}$$
 (4)

Where, H = 2.59 (m) is the shape factor which is typical for laminar flows [38], d_h is the hydraulic diameter of the channel (m).

Another mathematical model, by Ergun *et al.* determines the pressure drop in the foam material with spherical particles of diameter d_p . The Ergun equation is commonly utilized where the flow is through a dense bed, however, to draw a comparison between different mathematical models, this equation was also used.

242242

$$\frac{\Delta}{L} = AV + B\rho V^2 \tag{5}$$

244244

245 Where,

246246
$$A = \frac{150(1-\zeta)}{\zeta^3 d_p^2}$$
(6)

247247
$$B = \frac{1.75(1-\zeta)}{\zeta^3 d_p}$$
(7)

Research in the design and fabrication of metal foams with different manufacturing techniques has
also been undertaken [47], where Ashby *et al.* mathematically define the pressure drop in the metal
foams as,

251251
$$\frac{\Delta P}{L} = \varepsilon \left(\frac{1}{\omega}\right) \begin{bmatrix} \nu^{m} \rho \\ 1 & \nu^{m} \rho \end{bmatrix} V^{2-m} d_{L}^{-m}$$
(8)

Where, α is the absorption coefficient, d_L is the foam ligament diameter, ε and m are determined experimentally [47]. This equation is in the context of drop the in pressure with respect to transfer of heat, but for the purposes of correlating models, this equation was also used. The effect of the drag and friction due to flow in the foam material was explicitly described by Fourie and Du Plessis [48], where they make use of the tortuosity of the ligament structure, and thus determining the pressure drop as,

259259

 ΔP

0 4 7

260260
$$L = (3 - \tau)(\tau - 1) \left(\frac{\tau}{\zeta^3 d}\right) \left(\frac{\tau}{2} + \frac{\tau}{4}\right) \zeta$$
(9)

 $\rho \tau^2 V^2 = 3C_{dv} = C_{df}$

261 Where,

262262
$$C_{dv} = \frac{24v\zeta}{\rho(3-\tau)d_{-p}V}$$
 (10)

$$\rho V^2 d_p (\tau - 1)^{-0.667}$$
263263 $C_{df} = 1 + 10 \left(\frac{2v\zeta}{2v\zeta} \right)$ (11)

264264

265 Where, τ is the tortuosity, C_{dv} and C_{df} are drag and frictional coefficient.

Since the pressure drop in the channel is directly related to the pressure gradient and the channel permeability, the pumping power consumption can be approximated by the product of the pressure drop along the channel and channel flow rate [38]. Wang, 2005 establishes a pumping power parameter as a ratio of the pumping power for the cathode flow (the major part) of the electric power produced by a fuel cell. Unlike an equation that describes the fuel cell polarisation curve, a linear approximation is assumed to be a very good fit for practical operating conditions [38]. Here a modified form of the equation has been established to define a linearisation of a polarisation 15 273 curve,

$$274 V_{cel} = V_o - V_n (12)$$

Where, V_0 is the intercept of the polarisation curve, as the actual open circuit voltage is always higher, in the analysis, it has been maintained at 0.9 V. V_n is defined as the linear voltage drop as in equation (13).

278278
$$V = \underline{A_m v \rho LI} \left(\underbrace{\xi_c}{} \right)^2 \frac{1}{2}$$

$$^{n} 16\beta_{pump}A_c FCo_2 \gamma$$
(13)

Where, A_m and A_c is the area of membrane and cathode respectively (m²), v is the kinematic viscosity (m³/s), ρ is the density (kg/m³), L is the length (m), I is the current density (A/m²), ξ_c is the stoichiometric flow ratio, F is the Faraday constant (A/mol), C_{O_2} is the concentration of oxygen (mol/m³), β_{pump} is the pumping power ratio[38].

283 RESULTS AND DISCUSSION

One of the simplest means of analysing and optimising flow field configuration is through observation of the distribution of pressure and velocity in the fluid domain. As stated earlier, the selected design must be able to uniformly distribute pressure over the gas diffusion layer at a constant rate. The drop in pressure between the inlet and outlet of the flow channel must be less as well in order for the gas to reach the reactive site early for electrochemical reaction to occur.

289 DESIGN 1 OF FLOW CHANNEL (D1)

The first observation is the collision of the fluid with the foam as it flows from the inlet. This causes the speed at which the gas is travelling to increase but the obstruction causes a change in direction around the manifold. Convective flow is created along the porous domain. The D1 profile for the distribution of pressure and velocity is shown in Fig. 7. The purpose of this design was to 294 uniformly distribute the reactant gases over the open pore cellular foam material (OPCFM). The inlet of the design was created to have an obstruction that was oval in shape. This was done so that 295 the gas builds up momentum as it flows around the oval impediment. The downstream part of the 296 297 flow plate had same features as the upstream. Convective flows are observed as the gas leaves the 298 impediment into the porous fluid domain. From the pressure profile in Fig. 7(a), the pressure of 299 the gas entering the fluid domain is at 3.2 Pa. It reduces as the gas exit the fluid domain at 1.0 Pa, 300 indicating an overall pressure drop of 2.1 Pa. The mass transport which is linked to the efficiency of the fuel cell will also be seriously affected. A uniform pressure and velocity distribution are 301 302 observed, as shown in Fig. 7(a) and 7(b). The greater portion of the gas will flow through the foam, 303 meaning that the GDL, which will be in contact to the MEA, will have most of its surface in contact with the gas. Hence the release of electrons through the electrochemical reaction will be very high 304 305 thereby increasing the amount of energy produced. Water found in the pores or channels will be 306 carried to the outlet easily since large areas of the design will have gas flowing through them. This design will, therefore, be suitable for water management in the fuel cell and also the fewer dead 307 zones show the lesser possibility of water accumulation which affects the fuel cell negatively [40]. 308

309309

310 DESIGN 2 OF FLOW CHANNEL (D2)

The D2 design can be seen in Fig. 8. It consists of an obstruction which is perpendicular to the main inlet but the dimensions for each of the five(5) rectangular impediments are irregular. The design is similar to D1, with the downstream section of the fluid domain same as the upstream. The orientation of the inlet and outlet are diagonal to each other. The pressure distribution according to the pressure profile in Fig. 8(a) shows that D2 has the pressure of the fluid being high at the inlet but reduced at the outlet where the gas exits the fuel cell. From the profile, the mid 317 region of the design will have the pressure uniformly distributed. In comparison with D1, the inlet pressure for the D2 is lower. There is, therefore, the pressure drop between the inlet region and the 318 outlet of the cell. The efficiency of the fuel cell will be greatly affected due to the effect on mass 319 320 transport. Greater portions of the MEA will be utilised as the gas will travel through larger portions 321 of D2 compared to that of D1. The outlet velocity for D2 shown in Fig. 8(b) is higher than that of D1, hence any water in the fluid domain or channel will leave the D2 faster than it will D1. There 322 are some regions in the fluid domain of D2 that are low, which , creates dead zones and hence 323 more water accumulated in the fuel cell. It remains one of the major setbacks for this design. The 324 325 inlet and outlet orientation are also diagonal to each other.

326 DESIGN 3 OF FLOW CHANNEL (D3)

327 The D3 design, as shown in Fig. 9, has the orientation of the inlet and outlet being diagonal. The design comes with impediments at the inlet and outlet region of the cell. These obstructions are 328 designed to be both diagonal and perpendicular to the inlet and outlet. It allows the gas to flow to 329 the other parts of the fluid domain but from the pressure profile shown in Fig. 9(a), there is pressure 330 331 drop from the inlet to the outlet. This drop in pressure is fairly low when compared to those of D1 and D2. From Fig. 9(b), a uniform velocity distribution is observed through the bipolar plate. The 332 general design of D3 will have a negative impact on the efficiency of the PEM fuel cell. This 333 occurs because of the orientation of the inlet and outlet of the fuel cell. The impediment for this 334 335 design does not allow the fluid to flow through the entire surface of the fluid domain hence not all 336 the surface of the MEA will be utilised. Dead zones will however be created since the gas is unable to flow through every portion of the fluid domain. It indicates that only one-third of the MEA 337 surface may be utilised hence fuel cell performance will be low. 338

339 DESIGN 4 OF FLOW CHANNEL (D4)

340 The D4 design as shown in Fig.10, has the inlet and outlet of the design being symmetrically aligned to the mid portion of the design. From the design shown in Fig. 10(a), the gas travels 341 through each symmetrical section of the fluid domain due to the double impediment at the inlet 342 region on both the left and right side of the design. The obstruction is actually found at the edges 343 344 of the fluid domain. The gas travels freely from the inlet to the outlet with no impediment at the middle section of the fluid domain. The pressure drop from the inlet region to the outlet region of 345 346 D4 is low, hence it will have a positive effect on the mass transport of the fluid flowing through the domain. The efficiency will therefore be fairly better compared to the designs discussed earlier. 347 348 From the velocity profile in Fig. 10(b), there is a lower velocity at the inlet when compared with 349 other designs. There is also less or minimal restriction as the gas flow directly from the inlet to the 350 outlet. This is noticed around the mid-section of the fluid domain. It is also observed that the entire 351 MEA surface would not be utilised. The blue regions in the D4 are also high hence there would be more water accumulation of water which will affect the fuel cell performance. 352

353 DESIGN 5 OF FLOW CHANNEL (D5) (SERPENTINE FLOW PLATE)

354 The D5 design, as shown in Fig. 11, allows gas to travel through a greater portion of the MEA hence it is the popularly preferred flow plate design for most PEM fuel cells. The results from the 355 356 simulation performed as shown in Fig. 11 exhibited high pressure at the inlet for the first bipolar plate flow channel. As the gas flows through the rest of the channels, it drops gradually in terms 357 358 of pressure, which means that there would be high-pressure drop on the MEA. The implication is 359 that the mass transport will be affected and effectively lead to a reduction in fuel cell performance. 360 The velocity profile is shown in Fig. 11(b). It clearly shows that the velocity at which the gas travels will be distributed evenly across the whole flow plate design. Due to the nature of the 361 362 serpentine design, it is able to carry all water in the channel to the outlet hence very effective in

mitigating issues relating to flooding . The velocities of some of the layers at the boundaries are observed to be low particularly around the edges. Annular flows are therefore created as the water is moved to the channel walls. The area marked blue shows the part of the fluid domain where there dead zones could accumulate. Dead zones as defined earlier are sections on the fluid domain where the gas may not travel through due to the design of the flow plate.

368 VALIDATION OF RESULTS

Some specific velocities used in literature (1, 3, 6, 9, 12 m/s) [9] were integrated into ANSYS. The 369 370 simulation was carried out to give a detailed idea of various situations that may occur in the fluid 371 domain as the gas moved from the inlet to the outlet. It therefore showed the drop in pressure for 372 each design as the gas travelled through the fluid domain at different velocities. It was noticed that 373 the drop in pressure for the D5 (Serpentine design) was high compared to the other design that was aimed at using OPCF material. Fig. 12 shows the effect on pressure drop as the specific fluid inlet 374 375 velocities is varied in the range 1 m/s - 12 m/s for designs D1 - D5. It can be observed in Fig. 12, that D4 shows a very low-pressure drop, with a maximum of 20 Pa at a flow velocity of 12 m/s. 376 377 The inset in Fig. 12 shows the pressure drop for a serpentine flow channel at a range of flow velocity 1 - 12 m/s, where the pressure drop is very high even at low flow velocities. In contrast 378 to the traditional flow channels, the use of OPCF material shows better performance 379 characteristics. Table 2 shows the boundary conditions that were used to run the optimisation of 380 381 the flow plate.

382382

| Meshing Properties | | Boundary Conditions | | Solution Parameters | |
|--------------------|-------------------------------|---------------------|------------------------------------|-------------------------|-----------------------|
| Mesher | ANSYS meshing | Model | OPCF | Solver | CFX |
| Mesh | Proximity and Curvature | Viscous model | Laminar | Solver type | Pressure based |
| Relevance | Fine | Fluid | Hydrogen | Scheme | Simple |
| Size function | Fixed | Solid | Aluminium | Gradient | Least Square Cells |
| Smoothing | Fine | Temperature | 288 K | Discretisation pressure | Standard |
| Transition | Slow | Velocities | 1, 3, 6, 9, 12 ms ⁻¹ | Momentum | Second order |
| Elements | 250000 - 310000 | Pressure Outlet | 0 | Porosity | 0.90 |

Table 2 – Boundary conditions used in the simulation of the flow plates using Velocity

To obtain a comparison on the pressure drop in porous media, and to draw a contrast to the simulation results obtained by ANSYS, the proposed mathematical models were analysed using the values as shown in Table 3. Fig. 13 shows the pressure drop related to the different

- mathematical models and the simulation result for design D4 from ANSYS. It is found that for the
- same porosity $\zeta = 0.936$ and pore diameter, $d_p = 3.068$ mm, the Darcy model, has the lowest
- 391 pressure drop which follows a similar trend to that of the pressure drop for design D4.

| Parameters | Values | Reference |
|------------|---|-----------|
| ζ | 0.936 | [49] |
| υ | $1.838 \times 10^{-5} (\text{kg/s m})$ | [49] |
| Е | 4 | [48] |
| d_p | 3.068 (mm) | [7] |
| τ | 1.308 | [49] |
| ρ | 1.184 (kg/m ³⁾ | [49] |
| d_L | 0.35 (mm) | [48] |
| α | 0.4 | [48] |
| L | 5 (mm) | - |

Table 3: Parameter values used in the mathematical models

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Using the established result, that the Darcy model fits well with the ANSYS model simulation for design D4, further analysis on the mathematical model is therefore performed. The Darcy model in equation (2) relates to the pressure drop as a function of the permeability and the fluid velocity. The permeability as described in equation (3) relates to the pore diameter and the porosity.

Fig. 14 shows the effect of increasing pore diameter for a constant porosity, $\zeta = 0.93$. It is observed that the permeability of the material exponentially increases while the C factor reduces and approaches a constant value for higher pore diameter [39]. This suggests that the pressure drop for high pore diameter would have a linear response with increasing flow velocity. This can be observed in Fig. 15, where the effect of increasing pore diameter is shown with respect to the increasing velocity and the pressure drop. Further analysis on the effect of increasing porosity

suggest that for higher porosity, the pressure drop is lower. This effect can be observed in Fig. 15
(b) for a pore diameter of 100 μm.

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Further utilisation of the Darcy model is carried out by analysing the overall effect on pressure 408 409 drop in a 3D surface plot where the effect of varying pore diameter, porosity, and the flow velocity is considered. This can be observed in Fig. 16 (a), where a higher pore diameter and higher porosity 410 shows a low-pressure drop. There is, however, a trade-off with a low-pressure drop at higher pore 411 diameter, which is the flow regime of the operating fuel cell. For a fully functional PEMFC, it has 412412 been established that the flow through the channel is laminar. The Reynolds Number 413413 $(R_e =$ $\frac{\rho\sqrt{\gamma V}}{2}$) is a good measure of determining the flow in a channel, where, $R_e < 2300$ indicates a laminar 414414 flow and turbulent otherwise [59-60]. It is dependent on the flow velocity and the permeability 415415

(pore diameter and porosity) of the channel, assuming a constant viscosity and density. This key measure is analysed for varying porosity, pore diameter and flow velocity in Fig. 16 (b). It is observed that for a flow velocity above 6 m/s and pore diameter of greater than 2 mm, the flow in the channel would therefore be turbulent. This result indicate that in the design of OPCF channel for consideration in PEM fuel cells, with higher pore diameter to achieve a low-pressure drop, the flow velocity should be less than 6 m/s.

One clear way of analysing fuel cell performance is through the polarisation curve. It is expected that, due to a low-pressure drop, fuel cell performance to be better. Mathematical models that describe the polarisation curve has been extensively studied in the literature [38], however, the performance can also be measured using a linear approximation of the polarisation curve, as this works well for most fuel cells acting within their practical operating range [38]. In analysing such performance, the permeability of the flow channel is a key parameter, which depends on the pore 24 428 diameter and the porosity for porous media. A linear approximation of the polarisation curve is therefore developed which is dependent on the permeability of the channel as defined earlier in 429 equations (12) and (13). Fig. 17 shows a linear approximation of the polarisation curve for both 430 the porous medium and hollow (serpentine) channel. All of the terms in equation (13) are kept 431 432 constant for both types of channels except the permeability, which changes with the type of channel, as defined in equations (3) and (4). Fig. 17 shows the effect of using porous channel on 433 the current density and cell potential. The result for the porous channel was evaluated for a pore 434 diameter of $d_p = 0.25$ mm and porosity, $\zeta = 0.90$, whereas for the hollow serpentine channel, the 435 hydraulic diameter (calculated) $d_h = 0.5$ mm was taken. The calculated permeability of the 436 hollow channel was 2.02×10^{-8} m² and for the porous channel was 2.53×10^{-8} m². It is observed 437 in Fig. 17 that, due to a low-pressure drop because of the use of OPCF flow channel, the 438 performance of the PEM fuel cell is greatly increased. Based on the analysis carried out it can be 439 concluded that for a good performance of the PEM fuel cell using OPCF material, the permeability 440 should be greater than the traditional flow channel. 441

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443 TESTING OF FUEL CELL

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The fuel cell was also experimentally validated by testing the performance of the serpentine flow plate design with that of an open pore cellular foam material used in the new design. Fig. 18 shows the assembly process used in building the fuel cell with the open pore cellular foam material. The grooves were cut using a CNC machine to create the position where the aluminium open pore cellular foam will be placed. After the OPCFM is put in position, the membrane electrode assembly obtained from fuel cell store was also carefully placed on the foam. The cathode housing was also designed to have the foam as its flow channel. The fuel cell was carefully tightened and checked
for leaks, as any loss of hydrogen gas will compromise the economic efficiency of the new PEMFC
design. Once checks showed the fuel cell was well sealed, it was then placed in the experimental
set up as shown in Fig 19 and Fig.

455 The results obtained after using the open pore cellular foam material shown in Fig. 21 indicated that the fuel cell performance improved appreciably compared to the serpentine design and this 456 also validated the results obtained computationally in ANSYS. It must be noted that the hydrogen 457 was passed through a humidification chamber to keep the membrane moist to aid in good electro 458 459 osmotic drag and back diffusion for both experiments. All other parameters, like cell operating 460 temperature and pressure, were kept constant for both experiments. When the pressure drop 461 through the bipolar plate between the inlet and outlet is high, more pumping power will be needed 462 to overcome this, hence reducing the net performance of the fuel cell. The more gas is introduced 463 to the catalyst layer, the more electrons are released hence the reason for the high performance of the fuel cell when the open pore cellular foam was used. 464

465 CONCLUSION

466 The general performance of a fuel cell depends highly on the pressured rop as well as the velocity of the gas as it flows through the fluid domain. High drop in pressure indicates that the flow of gas 467 468 to the reactive site would be low. Therefore, the rate at which electrons will be released due to the electrochemical reaction will be lower, leading to a lower current produced. The work also 469 470 identified that the design of the flow plate affects the water management of the fuel cell. Having a 471 design where there are dead zones implies that not all portions (surface) of the MEA will be utilised 472 during the electrochemical reaction. The orientations of the inlet and outlet also played a key role 473 in determining the efficiency of the fuel cell. The drop in pressure of the foam was only subject to

the pores of the foam while that of the serpentine design experienced pressure drop in each arm of the flow channel. It explains the high-pressure drop for the serpentine flow plate design. The work finally concluded that, in comparison to the serpentine flow design, the open pore cellular foam material was a suitable option for a fuel cell with a minimum pressure drop of 22.5 Pa as compared to 10,000 Pa with the serpentine design at a velocity of 12 m/s.

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Fig. 1: Fuel cell with five (5) Stacks



Fig. 2: Exploded view of a Proton Exchange Membrane fuel cell.



Fig. 3: Nafion Membrane Electrode assembly



Fig. 4: PEM fuel cell with acetyl housing unit from obtained from fuel cell store.



Fig. 5: OPCF material and the PEM Fuel cell schematic



Fig. 6: The CFD model mesh using CFX.



Fig. 7: Fluid domain for flow channel D1: (a) - pressure profile (Pa), (b) - velocity profile(m/s)



Fig. 8: Fluid domain for flow channel D2: (a) - pressure profile (Pa), (b) - velocity profile(m/s)



Fig. 9: Fluid domain for flow channel D3: (a) - pressure profile (Pa), (b) - velocity profile(m/s)



Fig. 10: Fluid domain for flow channel D4: (a) - pressure profile (Pa), (b) - velocity profile(m/s)



Fig. 11: Fluid domain for flow channel D5: (a) - pressure profile (Pa), (b) - velocity profile(m/s)



Fig. 12: Graph of velocity against pressure drop for flow channel designs D1 to D5.



Fig. 13: Comparison of pressure drop using the different mathematical models and ANSYS simulation result for design D4.



Fig. 14: Effect of increasing pore diameter on the permeability and factor C.



Fig. 15: Effect of increasing velocity on pressure drop for (a) different pore diameter (b) different material porosity.



Fig. 16: Surface plot at varying pore diameter, porosity and flow velocity for (a) Pressure drop (b) Reynolds Number



Fig. 17: Current density vs cell potential for the porous and hollow channel.



Fig. 18 Building of Open pore cellular foam material PEMFC.



Fig. 19: Experimental set up a) Open pore cellular foam material b) Serpentine flow field design



Fig 20: Experimental set up for the texting of the fuel cell



Fig. 21: Polarisation curve for the serpentine flow field and the open pore cellular foam material