Review of operating condition, design parameters and material properties for proton exchange membrane fuel cells

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Published in:
International Journal of Energy Research

DOI:
10.1002/er.5810

E-pub ahead of print: 25/08/2020

Document Version
Peer reviewed version

Evaluation of parameters for Proton Exchange Membrane Fuel Cells (PEMFC) design

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Abstract

Studies into the effects of parameters used in the design of proton exchange membrane (PEM) fuel cell have been done. All the modelling parameters considered influenced the performance of the PEM fuel cells. The effect of the operating condition is shown to be significant. Increasing the operating temperature and operating pressure increases the mobility of ions and as a result the ionic conductivity is increased. In addition, the membrane is dried out when the correct humidity is not provided which increases membrane degradation. Adopting good design parameter is necessary for efficient transportation of both reactants (fuel and oxygen). With regards to the use of flow plates, the serpentine flow plate is highly recommended. Material properties are very important in material selection and new product development. For the membrane electrode area (MEA); the membrane, the ionic conductivity is very important and should be given an important consideration.

Keywords: PEM fuel cells, operating conditions, design parameters, material properties, cell performance.

1. Introduction

Using the right design parameters has helped in the advancement of polymer electrolyte membrane (PEM) fuel cells research [1,2]. Evidently, it has helped towards saving cost and time that would have been expended on expensive and time-consuming experiment. A polymer electrolyte membrane fuel cell (PEMFC) is a device used to generate energy for electrical applications [3]. The working principle relies on the direct and efficient conversion of energy stored in hydrogen fuel in form of chemical energy into electrical energy. This energy is

converted through certain electrical processes that results in the by-product of only water [4–11].

Energy and fuel extracted from fossil-based sources suffer depletion and raise serious concerns about climate change. For instance, in a fossil fuel internal combustion engine, specific fuel combustion rate for gasoline-powered is about 240 g kWh^{-1} which translates as about 34% system efficiency [12]. On the other hand, the fuel cells boast significantly greater efficiency and very low emissions as electrical energy conversion efficiency in fuel cells may reach up to 60% with specific fuel consumption rate falling below 60 g kWh^{-1}, generation of both electrical and thermal energy at 80% efficiency and pollutant emission at over 90% efficiency. apparently, at low temperature conditions, it takes only 1 g of hydrogen to produce the same energy as 2.37 g of gasoline [3][13].

Household utilization of fuel cells have been largely demonstrated and proven to provide flexibility, including increasing efficiency by the integration of both electrical and thermal outputs for energy generation, offering increased reliability, reduced noise and maintenance requirements and weight. Additionally, PEMFCs are reputed to operate optimally under high power density and low temperatures with scale-up flexibility. The application of a system such as the PEMFC in stationary, transportation and portable processes therefore promises a viable and effective alternative to fossil fuel, greatly reducing pollutant emissions and increasing energy efficiency significantly [3][13].

While the technology of PEM fuel cells holds great promises, it will remain inapplicable and impractical for industrial and commercial integration if it fails to out-play the already existing fossil fuel alternative in terms of cost. The effectiveness of either of the alternatives depends largely on the manufacturing or processing cost as well as the durability of PEMFC in the diverse operating conditions it will be exposed to. These factors coupled with the availability of hydrogen pose the greatest barrier to the innovation, development and commercialization of PEM fuel cells [3][13].

Having a better understanding of design parameters and their effects on the performance of PEM fuel cell increases the prospects for delivery of a better design that improves efficiency, reduce cost and give a cleaner environment. For this reason, this work was developed. An overview of the PEM fuel cell would be done followed by an analysis of important parameters necessary in the design of PEM fuel cells. Discussions on these parameters would be done

under three (3) categories; operating condition, design parameters and material properties. After proper analysis and evaluation has been done, conclusion would be made.

2. An overview of PEM fuel cells

A typical polymer electrolyte membrane fuel cell consists of an electrode assembly, an anode flow field and proton conducting polymer membrane (e.g., Nafion) which acts as a medium for electrical conductivity facilitated by some Platinum-based catalyst [3][3,14]. Fig. 1 is a schematic diagram of a two (2) stack PEM fuel cell showing all the components, electrical and chemical activities.

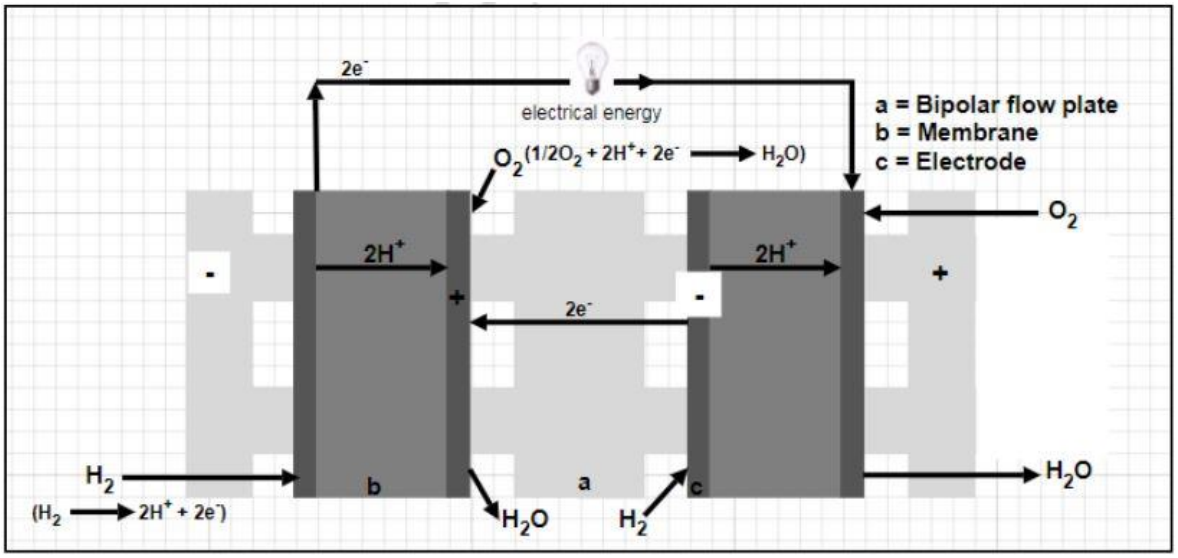

Fig. 1. Schematic of a two (2) stack PEM fuel cell [15]

As shown in Fig 2. The PEM fuel cell is divided into different components namely; anode/cathode collector, anode/cathode bipolar plate, anode/cathode gas diffusion layer (GDL), anode/cathode catalyst layer (CL) and a membrane at the centre. The major chemical reaction in the in the fuel cell is shown in Fig. 1 and the equation is as shown below.

$$2H_2 + O_2 \rightarrow 2H_2O + \text{Heat} + \text{Electricity} \qquad (1)$$

As shown in the Equation (1) above, after the reaction of hydrogen and oxygen, alongside water as product, heat and electricity is also produced. The reactions in the acid and basic electrolyte are simplified below in Table 1.

Table 1 PEM fuel cell chemical reactions in acid and basic electrolyte [1].

	Acid electrolyte	Basic electrolyte
Anode reaction	$H_2 \rightarrow 2H^+ + 2e^-$	$H_2 + 2OH^- \rightarrow 2H_2O + 2e^-$
Cathode reaction	$\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O$	$\frac{1}{2}O_2 + H_2O + 2e^- \rightarrow 2OH^-$
Overall reaction.	$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$	$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

Alongside the reactants; hydrogen, oxygen and water, the PEM fuel cell components plays an important role.

Cost and durability are a major concern for PEM fuel cell. Even though, the current technology of PEMFC has achieved over 35% cost reduction within recent years, the current cost of $61/kW still requires about 50% upgrade in order to compete effectively. A lifetime of about 2,500 hours was achieved in 2009 for PEMFC in transportation application and In 2018, 3,800 hours was achieved, yet this fails to meet the US Department of Energy [DOE] requirement of 5000 hours necessary to compete adequately [3][16]. A regular performance monitoring update for fuel cell technology is usually done by comparing the current achievement against the DOE recommendation for different applications. This is shown in Table 2.

Table 2 Laboratory achievement versus DOE recommended target for 2020 [16].

Fuel cell application	Recommended target by DOE (hours)	Laboratory achievement (hours)
Automotive	5,000	3,800
Public transportation	25,000	6,200
Stationary uses 1-10 kW 100 kW- 3 MW	 1,000 80,000	 11,900
Industry (forklift)	20,000	11,600

Alternative uses (Backup)	10,000	2,600

To reduce the disparity between the DOE recommended research target and the laboratory achievement, there is a need for innovation, research and development in the fundamental investigation of PEMFCs. Fields such as water management, heat regulation, optimization and design of materials used are important for the overall enhancement of PEMFC performance leading to more effective manufacturing and mass-production costs.

The properties exhibited by renewable energy sources provide vital enhancements to global energy needs, quality of life and sustainability which affects economies as well as environmental and welfare conditions. This led to the prediction that the global use of renewable energy sources will increase significantly from 15% to 50% in the year 2050. This prediction was further asserted while investigating and comparing the various mainstream renewable energy sources using criteria such as efficiency, durability, energy and power density, ease of integration and cost-effectiveness; the PEMFC storing energy in hydrogen form offered the greatest promise [17].

3. Design Parameters and their effects

Considering the components of a polymer electrolyte membrane fuel cell as shown in Fig. 1, studies have shown over time that a major factor responsible for the high cost of production is associated with the cost of material used for the membrane. In most commercially produced PEMFC, the proton conducting membrane is made of Nafion®, Aciplex® or Flexion®. Proper consideration when determining the design parameter can help to discover cheaper materials and better processes [18]. A well-designed model used to simulate an operation will adequately inform researchers on the performance of the system using specified parameters that are similar to the materials and component configurations necessary. This presents a powerful guide for researchers who aim to explore and understand the control strategies and contributions of the overall system to achieve enhanced performance. In addition, by the application of modelling and simulation, it is possible to adjust and regulate or omit specific parameters in the system in order to investigate and assess how variations could affect performance [19].

An illustration of a single PEM fuel cell showing all the various parameters that is solved during modelling is shown in Fig. 2. All the various components were considered in terms of material

properties and operating conditions. The parameters considered can be categorised as follows: water properties, hydrogen properties, oxygen properties and material properties for each of the layers. As a consequence of this, Spiegel et al [20] agreed that a slight change in any parameter affects at least two other parameters. To improve the performance of the system, parameters such operating temperature or pressure, can be changed which leads to a change in the state. Changes in system performance can be determined by monitoring the variation in the polarization curve. Fig. 3 below shows the figure of the polarization curve.

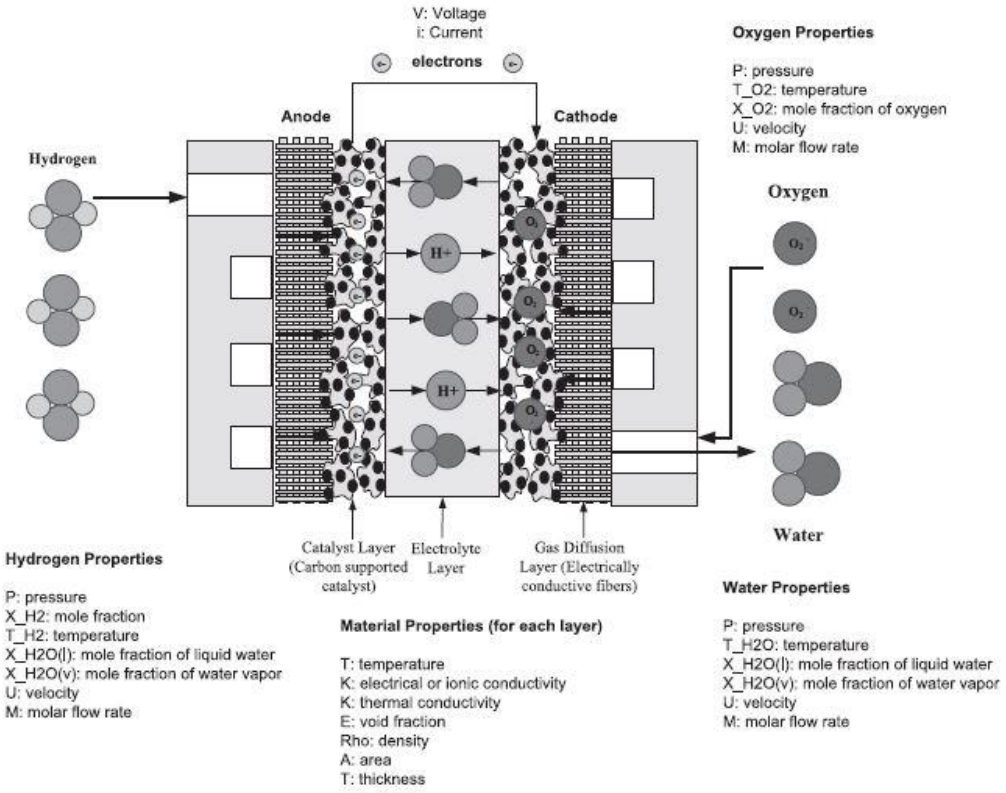

Fig. 2. Necessary parameters required for PEM fuel cell design [20]

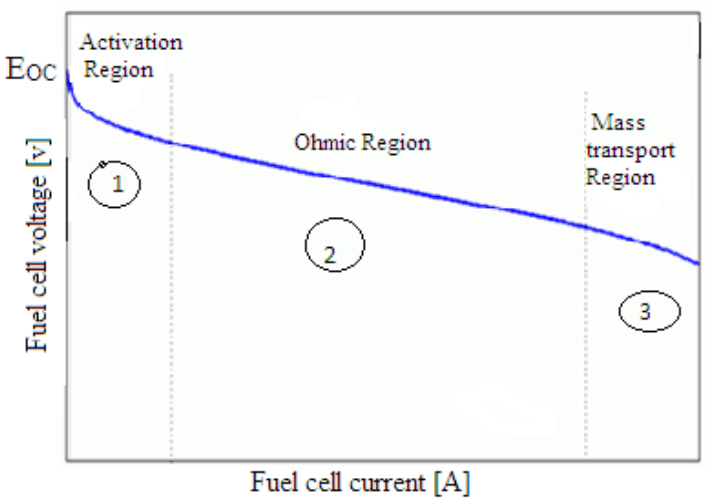

Fig. 3 Polarization curve [21]

A confirmation of the importance of accurate parameters during porous electrode preparation and performance monitoring in order to further the development of exchange membrane fuel cell technology was made by Carlson et al [22]. While maintaining a temperature of about 50°C, the study investigated Tokuyama AS-4 ionomer catalyst layer, Pt/C loading, relative humidity and thickness of the catalyst at the anodic and cathodic electrodes. It concluded that the loading thickness and catalyst layers at the cathode/anode junctures, affected fuel cell performance. It was also revealed that non-uniform current distribution across the electrodes was responsible for variations observed in the relationship between electrodes and current density and that the conductivity was affected by relative humidity in the electrodes.

Various tools, such as polarisation curves and Electrochemical Impedance Spectroscopy (EIS), were used in the investigation of homogeneity, overall stability, performance and resistance losses of a PEMFC subjected to changing operation parameters. The uniformity and chemical stability of the PEMFC using the segmented cell technique assess real-time spatial current density distribution was also studied. It was revealed that the optimal configuration of several parameters such as higher back pressure to enhance performance while maintaining uniformity and current distribution, increased relative humidity to enhance homogeneity, increased air stoichiometry for local stability which are necessary to design detailed models and simulations. Other vital parameters include water management and gas concentration [23].

Vital parameters that must be investigated in the design of a PEM fuel cell include the gas pressure, weight fraction, cell potential, cell temperature, fuel temperature, catalyst layers, water concentration, gas diffusion layers, backing layers, among others. The water, hydrogen

and oxygen are characterized by pressure, temperature, mole fraction, velocity, molar flow rate and mole fraction of liquid water and water vapour. The materials used in the design of each layer are characterized by the ionic and electrical conductivity, temperature, void fraction, density, area and thickness. The overall operating condition is determined by the operating temperature, cathodic and anodic pressure, cathodic relative humidity and stoichiometric factor. This is as shown in Fig. 2 with further analysis made in Table 3.

3.1. Operating condition

Recent research has shown the relative importance of operating conditions on the overall performance of PEM fuel cells. Subjecting fuel cells to varying operating conditions such as power density, permeability of gas diffusion electrode [GDE], operating temperature, electrode relative humidity, electrical conductivity and operating pressure, it revealed that different configurations of these modelling parameters significantly determine the soundness of a model constructed based on them. However, of the above modelling parameters, pressure of the fuel cell and the GDE conductivity were reported to have the most prevalent role in the optimal performance of the PEM fuel cell. A maximum power density of 870mW/cm^2 was achieved when the pressure is set 3.44 atm with GDE conductivity 9 of 997.7 s/m [24].

The cathode and anode are also important fuel cell operating conditions, as evidenced by Carlson et al while varying the thickness of the loading and catalyst layers at 50°C. This study submitted that conditions such as conductivity, non-uniformity of current distribution and relative humidity of the electrodes affected fuel cell performance. It showed relative humidity as a design parameter that greatly affects cell performance. This is ascertained by non-uniform current distribution when the relative humidity is varied from 95 to 70% [22]. Related work by Zhang et al [23] shows similar effects exhibited by back pressure and air stoichiometry.

In galvanostatic mode, Yang et al [25] noted that massive fuel cell performance issues such as the accumulation of water and nitrogen were recorded due to varying nitrogen and water accumulations and other parameters including electrode humidity, hydrogen pressure and current density distribution. The cathode inlet gas humidity and current density or the hydrogen pressure and air stoichiometry similarly affected cell voltage.

Benmouiza and Cheknane [26] investigated the operating parameters that majorly affected activation, osmic and mass transport voltage variations in PEM fuel cells. The study analysed current density, thickness of the electrolyte, transfer coefficient, operating temperature and useful cell area, the effects on voltage drop and efficiency of the fuel cell. It was noted that

while the drop-in mass transport decreased the voltage by about 1 V, the activation voltage dropped the voltage by 0.2 V and osmic voltage by about 0.8 V. This study also showed that increasing the hydrogen, oxygen and water pressure enhanced the cell performance. Detailed analysis is shown on table 3.

Applying the right operating condition can improve the performance of a PEM fuel cell. Using a tantalum micro resistive thermal sensor-based technique, chemically resistant, easy to integrate and versatile thermal sensors were used to investigate the in-situ temperatures and electrical conductivity of an operating PEM fuel cell in real-time. From this study, it was revealed that as a function of constant voltage or current of the fuel cell, the temperature of the active layer could vary significantly from the temperature measured in the bipolar plate, and it was possible to experience less important overheating [27]. This would improve durability and cost in real terms.

In a work by Nur et al [28], PEM Fuel cells with about 25 cm^2 active area were operated under varied conditions to assess the effects of temperature change on the performance of PEMFC. They were further characterized with additional cell resistance measurements and performance curves, the results showed that the increase in the inlet gas temperatures largely enhanced overall fuel cell performance.

PEM fuel cells of high temperature [HT-PEM], with a temperature operating range of 95°C to 200°C, were developed. This is because of the improvement associated with fuel cell performance when temperature is increased. Increasing the operating temperature, additionally, leads to increased conductivity and mass transfer of reactants, increased resistance of the electro catalysts to contamination and the improved electrode kinetics facilitating hydrogen oxidation reaction [HOR] and oxygen reduction reaction [ORR]. However, it is worthy of note that when the temperature is too high, membrane humidification drops, and the rate of hydrogen crossover increased. High temperature can also lead to reduced lifetime for PEM fuel cell due to the degradation of key components like gasket materials, bipolar plates and electro catalysts [29].

Fig. 6 below shows a fuel cell operating at humidity temperature 50°C but with varying operating temperatures between 30°C and 50°C, indicating the positive impact temperature increase has on cell performance owing to enhanced conductivity and electrode kinetics.

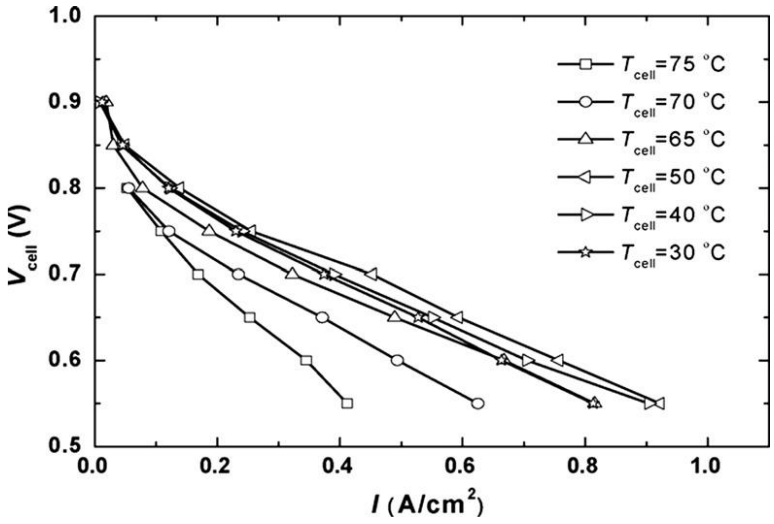

Fig. 6 Effect of cell temperature on cell performance at a humidification temperature of 50^0C [29]

Using a PBI-membrane MEA HT-PEM fuel cell, the electrical conductivity was assessed without extra humidification at between 120°C and 200°C. Fig. 6 below shows the linearly increased performance obtained by raising the temperature leading to enhanced current densities [29]. Strahl and Costa-Castello [30] developed a linear and nonlinear characterization model of an open-cathode PEM fuel cell and discovered the possibility of approximately equating linear and nonlinear behaviours of the models. It was concluded that in order to ensure adequate water management in a PEM fuel cell, one must employ advanced temperature regulation system.

Qin et al [31] experimented on a 20 kW PEMFC used in the automobile industry, investigated the operating pressure optimal configuration by integrating an air compressor in the system. The pressure optimization was assessed numerically and experimentally by investigating the fuel cell stack and the air compressor respectively. As a result, it can be argued that increased operating pressure led to increase power generation. A two-sided compression at 1.2 atmospheric temperatures is found to be the optimal pressure efficiency of the air compressor.

Studying active area of fuel cells operating under varying relative humidity, Nur et al [28] observed that the level of inlet gas humidification enhanced fuel cell performance, and an increase in the cathode gas humidification effects a more positive optimization on the cell.

In PEM fuel cells, the proton conductivity which largely determines power output is in turn greatly determined by the relative humidity [RH] of the fuel cell. As stated earlier, most PEM fuel cells are fitted with perfluorosulfonic acid [PFSA] membranes such as Nafion® or

Aciplex®. These membranes operate optimally only at relative humidity of greater than 80% in the inlet gases if H_2 and O_2 in order to contain enough water to enable optimal proton conductivity, activity of proton within the catalyst layers, mass transport and electrode reaction kinetics [32].

Fig. 7 below represents a schematic review of the balance of water in the cathode, anode and membrane components in a PEM fuel cell.

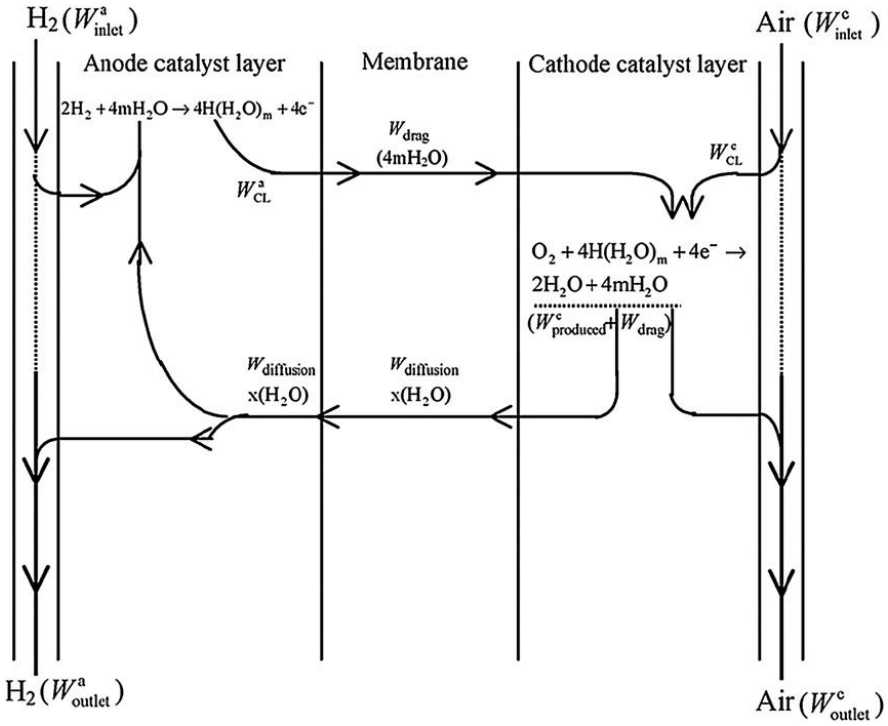

Fig. 7 Schematic of water balance inside an operating PEM fuel cell [32]

In conclusion, the relative humidity of a fuel cell affects the performance and impacts the cell thermodynamics, Tafel slope, current densities, mass transfer, and proton conductivity within the membrane, among other conditions. Using three-dimensional mathematical modelling to simulate an interdigitated flow field PEM fuel cell, Zhang et al [32] indicated that the flow characteristics and cell efficiency affect cell humidification. The computational fluid dynamics [CFD] experiment used a range of relative humidity from 0 to 100%, and measured fluid motion continuity equation, boundary layer theory and current distribution. From the simulation result, it can be deduced that in addition to its impact on current density, focusing on the anode electrode humidification had a more positive impact on achieving overall humidification and fuel cell performance.

In modelling a five single-celled PEM fuel cell stack, a single phase three-dimensional system that incorporates the membrane, gas diffusion layers, catalyst layers, current collectors and flow channels was used by Macedo-Valencia et al [33] to investigate the electrochemical reaction, transport parameters, heat transfer and fluid flow within the system. The results which were obtained by numerical model were instrumental to determining the heat sources and temperature as well as the distributions of the mass fractions of oxygen and hydrogen. It was discovered that the current density distribution was determinant of the heat sources in the MEA. The design was validated using polarization curves and experimental data.

Operating parameters include cathodic and anodic relative humidity, porosity and electrical conductivity of the gas diffusion electrode (GDE), pressure and operating temperatures. With the knowledge of the most effective and efficient parameters, balance can be achieved between couple characteristics such as the relationship between power density and operating conditions, as investigated in recent literature. To find this balance, Peng et al [24] employed the approach of artificial intelligence by a support vector machine (SVM). A power density model which corresponded to experimental data was successfully developed. With this model, the relationship between operating parameters and power density of fuel cell was studied, using simulation profiler to measure the insensitivity of the simulation to changes in the operating conditions. Though the process seemed laborious, the experiment revealed the major effects that the parameters of electrical conductivity of the gas diffusion electrodes and the fuel cell pressure has on the optimal performance of PEM fuel cell. This information is a vital guide for researchers who seek to develop model, simulate operating conditions and innovate the fuel cell technology.

3.2. Design parameters

In the construction of PEM fuel cell, design parameters such as channel geometry play an important role in the effective configuration of performance. One of the most powerful tools used to obtain the optimization of these parameters is the general algorithm [GA], using the fitness function calculation in an isothermal quasi-two-dimensional model [34]. Lee A et al [35] generated a model-based strategy to confirm the effects of geometric designs such as interconnector rib size and electrode backing layer thickness on overall fuel cell efficiency.

Flow channels are important parameters in the design of an efficient PEMFC. They are fabricated along the surfaces of the bipolar plates and are necessary for the distribution of gases

by ordering the transfer of gases and ensuring homogenous gas distribution. To avoid severe failure of the fuel cell, the flow channels must be designed with optimal geometric parameters [36]. Fig. 8 below compares different types of flow fields which have unique influences on design.

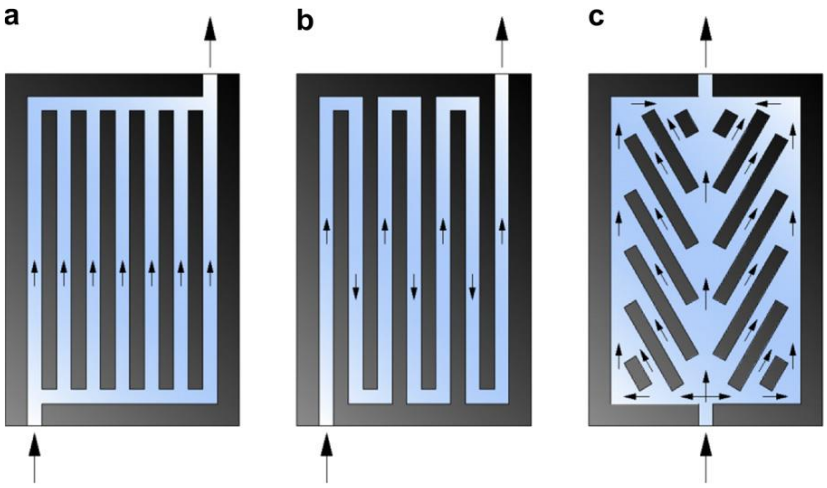

Fig. 8 Comparison of different flow fields: a) Parallel flow channels; b) Serpentine flow channels; c) Bio inspired flow channel [36]

Reshetenko et al [37] integrated 6-channel and 10-channel serpentine flow fields in a segmented fuel cell system and assessed the impact of these parameters on operating current distribution. For the 10-channel flow field, performance dropped at low current but increasing the number of channels at higher temperature enhanced cell performance due to a reduction in the rate of mass transfer voltage loss and increase in pressure drop. In addition, electrochemical impedance spectroscopy [EIS] indicated that the flow field design parameters affected fuel cell performance.

Similarly study by Carton and Olabi [38] analytically compared three configurations of flow plate parameters: serpentine flow plate, maze flow plate and parallel flow plate and assessed how the design parameters affected efficiency, current, power and voltage using polarization curves and other experimental tools. The findings revealed that while the serpentine design proved more effective in all conditions, the parallel design exhibited considerably well at high pressures. Fig. 9 below shows the three flow plate designs in the experiment.

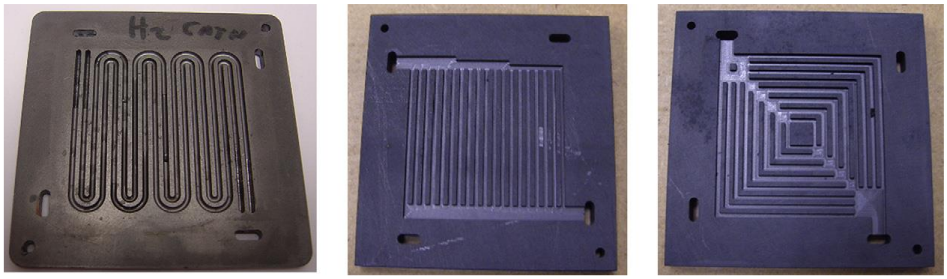

Fig. 9 Serpentine flow plate, parallel flow plate and maze flow plate designs (39)

Fuel cell performance and channel under rib convection can be significantly increased by increasing the pressure of the gas flow between side-by-side channels. This can be achieved by fitting longer straight serpentine flow channels in rectangular flow fields [36]. Fig. 10 below shows channels of different lengths achieved by varying the number of channels arranged in parallel, showing that the length of flow channels affects fuel cell performance.

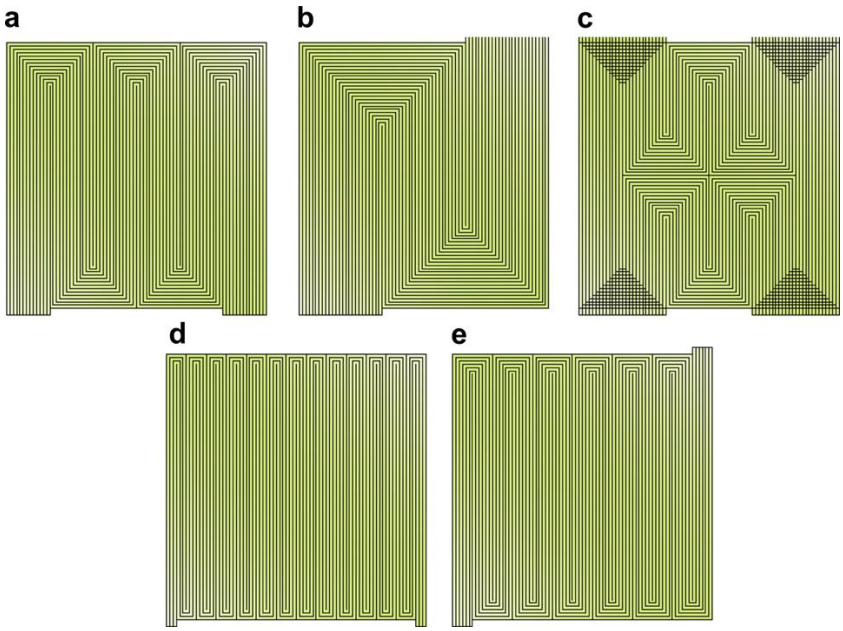

Fig. 10 Flow field patterns of anode and cathode on 200 cm^2 PEMFC: a) 3-channel multiple serpentine flow-field; b) 6-channel multiple serpentine flow-field; c) 13-channel multiple serpentine flow-field; d) 26-channel multiple serpentine flow-field; e) 26-channel multiple symmetric serpentine flow-field [36]

Many investigations have concluded that the width of flow channels offer significant effect on fuel cell performance howbeit at low operation potentials only. Manzo et al [36] designed a model integrated with a parallel flow field and a counter flow field with about 100 cm^2 active area. Using a basic flow field design, it was found that the optimal width for the flow channels

was between 0.7 mm and 1 mm. In general, channel width should increase with decrease in current density.

The flow in a fuel cell and its effects on fuel cell performance was assessed by Kamaruddin et al [39] using 24 full-factorial designs to observe the relationship between diameter of the inlet flow, height of storage vessels, direction of flow and fuel cell orientation. While maintaining vertical flow direction, the inlet flow diameter was varied to 1.5 mm, 2.38 mm and 4 mm, vertical/horizontal orientation and height of storage tank ranging from 50 mm to 70 mm. The flux was significantly affected by the inlet diameter and height of storage tank.

Manzo et al [36] reported that the reduced depth of the flow channel along the cathode stream wise direction induced higher reactant gas inflow into the gas diffuser and catalyst layers which in turn enhance fuel cell performance. However, the pressure drop increases due to this reduction. Lee et al [35] concluded that the reduction in the thickness reduced cell performance due to uneven distribution of reactant species.

The Gas Diffusion Layer [GDL] is a component in the fuel cell that cast as energy conductor to facilitate the transportation of gases and the management of water. It possesses both hydrophobic and hydrophilic properties and is generally made of woven carbon fibre. Previous researches has investigated and confirmed the impact of Gas Diffusion Layer [GDL] on fuel cell performance[40,41]. Fig. 11 below shows the application of GDL on fuel cell membrane [42].

Figure 11: GDL is applied to the membrane in the hot press [42]

Studying a fuel cell performance with varying catalyst layer [CL] thickness at both electrodes at 50°C led to further understand the relationship the catalyst layer thickness has on overall PEM fuel cell performance. The results showed that simultaneously increasing the thickness of the catalyst layer and the loading layer affected how the cathode and anode are optimized to improve fuel cell performance [22].

The membranes installed in PEM fuel cells are largely responsible for the transfer of gases and the electrical conductivity of the fuel cell. Liu et al [43] investigated the effects of varied membrane thickness on fuel cell performance, changing the thickness by fitting Nafion 117 at 175 μm thickness, 115 at 125 μm thickness and 112 at 50 μm thickness. The study evaluated methanol concentration at 2.0 M and it was revealed that the membrane with more thickness positively affected the performance at low current density while it had negative impact on performance at higher current density. The result was different for methanol of 4.0 M concentration, as varying the current densities largely across the three thicknesses of the Nafion samples did not change the cell voltages exhibited by the three membranes. Finally, it was found that increased membrane thickness improved the fuel efficiency of the fuel cell.

In 2015, Yilma and Ispirli [44] experimentally discover the performance of fuel cells by developing a model in Finite element method program. At 25°C across 13 different electrical conductivities and 6 different membrane thicknesses, it is observed that the current density from the anode exhibited best result at the smallest thickness.

Karpenko-Jareb et al [45] investigated the time-dependent changes that occur within the operating lifetime of fuel cells. Utilizing a semi-empirical model and observing the physical and chemical changes in the PEMFC, it was discovered that the oxygen crossover rate mostly affected the rate if degradation the membrane thickness. The time-dependent degradation in a PEM fuel cell was measured using a semi-empirical model showed that the thickness of the membrane was dependent on the oxygen crossover rate.

An isothermal, single-phase and single domain three-dimensional model was developed and integrated using CFD by Kahroba and Shirvani [46] to investigate the thickness of the membrane., It was found that while proton conductivity increased with membrane thickness, cutting the membrane thickness from 0.178 mm to 0.089 mm the fuel cell potential is positively affected by decrease in membrane thickness.

In an interrelated research by Dehsara and Kermani [47] which involved the design of a two-dimensional numerical model of the single-phase flow of gases in the electrode of a PEMFC operating at relative humidity of 100%, temperature of 80°C and pressure of 5 atm. Physical parameters such as channel length and height, gas diffusion layer [GDL] thickness, catalyst layer [CL] height, hydraulic permeability, open circuit voltage and osmic resistance were considered in the modelling. Due to their involvement, they all influence the outcome of the experiment and the overall performance of the system.

3.3. Material properties

The different physical and chemical components of a PEM fuel cell stack exhibit various physical, chemical or physio-chemical properties each impacting file cell performance in specific ways. It was revealed that an example of such are the thickness and porosity of the gas diffusion layer [GDL] which influences the transportation properties of porous components [48].

Analysis by Gao et al [48] showed that the anisotropic properties of the GDL should be increased since the permeability was more significantly affected through the principal flow direction than the non-principal flow direction. It was also discovered that increasing the number of fibres affected permeability than increasing the thickness.

Further investigation by Hovorka et al [49] involved the measurements of the coefficients of diffusion and permeability in a two-compartment horizontal diffusion cell. The system consisted low density polyethylene [LDPE], toluene, chiral D- and L-methyl lactates. It was made such that the membrane does not absorb the solvent. The Nafion membrane exhibited considerable difference from the cellophane membrane in terms of transportation and absorption of the methyl lactates. A difference of about 50% was observed and permeability coefficient of the methyl lactate enantiomers and diffusion coefficients in the Nafion membrane. However, the diffusion coefficients changed fifteen-fold when the permeability coefficient difference of the two enantiomers was raised to ten-fold across the two membranes.

A study by Mangal et al [50] in 2015 utilised a diffusion bridge experimented on the porous components of a PEM fuel cell, investigating the transport system and the viscous permeability and molecular diffusivity within various gas diffusion layers [GDL]. Controlling convective transport by regulating the differences in pressure, a combination of Fick's and Darcy's model was used to determine the diffusivity while an oxygen sensor was used to measure oxygen transport within the porous components. At the end if the study, it was discovered that only

with PTFE loading varying between 1.13 x 10^{-11} to 0.35 x 10^{-11} m^2 and diffusivity varying between 0.209 to 0.071 does the permeability show changes, and that both the diffusivity and permeability suffered change with increasing GDL PTFE content.

Another study by Orogbemi et al [51] showed reducing GDL permeability when carbon loading increases in a PTFE loading of the microporous layer, owing to increased thickness of the microporous layer. Across PTFE loading by weight from 10% - 50%, the GDL permeability was minimum at 20%, but showed increase between 10% - 20% and between 20% - 50%. In the 0% - 10% PTFE loading interval, the carbon loading in the microporous layer affected the GDL permeability.

In 2016, Zhang et al [23] identified certain key parameters that are important for the development of fuel cell with homogeneity, overall stability, performance and resistance losses. They reported that water management and reactant gas concentration are vital parameters for an efficient fuel cell.

In a research experiment by Liu et al [43], the impact of methanol concentration was assessed across three (3) membranes with varying thickness of 175 μm, 125 μm and 50 μm. Changing methanol concentration from 2.0 M to 4.0 M revealed that while cell voltage varied at 2.0 M, the three membranes maintained equal cell voltages at 4.0 M.

Systematic [52] explored the transport properties of a polymer electrolyte membrane fuel cell generated a thermodynamic description of the transport system in two setups of fuel cell membrane. In this analysis, the mass and charge transport system showed significant effect on the permeability of the system.

Conductivity, both thermal and ionic, is one of the most important properties needed in materials used in the PEM fuel cell. For this reason, researchers continue to explore various materials with potentials for use. For instance, a perfluorosulfonic acid MF-4SC membrane was investigated in hydrogen and sodium ion forms. Varying the values of the relative humidity from 0% to 95%, the proportional limit stress and the Young's modulus were found to peak when relative humidity ranged between 32% and 58%. Above relative humidity of 32%, conductivity was higher parallel to the strain than perpendicular to the strain and vice versa for relative humidity less than 32%. The ionic conductivity at 0° and 90° to the strain were measured. Results showed that the ionic conductivity dropped below the value before it was deformed after irreversible straining occurred. However, 2 hours after straining, the

conductivity was restored to original value. Anisotropic effects characterised the iconic transfer within broken membranes and at 9% relative humidity, broken membranes exhibited better ionic conductivity than original values [53].

Another group of researchers, Ma et al [54], introduced membranes made of Ag-silica nanocomposite using acetonitrile as both metal ion stabilizer and solvent and investigated the effects high loading of nanoparticles of Ag with electrical conductivity. Reaching beyond 6800 s/cm, the conductivity and the positive conductivity-temperature coefficient rose simultaneously. This extends the application of fuel cells in high temperature operating conditions.

Considering an alkaline media, the ion conductivity of membrane members was measured in anion exchange membrane and cation exchange membrane. In the bid to predict the overall performance of the alkaline borohydride fuel cell, a cell model was used to generate an expression for the conductivity. It was concluded that the cell performance was largely dependent on membrane conductivity [55].

Various characterisation methods have been used to analyse materials to have a better understanding of their ionic capabilities. Three-dimensional (3D) x-ray computer tomography [CT] was used to investigate three gas diffusion layers and the thermal conductivity of components were assessed. Results by Pfrang et al [56] showed that the average thermal through-plane conductivity was about 4 to 12 times lesser than the average thermal in-plane conductivity, when the macroscopic and anisotropic effective thermal conductivity was measured. It was also revealed that the thermal conductivity at the macro-level was significantly affected by the contact area between the spatial distribution of PTFE and carbon fibres. The success of this investigation is huge as it shows the best way to maximise the thermal conductivity properties of the materials thereby ensuring that the system becomes more cost effective.

Water uptake and membrane swelling are some of the important properties of the membrane which has been used to determine it performances and durability. Comparing two lactates materials, Hovorka et al [49] showed that in dilute solutions, L-methyl lactates have less mass sorption but higher area swelling versus D-methyl lactate. Studies of this nature assist to determine the best materials in the PEM fuel cells. Similarly, in developing a membrane-hydration model in order to characterise the properties of water transfer in a single cell PEM using saturated hydrogen and dry air, Misran et al [57] revealed that the level of water uptake

in the membrane significantly affected key parameters. These parameters include water back-diffusion flux, water diffusion coefficient, electro-osmotic drag coefficient and membrane ionic conductivity. In turn the gas channel relative humidity determined the water content. Large water uptake gradient between both electrodes inhibits PEM fuel cell flooding by preventing the transfer of water from the cathode to the anode and resulting in a negative water back-diffusion flux. Understanding the behaviour of the materials when exposed to water is very useful for effective water management.

The sigmoidal dependence that water uptake has on relative humidity at uniform temperature were investigated using mesoporous acid-free hematite ceramic membranes. The ceramic membranes recorded linear increase in conductivity as relative humidity was raised, at 2.76 x 10^{-3} S cm^{-1} between RH ranges of 81% to 90% [58]. An increase in conductivity usually results in an increased performance and durability making the system cost effective.

1 Table 3: Showing the influence of various modelling parameters on the fuel cell performance

Parameter Investigated	Method	Findings	Ref
Flow plates (serpentine channels)	A 3D numerical model (VOF method)	The experiment shows the best arrangement for the flow plates to get the highest pressure and parasitic power.	[59]
Material properties and humidity	Application of hydrophilic MPL coating to a hydrophobic GDL was done and the resulting effects were monitored through X-ray visualization.	The performance of the fuel cell improved and the following observed; reduced resistance of the membrane even without humidification, the catalyst layer-MPL interfaces water retention increased, the accumulation of water within the GDL and oxygen transport resistance increased when the densities were high. The potential of the cell increased by 14% (0.07 V at 1.5 A/cm2)	[60]
Flow channel design	The use of three-dimensional numerical simulation was adopted and the flow field and heat transfer rate in square area cooling plates were obtained.	A model called the zigzag channel model was developed and compared with the straight channel model. Reduction in the maximum surface temperature, surface temperature difference and temperature uniformity index were observed showing a better cooling performance by the zigzag channel model.	[61]
Number and arrangement of separator electrode assembly (SEA)	The development of four different configurations towards the determination of the effect of intermediate electrode on the performance of the square tubular PEMFC.	The introduction of intermediate electrode leads to an increases current density, higher consumption of reactants and an overall increase in the PEMFC performance. Additionally, it does not lead to additional cost and only one intermediate electrode layer should be added as adding more leads to a huge pressure drop.	[62]

Operating conditions and channel structure	Optimisation of operating temperature, anode pressure, cathode pressure, current density and channel structure (heights of channel inlet and outlet) of PEMFC using multi-objective genetic algorithm.	The new channel described as tapered is better when compared with the conventional straight channel. It produced enhanced gas reactant transport and the power output is increased.	[63]
Internal water transfer behaviour	Modelling and analysis of internal water content behaviour in a fuel cell having large surface area.	With the help of simulation results, the influence of the net water transfer coefficient on the fuel cell performance was varied. Furthermore, when the fuel cell is in counter-flow mode, back-diffusion of water enhances the membrane performance.	[64]
In-line and staggered blockages in parallel flow field channels	Numerical simulation is used to compare different effects of in-line and staggered blockage configurations within a parallel flow field with unblocked flow field.	The result of this experiment shows that changing the flow field design affect the pressure and hence overall performance of the fuel cell.	[65]
GDL compression	Lattice Boltzmann pore-scale simulation technique was used to determine the GDL compression role.	The result of this experiment shows that GDL compression affect the current density and hence overall performance of the fuel cell.	[66]
Operating pressure	Numerical and experimental investigation of fuel cell stack.	The result of this experiment shows that the power generated by the fuel cell stack is increased when the operating pressure is increase hence overall performance of the fuel cell is enhanced.	[67]

Material properties (carbon nano-forms as supports for Pt catalyst)	Characterization of different synthesized Pt supported with various carbon nano-forms to be used as catalyst layer	Addition of carbon noticeably improved fuel cell performance. A material tagged MWCNT gave the best carbon support for the Pt catalyst based on the experimental result.	[68]
Catalyst layers (CL)	Comparison of hydrophobic CL using physical and electrochemical characteristics.	It can be deduced that the material used as CL can affect it overall performance. Catalyst layers with more Pt and hydrophobic power performed better both for the CL made with Tanaka and the conventional CL.	[69]
Pore structure and effective diffusion coefficient of catalysed electrodes	Experimental investigation of the pore structure and EDC of the catalyst layers through characterization by standard porosimetry.	The result of this experiment shows that Pore structure and effective diffusion coefficient of catalysed electrodes is directly impacted by the Pt loading hence overall performance of the fuel cell is influenced.	[70]
Bipolar Plate Materials	An investigation into different materials used as bipolar plates.	The author argues that the type material used as a bipolar plate have an influence on the performance of the fuel cell.	[10]
Operating temperature, membrane's thickness and catalyst layer thickness	A 3D model in COMSOL was used to investigate the effect of operating temperature, membrane's thickness and catalyst layer's thickness on the performance of HT-PEMFC and analysis done using the polarization curves.	The physical parameters investigated had huge influence on the HT-PEMFC. The performance of the fuel cell improved at the following condition; when temperature is increased, thinner membrane is used, and CL thickness is reduced.	[71]
Channel to rib width ratio with various flow field designs	The application of 3D CFD model in the investigation of the influence of geometry designs and flow field	It can be concluded that geometry designs and flow field dimensions have influence on the performance of PEM fuel	[72]

	dimensions on the performance of PEM fuel cells.	cells. Although the influence varies depending on the other operating condition especially the operating voltage.	
Temperature, pressure, relative humidity and conductivity	The use of simulation profiler to determine the sensitivity of varying operating conditions.	Considering the simulation results, pressure and conductivity emerged as the two most leading inputs for effective PEMFC performance.	[73]
Flow-field layout (Design)	Experimental investigation into the effect of flow-field layout on the membrane electrode area.	It was established that Flow-field layout (Design) have huge impact on the performance. This is demonstrated with the serpentine flow-field layouts side performing better than straight-parallel flow-field layouts.	[74]
Operating condition	Experimental investigation of the influence of fuel cell operating constraints in galvanostatic mode.	All the operating conditions such as cathode humidity, air stoichiometry, hydrogen pressure and operating current density had influence on the system activities.	[75]
GDL deformation and transport phenomena in an interdigitated flow field	A 3D mathematical model is developed and applied to investigate the effect of the GDL deformation performance of PEMFC.	The result of this numerical experiment shows that increase in the assembly forces lead to an increased performance of the fuel cell. Pressure is also affected as it drops. A high level of consideration needed to make such decision.	[76]
Current density, platinum loading and GDL porosity	A mathematical model was used in the numerical analysis of the inhomogeneous platinum loading within the catalyst layer (CL) and porosity inside the gas diffusion layer (GDL) at the cathode of a PEMFC.	The interaction between the platinum loading and GDL porosity is strong and both have significant impact on the current density. Hence effective design of Pt loading and GDL porosity is crucial.	[77]
Voltage drops, exchange current density, transfer	Computer fluid dynamics (CFD) is used to determine the effect operating	The result of this experiment shows that Voltage drops, exchange current density, transfer coefficient, electrolyte thickness, cell useful area and temperature affect voltage	[78]

coefficient, electrolyte thickness, cell useful area, temperature effect	parameters have on the voltage-current density curve.	and efficiency of the cell. Hence, the overall performance of the fuel cell is influenced.	
Humidity	Self-humidified operation of a Polymer Electrolyte Membrane (PEM) fuel cell with dry feed conditions is experimentally investigated.	This work established that there is an optimum temperature and flow rate at which the performance it highest. After which a further increase decreases the performance of the fuel cell. A minimum flow rate is also established for Hydrogen.	[79]
Elevated current densities	Current-voltage polarization curves measured considering membranes with different thicknesses and operating condition.	Important parameters like internal cell resistance, charge transfer exchange current densities and roughness factors have been affected by applying elevated current densities hence, overall performance of the system.	[80]
Inlet flows under simulated driving cycle conditions	The use of computational fluid dynamics (CFD) to determine PEM fuel cell stack performance during a driving cycle.	Variable inlet flows have considerable effect on water, thermal and gas management. It also has effect of the total power generated.	[81]
Pressure, relative humidity and cell voltage	A physical 2D model for chemical membrane degradation has been developed.	Membrane degradation has a huge influence on the fuel cell performance. This investigation submits that membrane deteriorates more when the following operating condition; pressure, relative humidity and cell voltage, is high.	[82]
Partially restricted cathode flow channels and metal foam as a flow distributor	The influence of three (3) different flow channels on the PEMFC performance is investigated.	Different level of performances was recorded on each case showing influence on the fuel cell performance. However, metal foam gave the best result.	[83]

Materials for metal foam flow distributor	Chemical vapour deposition method was used to grow graphene on a nickel foam and characterization by scanning electron microscopy and Raman spectroscopy.	Analysis using Tafel model showed that graphene-coated samples were more resistant to corrosion when compared with the uncoated ones. Their electrical conductivity and hydrophobicity is also enhanced.	[84]
Enhancement of proton exchange membrane (PEM) properties	Polyethersulfone (PES), sulfonated poly (ether ketone) (SPEEK) and nanoparticles were used to synthesise a PEM.	The synthesized membranes showed great improvement in properties such as water uptake, ion exchange capacity and proton conductivity compared to pristine PES membrane.	[85]
Pressure difference between adjacent channels in an adjustable flow field	Used computer simulation to design an adjustable flow field which could be transformed to either serpentine flow field or interdigitated flow field.	The result proved the existence of an optimum pressure difference between two channels and it contributes to the overall performance of the PEMFC. More information on optimizing a hybrid flow field is discovered.	[86]
Charge transfer coefficient (CTC) and the operating voltage	Used computer simulation to examine the influence of operating temperature and CTC on the operating voltage.	The result showed a decrease in activation overvoltage at both sides of the electrodes when there is an increase in CTC from 0.1 to 2.0. It further shows that pressure has no effect on CTC.	[87]
Materials (sulfonated TiO2-Poly (Vinylidene fluoride-co-hexafluoropropylene) nano composite membranes)	Investigations such as FT-IR, SEM, EDX, AFM, Proton conductivity, contact angle measurement, IEC, TG, water uptake, tensile strength were conducted.	The addition of composite ensured the fabricated composite membranes have increased high proton conductivity, good water uptake and a maximum fuel cell power density of 85 Mw/cm^2 when used for PEM fuel cell.	[88]

2

4. Conclusion

Investigations into the effects of modelling and simulation parameters on the design of cost-effective proton exchange membrane (PEM) fuel cell have been done. Attempt has been made to classify the parameters into operating parameters, design parameter and material properties. In this work, operating parameters includes the temperature, pressure and relative humidity. Design parameters considered includes geometry parameter like channel length, channel width, channel height, GDL/CL/membrane thickness and surface area. For materials, properties such as porosity, permeability, diffusivity, concentration, mass and water transport, ionic and thermal conductivity, water uptake and membrane swelling were evaluated.

All the modelling parameters influenced the performance of the PEM fuel cells. The influence shown by the operating condition is huge. An increase in operating temperature and operating pressure increases mobility of ions hence the ionic conductivity is increased. In addition, not having the right humidity increases membrane drying thereby encouraging membrane degradation.

Adopting good design parameter is necessary for efficient transportation of both reactants (fuel and oxygen). In the case of flow plates, the serpentine flow plate is highly recommended. The amount of changes in output due to varying parameters like membrane/ catalyst layer (CL)/gas diffusion layer (GDL) thickness and flow plates channel length/width/height is huge and cannot be overestimated.

The material properties are very important in material selection and new product development. For the membrane electrode area (MEA), in case of the membrane, the ionic conductivity is very important and should be highly considered.

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