

Одним з факторів, які можуть підвищити властивість поверхневого перенесення для дифузії газу з матеріалу мембрани в ПЕПОМ, є пористість матеріалу газодифузійного шару, що впливає на розподіл часток на електродах. В даному дослідженні проводиться моделювання продуктивності ПЕПОМ шляхом чисельного дослідження впливу пористості ГДШ в деяких комерційних ELAT-ТЕК-1200W ($\varepsilon=0,31$) і SIGRACET 25BA ($\varepsilon=0,63$), а також органічних матеріалів, таких як кокосова койра ($\varepsilon=0,88$). Для цього використовували COMSOL Multiphysics 5.3a у вигляді масових концентрацій частинок, нанесених на профіль поверхні і точок розрізу на електродах за минулий час. Потім отримані результати були використані для визначення продуктивності ПЕПОМ шляхом розрахунку деяких втрат; активаційних, омичних і масової концентраційної поляризації. Результати показали, що на продуктивність ПЕПОМ впливає тільки масова поляризація. Це означає, що питома потужність сильно залежить від концентрації частинок в анод і катод. Масова концентрація сильно залежить від розподілу часток; в ході реакції утворюються H_2 , O_2 і H_2O . Найбільша концентрація H_2 на аноді спостерігається в ГДШ з використанням ELAT-ТЕК-1200W, що має найменшу пористість, що забезпечує найвищу питому потужність в порівнянні з іншими матеріалами ГДШ. Це полегшує процес дифузії між частинками H_2 і O_2 . Однак кокосова койра як органічний матеріал може в майбутньому стати перспективним ГДШ завдяки своїй ефективності в порівнянні з іншими

Ключові слова: чисельне дослідження, ПЕПОМ, продуктивність, пористість, газодифузійний шар, матеріал, COMSOL Multiphysics

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1. Introduction

One of the energy sources that promise in the future is a fuel cell. It is an electro-chemical device that produces direct electrical current from the chemical energy stored in a fuel [1]. It is the most promising energy conversion device because it has the cleanest technology, relatively low operating temperature (around 80 °C), almost no noise, and has a high efficiency to generate electricity (around 70 %). The exhaust emissions are water and heat, which are used as “fuel cell by-products”. At present, it is used in various applications including electricity for households and trans-

portation [2]. From several types of fuel cells, the Proton Exchange Membrane Fuel Cell (PEMFC) is the type that is very suitable for power plants because it uses a membrane on the stack. It is a very practical certainty compared to after fuel cell types.

The PEMFC basic elements are bipolar plates, diffusion layers, electrodes and an electrolyte [3]. In the components, the membrane electrode assembly (MEA) is composed by a proton exchange membrane, catalyst layers, and gas diffusion layers (GDL) sandwiched in between flow field plates. The GDL is one of PEMFC parts, a vital electrode part located at Membrane-Electrode Assembly (MEA) [4–6]

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A NUMERICAL STUDY OF PROTON EXCHANGE MEMBRANE FUEL CELL PERFORMANCES AFFECTED BY VARIOUS POROSITIES OF GAS DIFFUSION LAYER MATERIALS

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that functions to provide a good pathway for reactants to catalysts [6]. Another function of the GDL is as gas diffuser and provides additional mechanical strength (mechanical support) for the membrane [6]. Consequently, the main requirements in selecting materials for GDL are:

- 1) having high electrical conductivity;
- 2) having high permeability;
- 3) having corrosion resistance;
- 4) facilitating water and CO₂ disposal;
- 5) having good mechanical properties, good porosity for the inlet and outlet of the reactant and products;
- 6) a cheap price [7].

Various improvements and developments continue to be made to expand the efficiency of PEMFC because one of the weaknesses is the high water content in each electrode due to the trapping of water from the reaction between H₂ and O₂. Therefore, there have been many efforts focused on developing conductor membranes, including the GDL material with high conductivity and can operate at higher temperatures to expand the ability of H₂ diffusivity can cause further surface transfer properties.

To meet the requirements of the GDL material, it is necessary to choose materials that meet the requirements that the availability of material that is easy and abundant, high permeability, and also has a cheap price. An organic matter that meets these criteria seems to be a material composed of compounds containing carbon. As we know, carbon has allotropic properties so that it can be used as a catalyst or material that is easy to absorb the water content. The GDL material must also transfer the generated heat on the catalyst away from the MEA. Therefore, the use of organic materials by the GDL must be done. Recently, the most widely used materials for GDLs is carbon in the form of commercial carbon [8] and organic carbon.

2. Literature review and problem statement

The commercial GDL used is generally produced using carbon-based polyacrylonitrile materials, which are derived from non-renewable energy materials having high production costs [9]. This problem makes some researchers develop the GDL by using carbon materials derived from biomass which is very abundant and is a renewable material. One of the promising biomass as the GDL materials which has been studied is coconut fiber [10]. It was observed that carbon coconut coir can be useful in distributing reactant gas. It has many parallel hollow tubes and functions as porous media material. It has a certain size porosity which is capable of distribution of the reactants throughout the catalyst layer. Coconut coir is also able to eliminate water and CO₂ out of the cell. Besides, it is able to transfer the generated heat on the catalyst away from the MEA.

One of the factors that can increase the surface transfer property for gas diffusivity apart from the membrane material itself is the H₂ mass distribution of the catalyst [11] which states that the reduction in membrane porosity size can increase the electronic conductivity of GDL. The size of porosity will also significantly affect the uniformity of reactant gas distribution, so that it will affect the generated electric current which shows the PEMFC performance. Besides the porosity is one of significant factors in determining gas and water transport through/in the GDL, the

distribution and variation in porosity give the effect on the capillary pressure driving the water out of the PEMFC [12]. Therefore, in the present study, various porosities of the used organic materials as GDL will be considered. Some effects of the reactant transports in the PEMFC electrodes will be compared.

The porosity can be defined as the ratio of the volume of empty space in a material [13]. It can also be defined as the ratio of non-fiber volume to the total volume of material [14]. In the recent study, the effect of porosity that greatly affects the performance of GDL in 3 types of organic matter will be observed using COMSOL numerical simulation. The numerical simulation will investigate the diffusion of reactants that greatly affect the mass and mass transport that occurs in the electrodes (Anode and PEMFC cathode). Therefore, the study will compare the porosity effects of coconut carbon fiber ($\epsilon=0.74$) [10] with the two of commercial GDL materials; SIGRACET 25BA ($\epsilon=0.88$) [7] and ELAT-TEK-1200W ($\epsilon=0.31$) [12] using COMSOL Multiphysics 5.3a software. In the simulation results, the species mass concentration at the anode and cathode in the Gas Diffusion Layer (GDL) will be presented. If the previous studies [15] observed the gas velocity and the mass conservation in the steady conditions, however, in this study, the mass concentration will be simulated under transient conditions until the reactants reach the equilibrium state.

3. The aim and objectives of the study

The aims of the study are to determine the PEMFC performance due to different porosities among three GDL materials affecting the surface transport properties of gas diffusivity causing some losses or polarizations or overpotentials.

On the other hand, the transport properties make some losses in the PEMFC, so that it will give an impact on the PEMFC performance.

To achieve this aim, the following objectives are accomplished:

- by calculating the performance of PEMFC by investigating the effect of GDL porosities in some commercial ELAT-TEK-1200W ($\epsilon=0.31$), and SIGRACET 25BA ($\epsilon=0.88$), also an organic material coconut coir ($\epsilon=0.74$) numerically using COMSOL Multiphysics 5.3a;
- by determining the species mass distribution represented by the gas flow velocity and total mass conservation at the anode and cathode of the Gas Diffusion Layer (GDL);
- by calculating the electricity voltage to get the power density of the fuel cell. It explains that the PEMFC performance curve was influenced by three polarizations:
 - 1) an activation polarization;
 - 2) an ohmic polarization;
 - 3) a concentration polarization.

4. Numerical simulation for GDL species transport

There are some assumptions for analysis conditions in the present study considering that the PEMFC (Fig. 1) is operated in unsteady (transient) and isothermal conditions. Then, pressure drops are ignored. It works in adiabatic conditions. It is only H₂ that reacts electrochemically, while all gases and water obey ideal gas law.

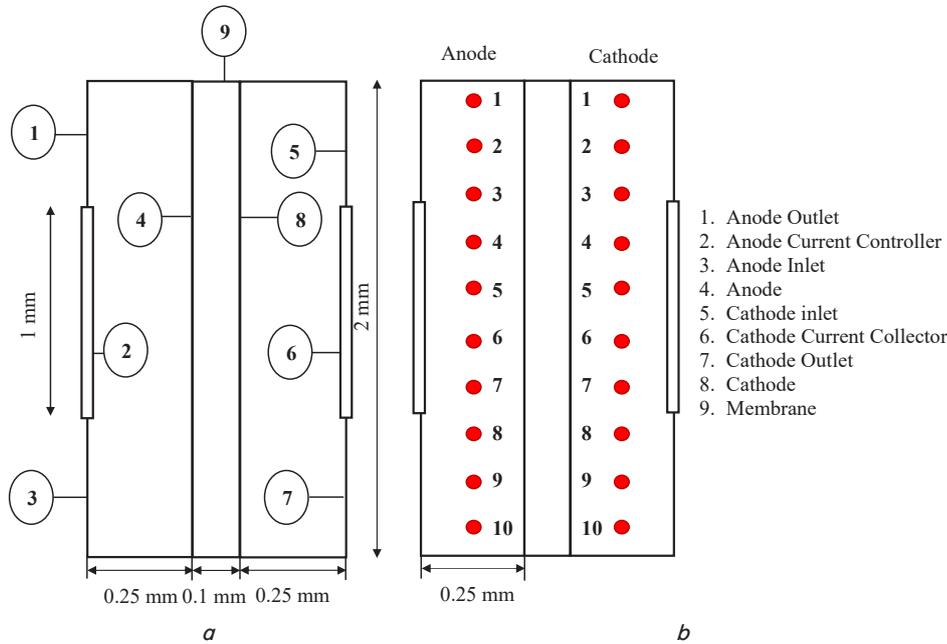


Fig. 1. Geometry model of PEMFC: *a* – size, domain, and boundary layers; *b* – cut point method measuring mass concentration

Table 1

Dimensions		
Parameters	Value	Unit
Cell height	2	mm
Cell width	0.25	mm
Membrane thickness	0.1	mm
Current collector height	1	mm

Table 2

Operating conditions		
Parameters	Anode	Cathode
Reactant	H ₂	O ₂
Pressure, P_a/P_c	1 atm	1 atm
Relative moisture, RH_a/RH_c	100 %	100 %
Operating temperature T_a/T_c	333 K	333 K

4. 1. Modeling approach

The physical properties of various organic matters for GDL materials are assumed to have the same mathematical parameters. However, the usage of different materials causes a difference in terms of porosity. Modeling of porosity effects of PEMFC has an essential material for the optimization of parameters affecting the performance of the fuel cell. The present study predicts the mass fraction effects and the transport phenomena in the transient conditions. The model is developed as having a single flow channel presented in Fig. 1, *a* and using model parameters given in Table 1, 2. In addition, some parameters and physical properties are listed in Table 3, using recent work assumptions and the other previous research.

The recent study uses a two-dimensional model, two-phase flow, ideal gas, non-isothermal PEM Fuel Cells and uses the agglomeration model simulated with COMSOL Multiphysics 5.3a. The model is divided into 3 domains; an anode, a membrane, and a cathode. Each GDL material is integrated directly with the gas distributor that has an inlet channel, a current collector, and a channel outlet. The same notation is used for the cathode side (Table 1).

Furthermore, the anode side is divided into 10 cut points to investigate the H₂ mass concentration that occurs during PEMFC operation as shown in Fig. 1, *b* (Table 2).

List of parameters for governing equations

Table 3

Parameter	Value	Unity
Conductivity, solid phase, k_s	5,000	S/m
Conductivity, membrane, k_m	7.2	S/m
Cell voltage, V_{cell}	0.6	V
Fluid viscosity, μ	2.10×10^{-5}	Pa s
Reference pressure, P_{ref}	1	atm
Anode inlet pressure, $P_{a,in}$	1	atm
Cathode inlet pressure, $P_{c,out}$	1	atm
Equilibrium potential, anode	0	V
Equilibrium potential, cathode	1	V
Proton-water drag coefficient through membrane, D	3	–
Exchange current density, anode, $i_{0,a}$	9.23×10^8	A/m ²
Exchange current density, cathode, $i_{0,c}$	1.05×10^6	A/m ²
Specific surface area, S	1.04×10^7	m ² /m ³
Aggregate radius, R_{agg}	0.1	μm
Faraday constant, F	96,487	C/mol
Microscopic porosity inside agglomerates, ϵ_{mic}	– ELAT-TEK-1200 W=0.31; – coconut coir=0.74; – SIGRACET 25 BA=0.88	–
Macroscopic porosity between agglomerates, ϵ_{mac}	– ELAT-TEK-1200 W=0.31; – coconut coir=0.74; – SIGRACET 25 BA=0.88	–
Anode inlet weight fraction H ₂ , $w_{H_2,in}$	0.2	–
Cathode inlet weight fraction O ₂ , $w_{O_2,in}$	0.168	–
Cathode inlet weight fraction, H ₂ O, $w_{H_2O,in}$	0.2	–
Molar mass, H ₂ , M_{H_2}	2	g/mol
Molar mass, O ₂ , M_{O_2}	32	g/mol
Molar mass, H ₂ O, M_{H_2O}	18	g/mol
Molar mass, N ₂ , M_{N_2}	28	g/mol
Henry's law constant, H ₂ in agglomerate, H_{H_2}	4.56×10^3	Pa m ³ /mol
Henry's law constant, O ₂ in agglomerate, H_{O_2}	0.101×10^{12}	Pa m ³ /mol
Active layer thickness, I_{act}	10	μm

4. 2. Model equations at porous media fluid flow of GDL

To model the gas flow, the reactant gas velocity can be calculated using Darcy’s law based on the law of continuity determined by:

$$\nabla \cdot (\rho u) = 0 \text{ at the anode and cathode,} \tag{1}$$

where ρ is the mixture density of the gas phase (kg/m³) and u is the velocity of the gas (m/s). Then, the ideal gas law states the density in the gas phase mixture:

$$\rho = \frac{P}{RT} \sum_i M_i x_i \tag{2}$$

At the electrode boundary aimed at the anode and cathode, the gas velocity was calculated from the total mass flow agreed by the stoichiometric coefficients using Faraday’s law, resulting:

$$-n \cdot u_{\text{anode}} = \frac{j_{\text{anode}}}{\rho F} \left(\frac{M_{\text{H}_2}}{2} + \lambda_{\text{H}_2\text{O}} M_{\text{H}_2\text{O}} \right) \tag{3}$$

$$-n \cdot u_{\text{cathode}} = \frac{j_{\text{cathode}}}{\rho F} \left(\frac{M_{\text{H}_2}}{4} + \left(\frac{1}{2} \lambda_{\text{H}_2\text{O}} \right) M_{\text{H}_2\text{O}} \right) \tag{4}$$

By combining all the boundary conditions, Darcy’s law calculates the gas flow velocity and preserves the total mass conservation in the anode and cathode.

Further, in the anode, there are two gases; H₂ and H₂O while in the cathode, it presents three gases; O₂ and N₂ (air), as well as H₂O. The model used one instance of the transport of concentrated species interface for each electrode side, then each electrode was focused in some cut points illustrated by Fig. 1, b.

4. 3. 2D Comsol Multiphysics model simulation procedures

In the recent study, Fuel Cell and Battery module were selected for the PEMFC system. The PEMFC model was modeled by adding Electrochemical in Secondary Current Distribution (CD) to model electrochemical currents using Ohm’s law and the Butler-Vormer equation. Using the equations, some polarization plots and distributions of current density will be obtained. Then, determining the velocity of fluid flow in the GDL, the physics was selected in Fluid Flow in Porous Media and Subsurface Flow in Darcy’s Law (dl). Meanwhile, finding out mass transportation that occurs at PEMFC, Transport Species Materials in Transport of Concentrates Species (tcs) was added. The physics was added twice at the anode and cathode sides because the mass transport at the anode is H₂ and H₂O, while at the cathode there was the mass transport of O₂ and N₂ (air). The Maxwell-Stefan equation was used to solve the mass transfer in the porosity of GDL. The Navier Stokes and the Brinkman equations are also used in the GDL and electrodes. The equations were also used to obtain the mass concentration profiles of substances at the anode and cathode in the physics.

5. Performance assessment of PEMFC using various organic materials

In addition, the study also calculates the PEMFC performance considering numerical simulation results of the mass

concentration influenced by the use of three GDL materials with different porosity. Then, the PEMFC performance will be represented by the power density versus the resulting current. Before getting the result, several parameters need to be calculated.

Initially, the PEMFC operating voltage can be determined by the result of ideal voltage reduced by all three types of polarizations [16]:

$$V_{\text{cell}} = E - \eta_{a,a} - \eta_{a,c} - \eta_r - \eta_{m,a} - \eta_{m,c} \tag{5}$$

where E is open-circuit voltage (OCV), η_a , η_r , η_m , respectively, are the activation polarization, the ohmic polarization and the mass concentration polarization.

E , the open-circuit voltage, is the ideal potential known as the theoretical potential which is not possible to be obtained in actual applications due to its irreversibility. Later, it is referred to as the polarization or the losses or the overpotentials.

5. 1. Activation overpotential

This polarization is the amount of voltage needed to generate the activation energy of an electrochemical reaction expressed with the ButtlerVolmer equation:

$$J = J_0 \left[\begin{array}{l} \exp\left(\frac{azF\eta_{act}}{RT}\right) - \\ - \exp\left(-\frac{(1-a)zF\eta_{act}}{RT}\right) \end{array} \right] \tag{11}$$

where a is known as the transfer coefficient (or symmetry factor) and the value changes in the range $0 < a < 1$. Experimentally, the value often used for the value of a is around 0.5. Meanwhile, $J_{0,i}$ is exchange current density and represents the readiness of the electrodes to form electrochemical reactions. Then, the activation overpotential for the anode and cathode can be calculated as follows:

$$\eta_{act,i} = \frac{2RT}{zF} \sinh^{-1} \left(\frac{J}{2J_{0,i}} \right), i = a, c. \tag{12}$$

5. 2. Ohmic overpotential

Charge transport regulates the charge of the electrons and the ions from the production to the consumption. The resistance to the charge transport results in a lost voltage (the ohmic loss) [16]. For excess PEMFC resistance by considering the contribution of each cell component; anode, cathode, electrolyte, and interconnector, Ohm’s law can be determined as follows [17]

$$\eta_{ohm} = J(d_a \rho_a + d_e \rho_e + d_c \rho_c + d_{int} \rho_{int}), \tag{13}$$

in which, d and ρ are thickness and resistivity for anodes, cathodes, electrolytes and GDL.

5. 3. Concentration overpotential

The mass transfer process of uncharged species of both H₂ and O₂ is an important matter because the reactants and products mixing in the catalyst layer ensure the performance of the fuel cell. In order to minimize overpotential (concentration loss), it is able to be optimized at the electrode. The mass transport in a porous solid is eventually studied as a complex phenomenon. Knudsen diffusion re-

gards the diffusion of gas molecules over some very small capillary pores. An effective Knudsen diffusion takes into account the porosity and tortuosity of the electrodes as follows:

$$D_{i,k}^{eff} = \frac{2}{3} \cdot \frac{\epsilon}{r} \cdot \sqrt{\frac{8RT}{\pi Mi}} \cdot r_p, \quad (14)$$

where ϵ , r and r_p represent porosity, tortuosity, and pore average radius of porous media. M is the molecular mass of species.

The difference in concentration of the two gas species between the electrode interface and the bulk becomes the concentration overpotential written by the equation as follows:

$$\eta_{con, a} = \frac{RT}{2F} \ln \left(\frac{P_{H_2}}{P'_{H_2}} \right), \quad (15)$$

$$\eta_{con, c} = \frac{RT}{2F} \ln \left(\left(\frac{P_{O_2}}{P'_{O_2}} \right)^{0.5} \frac{P'_{H_2O}}{P_{H_2O}} \right). \quad (16)$$

Afterward, the partial pressure of the electrode-electrolyte of the gas species is explained by the Fickian diffusion [16].

Finally, after finding the appropriate parameters in some of the equations above, we will come at the purpose of the research, which is to get the PEMFC performance which can be formulated as follows :

$$P = JV_{cell}, \quad (17)$$

where P stands for power density, J is commonly used as current density and V_{cell} is the fuel cell operating voltage.

Finally, from some equations, the performance of PEMFC based on the effect of the porosity from the 3 different organic materials will be found.

6. Results

6.1. Effect of porosity on the mass concentration profiles in elapsed time

In the concentration profiles, the surface contour and mass concentration of species at the anode and cathode for H_2 , O_2 , and H_2O will be presented. The surface contour illustrates the mass concentration distribution during the reaction process, then it will present at the mass concentration profiles at each cut point measuring the mass concentration as illustrated in Fig. 1.

6.2. Concentration profiles of H_2

Due to H_2 inlet through the anode, the H_2 mass concentration is shown their surface contour and mass concentration as illustrated in Fig. 2. It is represented by one of the organic material; the coconut coir.

Then, the H_2 mass concentrations of three GDL materials are plotted in Fig. 3 from each cut point method measuring illustrated in Fig. 1, b.

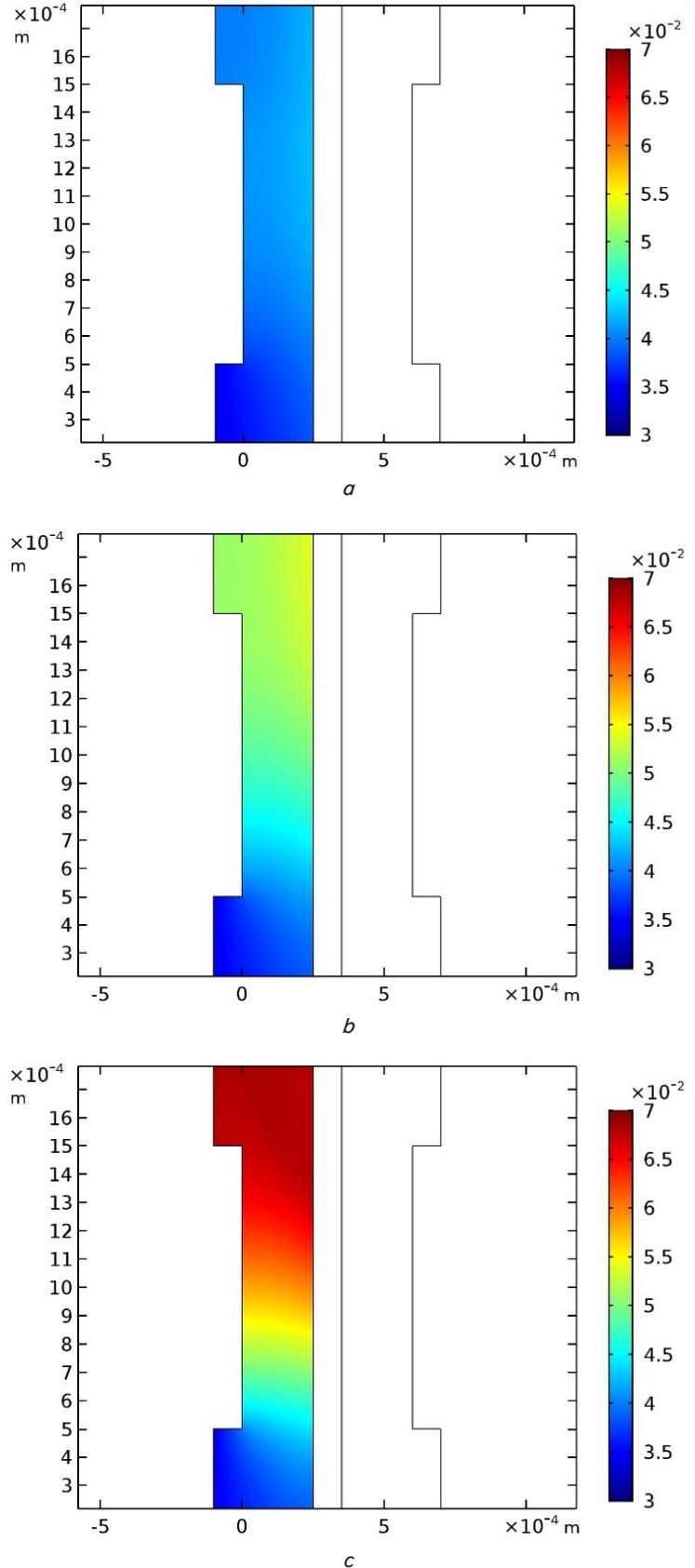


Fig. 2. Hydrogen mass concentration at anode of Coconut Coir: $a - t=0.02$ s; $b - t=0.05$ s; $c - t=0.09$ s

Afterward, the mass concentration of H_2 in each material having different porosities can be compared as shown in Fig. 4.

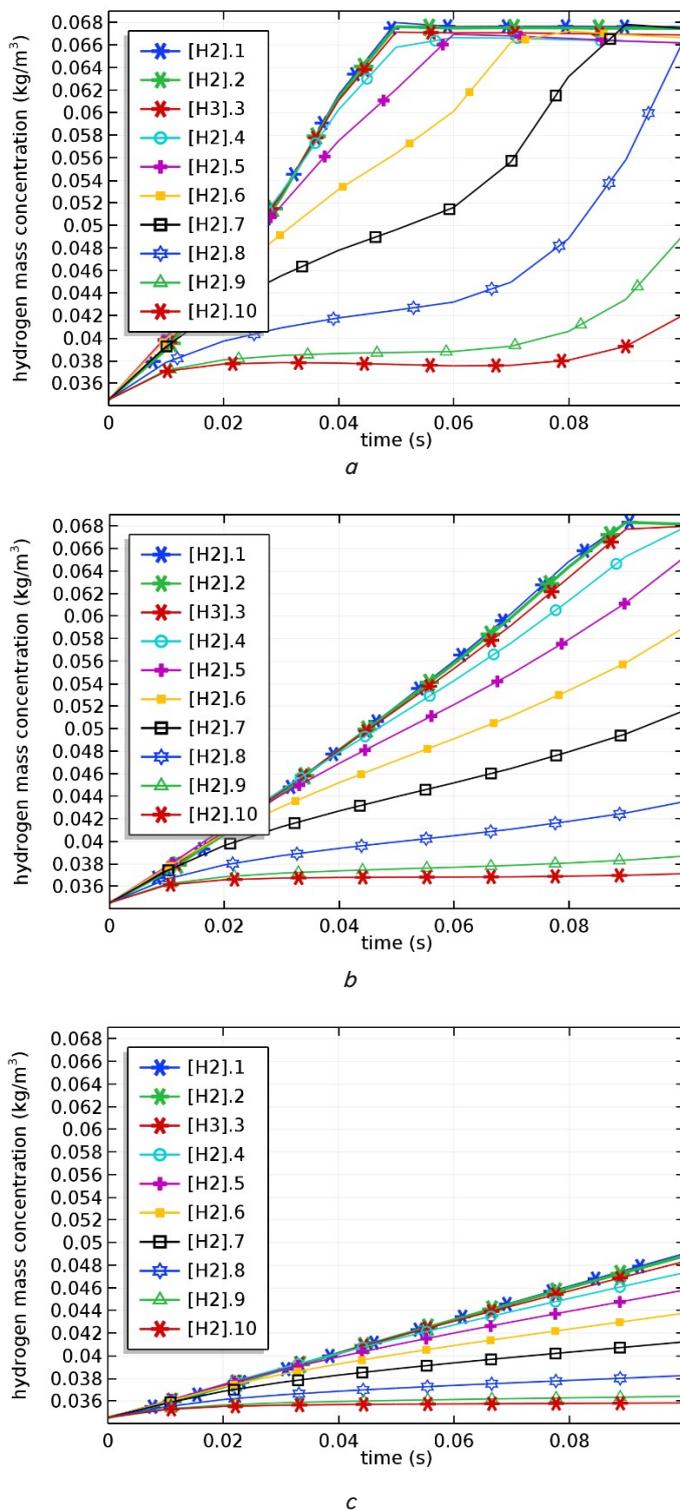


Fig. 3. H₂ mass concentration at anode: *a* – ELAT-TEK-1200W; *b* – Coconut Coir; *c* – SIGRACET 25BA

Fig. 3 explains that the H₂ mass concentration increases in elapsed time. It increases with the time, even it is close to the anode outlet, the H₂ concentration tends to be constant. It is due to H₂ has reacted on the electrode to release the protons in the electrolyte membrane toward the cathode. The conditions are different from the area

that is far from the inlet. In the area, the H₂ concentration increases significantly because the unreacted H₂ flows upward, causing the increase of the H₂ mass concentration at the anode outlet. Correspondingly, if we look at the surface contour in Fig. 2, it can be understood that there is an increasing H₂ concentration in elapsed time and pile up in the anode outlet. Automatically, in the steady state conditions (after *t*=0.09 s), the anode outlet has the highest mass concentration of hydrogen.

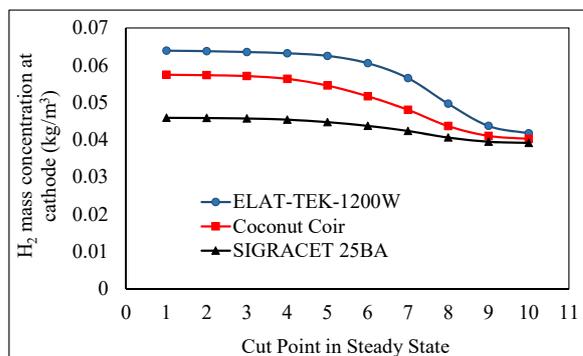


Fig. 4. The effect of different porosities of Hydrogen mass concentrations

Initially, at the anode inlet (point 10), the H₂ concentration is the highest if it is compared to other points. Afterward, after point 7, it begins to decrease because H₂ has reacted with electrodes to break down the protons and the electrons. At the points 10 to 8, it tends to be constant because the fuel cell is a reversible system in which the reactants (H₂) will continue to be supplied through the anode inlet.

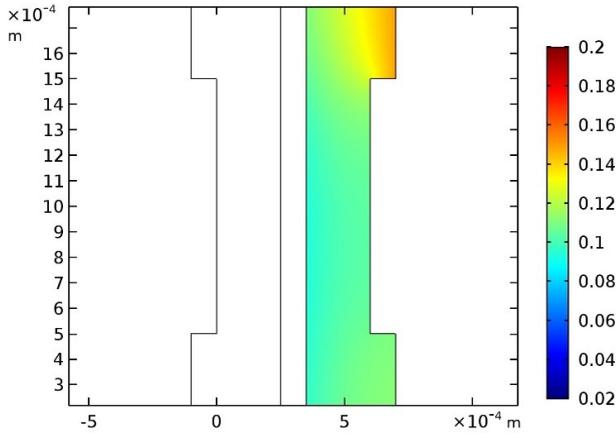
Afterward, Fig. 4 compares the H₂ mass concentration among three GDL materials. It shows that the highest hydrogen concentration was owned by ELAT-TEK-1200W which had a porosity of 0.31 followed by coconut coir and SIGRACET 25BA.

6. 3. Concentration profiles of O₂

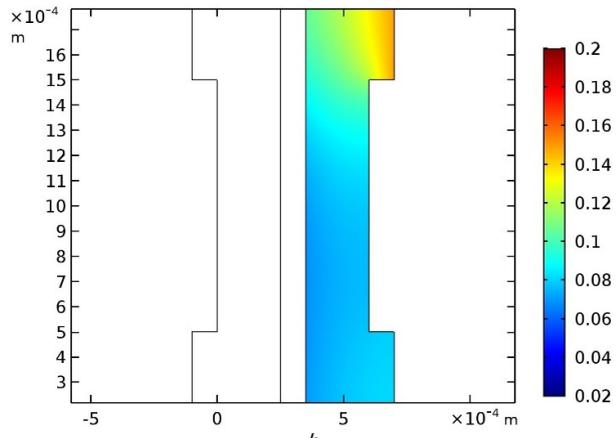
At the cathode, the flow rate of O₂ can be observed in the form of the O₂ mass surface contour in Fig. 5 and also the mass concentration profiles for each cut point in Fig. 6. Then, the effect of each type of material with different porosities can be compared in Fig. 7.

Fig. 5 illustrates the surface contour changes of the O₂ mass concentration in surface contour to calculate the mass concentration plotting in Fig. 6. The figure represents the O₂ mass concentration in elapsed time for the 3 GDL materials. From the cathode inlet (point 1), the O₂ mass concentration decreases significantly over time approaching 0 (runs out).

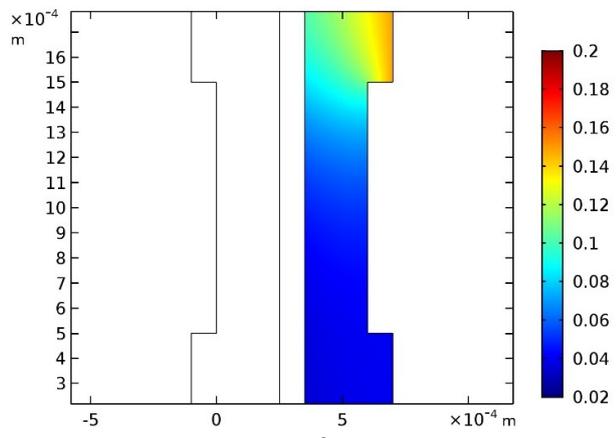
In all porosities, based on the surface contour, the highest mass concentration is at the cathode inlet. Then, they were plotted in Fig. 7 to describe the comparison of the O₂ mass concentration in the difference porosities. The result shows that the highest O₂ mass concentration is SIGRACET 25BA, then coconut coir, and finally ELAT-TEK-1200W.



a

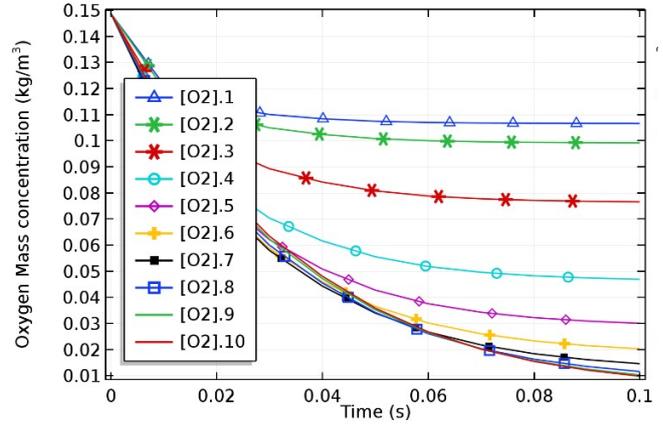


b

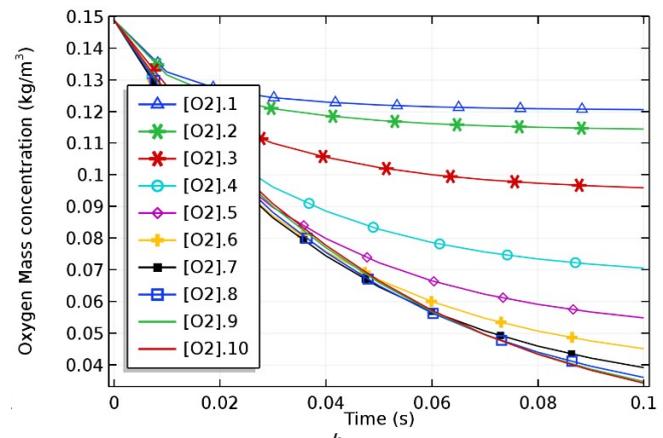


c

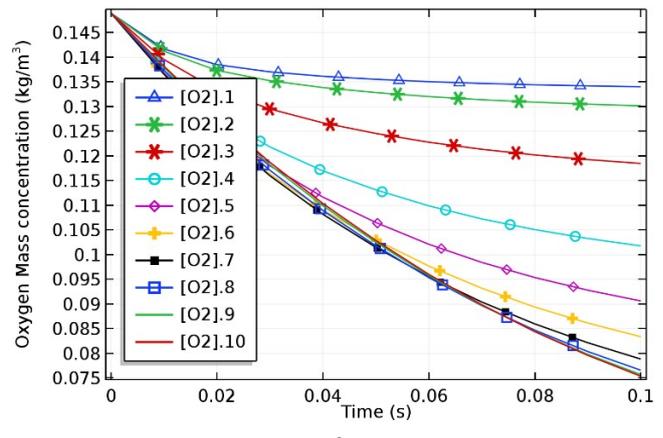
Fig. 5. Oxygen mass concentration at anode (kg/m^3) of Coconut Coir: a - $t=0.02$ s; b - $t=0.05$ s; c - $t=0.09$ s



a



b



c

Fig. 6. Oxygen mass concentration at anode: a - ELAT-TEK-1200W; b - Coconut Coir; c - SIGRACET 25BA

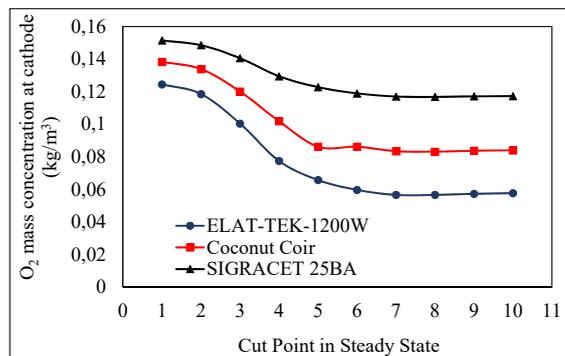


Fig. 7. The effect of different porosities of Oxygen mass concentrations

6. 4. Concentration profiles of H₂O

The insufficient PEMFC that cannot be avoided is the water formation in the electrode; cathode and anode. Like H₂ and O₂ species, the surface contour and the water mass concentration at each electrode point are also plotted in the comparison graph among the GDL materials shown in Fig. 8.

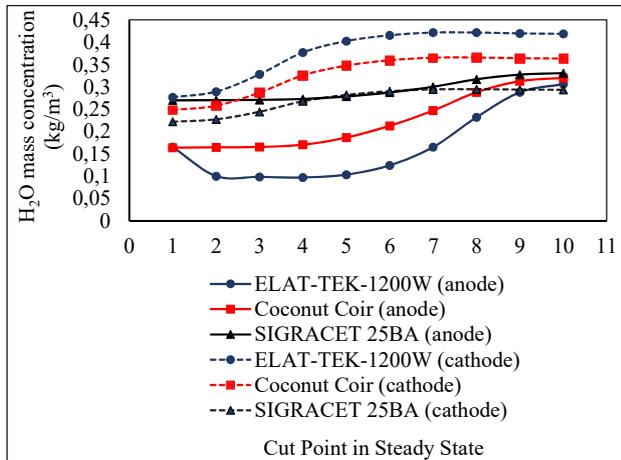


Fig. 8. The effect of different porosities of water mass concentrations at the anode

From Fig. 8, it can be seen that the porosity of the GDL also influences the water mass concentration distribution at each point.

At the anode, the water concentration at each point decreases in elapsed time. Meanwhile, the highest water content in each GDL material is located at point 10, in which it is the anode inlet. If the GDL that is a part of the electrode has high porosity, the displacement of protons containing water molecules will be inhibited, so that the diffusion velocity will slow down. It will cause the water in the GDL to be retained [17]. It is illustrated in Fig. 8 that the lowest water mass concentration is located at the anode outlet.

The water mass concentrations for the three different GDL materials at the cathode also are illustrated in Fig. 8 using the dash line in which it tends to increase. It opposites to the H₂O mass concentration at the anode due to the different inlet/outlet of the anode and the cathode.

6. 5. Performance of PEMFC affected by various GDL porosities

After finding the numerical simulation results in the mass concentration of the three different GDL porosities, both in the surface contour and the cut point of mass concentration at the anode and cathode, then the PEMFC performance influenced by the GDL materials with different porosities will be calculated based on the data written on the physical parameters in Table 1–3 by using equations (5)–(17).

Initially, before calculating the PEMFC performance determined using eq. (17), the losses (overpotentials) had been calculated. The overpotentials of the PEMFC operation will reduce the ideal cell potential stated in eq. (5). After considering the three overpotentials of PEMFC operation, it can be illustrated by the following graphs as shown in Fig. 9–11.

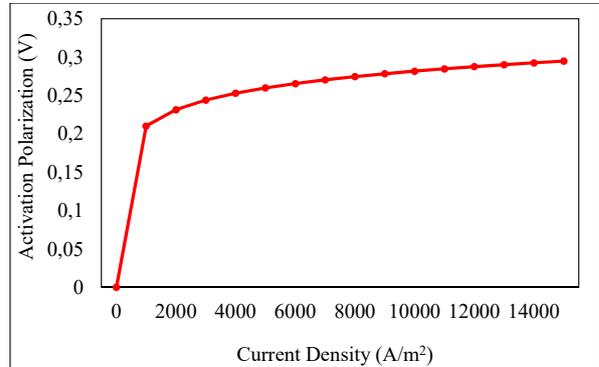


Fig. 9. Activation overpotential in the different GDL porosities

6. 6. Activation overpotential

The activation overpotential represents the activation polarization among three materials having the same values shown in Fig. 9, the activation polarization for both the anode and cathode. In fact, the three different materials show the same changes from 0 to 0.295 V.

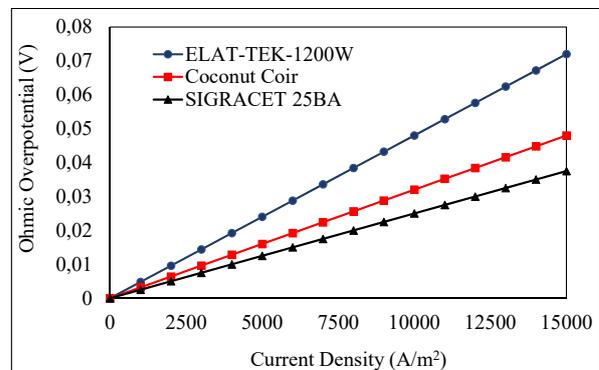


Fig. 10. Ohmic overpotential in the different GDL thickness

6. 7. Ohmic overpotential

Fig. 10 presents the ohmic overpotential that depends on the thickness and the resistivity for anodes, cathodes, electrolytes and GDL. The porosity of GDL materials does not affect the ohmic overpotential, however, each material has a different thickness and resistivity, which greatly affects the ohmic overpotential value.

6. 8. Concentration overpotential

After finding the mass concentration values plotted in Fig. 2–8, the overpotential activation is illustrated in Fig. 9.

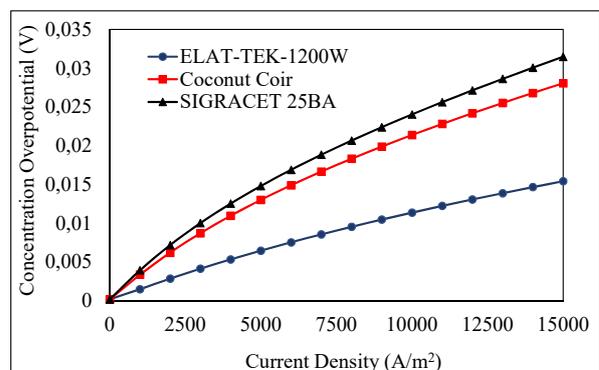


Fig. 11. Concentration overpotential in the different GDL porosities

Meanwhile, the excess concentration of the anode concentration can be neglected, but the excess concentration of the cathode concentration is considered at high current densities as shown in Fig. 11.

Table 4

Thickness and resistivity of GDL materials

	Unit	ELAT-LT-1200W	COCONUT COIR	SIGRACET 25 BA
d_a	m	0.0003	0.00025	0.0002
ρ_a	$\Omega\cdot\text{m}$	8,000	5,000	8,000
d_e	m	0.00001	0.00001	0.00001
ρ_e	$\Omega\cdot\text{m}$	9	9	9
d_c	m	0.0003	0.00025	0.0002
ρ_c	$\Omega\cdot\text{m}$	8,000	5,000	8,000

In Fig. 11, it looks that porosity greatly influences the concentration losses which are very significant results. The biggest losses occur in SIGRACET 25BA which has the biggest pores.

6. 9. Power density (PEMFC performance)

After calculating the amount of losses/polarization occurring in the fuel cell stack using eq. (17), finally the PEMFC performance can be illustrated in Fig. 12. At different porosities, the concentration polarization has great losses affecting the PEMFC performance.

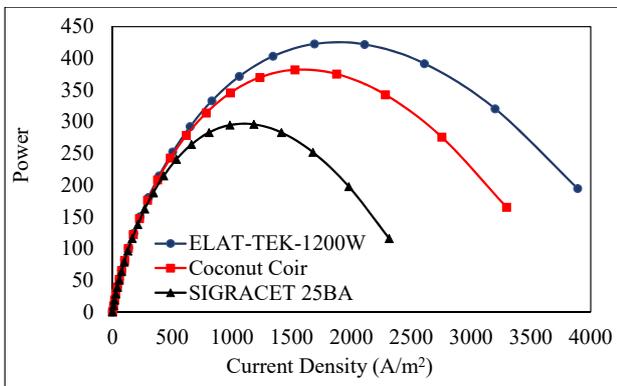


Fig. 12. PEMFC performances of the various porosities GDL materials

7. Discussion of PEMFC performance influenced by the porosities of the GDL materials affecting various activations

In the concentration profiles depicted in Fig. 2–8, the surface contour and mass concentration of species at the anode and cathode for H₂, O₂, and H₂O were presented. The surface contours illustrate the mass concentration distribution during the reaction process. The H₂ mass concentration increases in elapsed time. However, the H₂ concentration close to the anode outlet tends to be constant due to H₂ has reacted on the electrode to release the protons in the electrolyte membrane toward the cathode. The conditions are far different from the outlet area because the unreacted H₂ flows upward, causing the increase of the H₂ mass concentration at the anode outlet. Correspondingly, if we look at the surface contour, the anode outlet has the highest mass

concentration of hydrogen. Then, if to compare the H₂ mass concentration among three GDL materials, it shows that the highest hydrogen concentration was owned by ELAT-TEK-1200W which had a porosity of 0.31 followed by coconut coir and SIGRACET 25BA. It means that the porosity factor certainly plays an important role to influence it. The higher the porosity, the more difficult for H₂ to release protons and even the anode outlet function to release the protons. As a result, the less proton production, H₂ is more difficult to flow into the membrane then it will bond with O₂.

The surface contour of the O₂ mass concentration represents the O₂ mass concentration that decreases significantly over time in the cathode inlet. It is because O₂ reacts with protons and electrons to form H₂O. Among the three GDL materials, they have the same trend, which decreases in elapsed time. In all porosities, based on the surface contour, the highest mass concentration is at the cathode inlet. Then, after regarding comparison among them, the result shows that the highest O₂ mass concentration is SIGRACET 25BA, then coconut coir, and finally ELAT-TEK-1200W. At the cathode, the porosity affects the distribution of O₂ significantly. The greater the porosity, the smaller the O₂ diffusivity ability.

Afterwards, the insufficient PEMFC that cannot be avoided is the water formation in the electrode; cathode and anode. Like H₂ and O₂ species, the surface contour and the water mass concentration at each electrode were compared. It can be seen that the porosity of the GDL also influences the water mass concentration distributions. At the anode, the highest water concentration is the anode inlet. If the GDL that is a part of the electrode has high porosity, the displacement of protons containing water molecules would be inhibited, so that the diffusion velocity will slow down. It will cause the water in the GDL to be retained [17]. On the contrary, the lowest water mass concentration is located at the anode outlet. It means that the mass of water has not accumulated at the anode outlet, then it makes easier to flow H₂. Afterward, beside the H₂ mass is enough to initiate the reaction, some of them move to the cathode through the membrane.

Then, the water mass concentrations for the three different GDL materials at the cathode opposites to the H₂O mass concentration at the anode due to the different inlet/outlet of the anode and the cathode. In fact, the water mass concentration at the cathode is much greater than at the anode one. This is the result of the effects of “electro-osmotic drag” transport, in which together with the electrochemical water production resulting in an accumulation of water at the cathode [18].

After finding the numerical simulation results in the mass concentration of the three different GDL porosities, both in the surface contour and the cut point of mass concentration at the anode and cathode, the PEMFC performance influenced by the GDL materials with different porosities was calculated based on the data written on the physical parameters in Table 1–3 by using equations (5)–(17). Initially, before calculating the PEMFC performance determined using eq. (17), the losses (overpotentials) had been calculated. The overpotentials of the PEMFC operation reduce the ideal cell potential stated in equation (5). Firstly, the activation overpotential represents the required energy to initiate the reaction at PEMFC. It is also illustrated as a barrier that the reactants must overcome. It will influence the electrochemical reaction involving the absorption process among

species on the electrode surface. However, the results show that the activation polarization among three materials has the same values shown in Fig. 9. It is the fact that, based on equation (11), (12), the activation polarization only depends on the operating temperature, thus the porosity does not affect the activation losses. In the present study, the activation polarization for both anode and cathode and also from the three different materials show the same changes from 0 to 0.295 V.

The other overpotential, the ohmic overpotential depends on the thickness and the resistivity for anodes, cathodes, electrolytes and GDL. Here, the ion transport is more difficult and complex than electricity transmission. In the electrolytes, it is a dominant loss and is caused by an excess of resistance (ohmic overpotential). Therefore, it depends on some parameters, such as the proton conductivity, the electrolyte thickness and the current density, as presented in eq. (13), (14). The porosity of GDL materials does not affect the ohmic overpotential, however, each material has a different thickness and resistivity, which greatly affects the ohmic overpotential value. In addition to the size of the thickness and resistivity of each material calculated in eq. (13), it can be seen in Table 4 giving some different properties of materials.

After finding the mass concentration values, the overpotential activation was illustrated in Fig. 9. The mass transportation is simultaneous activity in the fuel cell in which the reactants sent to the electrochemical reaction area producing the product must be quickly removed from the reaction to get a stable electricity production. Some species appear to be overreacting, such as unexpected water formation. Thus, one of the main reasons for excess concentration is the convective mass transfer from the gas channel to the porous electrodes. The anode consists of H_2 and O_2 for the cathode side. However, there are H_2 , O_2 , and H_2O flowing in porous electrodes. H_2 can pass to the interface of the electrodes quickly on the anode side due to its high effective diffusion coefficient. On the other hand, O_2 and H_2O , which have a high molecular weight, diffuse at the cathode side with a lower diffusion coefficient. Meanwhile, the excess concentration of the anode can be neglected, but the excess concentration of the cathode is considered at high current densities as shown in Fig. 11. It looks that the effect of the porosity greatly influences the concentration losses which are very significant results. The biggest losses occur in SIGRACET 25BA which has the biggest pores. It is due to the big porosity will produce the overreacting process, such as unexpected water formation, it gives an effect in an accumulation of species concentrations at the electrode.

After calculating the amount of losses/polarization that occurs in the fuel cell stack using eq. (17), finally the PEMFC performance can be illustrated in Fig. 12. At different porosities, the concentration polarization has great losses

affecting the PEMFC performance. It has a significant loss besides the ohmic and activation losses. As a result, the ideal power density of the maximum power density cannot be achieved due to the polarizations. The highest power density is achieved by the smallest porosity material (ELAT-TEK-1200W). If it is look at the mass concentration species in Fig. 2–8, ELAT-TEK-1200W is capable of producing very high-power densities because the H_2 concentration in the anode generates the highest concentration compared to other GDL materials. As a result, the supply of fuel is very large to react with O_2 . This is evidenced by the lowest O_2 concentration at the cathode side. It means the best H_2 and O_2 reactions compared to coconut coir and SIGRACET 25BA. On the other hand, the H_2O formation at the anode for ELAT-TEK-1200W is the lowest one. It makes an easier way for the diffusion between H_2 and O_2 species to work properly. Finally, ELAT-TEK-1200W produces a high generated power density for PEMFC. In the study, coconut coir as an organic material nevertheless has the potential GDL material to replace other commercial GDL such as ELAT-TEK-1200W and SIGRACET because it has a quite promising performance. Coconut coir can be a promising GDL material in the future because of its performance and environmentally friendly materials.

The future work needs to investigate the performance of PEMFC comparing GDL materials among other some derived organic materials, coconut coir, and commercial materials. The other physical properties of the GDL need to be considered in the numerical simulation properties to predict the PEMFC performance more accurately due to this research only examines the porosity effects. Hence, further research will be needed to calculate all the physical properties of organic materials having some potencies to become GDL. Afterward, the effect of temperature and pressure that is currently under STP conditions will be able to be varied in real terms according to experimental conditions.

8. Conclusions

1. The highest H_2 mass concentration was owned by ELAT-TEK-1200W which had a porosity of 0.31, however, the highest O_2 mass concentration is SIGRACET 25BA.

2. The greater the porosity, the smaller the O_2 diffusivity. The porosity does not affect the activation and also the ohmic overpotential. It only influences the concentration polarization that gives an impact on the PEMFC performance.

3. The biggest losses occur at SIGRACET 25BA, so that ELAT-TEK-1200W produces the highest generated power density for PEMFC. Coconut coir can be a promising GDL material in the future because of its performance and environmentally friendly materials.

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