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Conceptual Design of 5 kW PEM Fuel Cell Stack

Siti Kartom Kamarudin, Wan Ramli Wan Daud, Ayub Md. Som and Mohd. Shahbudin Masdar

Jabatan Kejuruteraan Kimia dan Proses
Fakulti Kejuruteraan
Universiti Kebangsaan Malaysia
43600 UKM Bangi
Selangor
Malaysia

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ABSTRACT

The main objective of this paper is to conceptually design the stack of Proton Electrolyte Membrane (PEM) fuel cell taking into consideration the voltage for a single cell, number of cells required, current density, power density and finally the current flow in the stack. A part from that, effect of important parameters such as temperature, pressure, voltage, current density and distance gas flow channel were presented in this paper. From the result, it was observed that 32 numbers of cells (0.7 V for each single cell) with a current flow of 260A were required for power output of 5 kW after considering the parasitic load of 8% from the total power output. The active area of the single cell was found to be about 250 cm^2. The current density and power density were determined as 900 mA/cm^2 and 660 mW/cm^2, respectively. The cell efficiency is expected about 65%. Finally, the electricity cost in this study was calculated as RM 0.152/ kWh^{-1}.

Keywords: Conceptual design, PEMFC, current density, power density

ABSTRAK

Objektif utama kajian ini adalah untuk mereka bentuk konsep stak sel bahan api membran elektrolit polimer (PEMFC) dengan mengambil kira voltan untuk sel tunggal, bilangan sel, ketumpatan arus, ketumpatan kuasa dan jumlah aliran arus dalam stak. Selain daripada itu, kesan parameter penting seperti suhu, tekanan, voltan dan jarak aliran gas ke ruang aliran juga di tunjukkan di kajian ini. Daripada keputusan yang diperoleh, didapati bilangan sel yang diperlukan adalah 32 (0.7 V untuk setiap sel tunggal) dengan aliran arus sebanyak 260A diperlukan untuk kuasa keluaran 5 kW selepas mengambil kira beban parasitik 8% daripada jumlah kuasa keluaran. Luas permukaan aktif untuk satu sel adalah 250 cm^2. Ketumpatan arus dan kuasa masing-

masing adalah 900 mA/cm^2 and 660 mW/cm^2. Keberkesanan sel dianggarkan sebagai 65%. Akhir sekali kos elektrik yang dikira dalam kajian ini adalah RM 0.152/ kWj^{-1}.

Kata kunci: Reka bentuk konsep, PEMFC, ketumpatan arus, ketumpatan kuasa.

INTRODUCTION

The performance of PEMFC is limited by polarizations. A good understanding of the effect of design and operating conditions on the cell potential is required in order to reduce the polarization. Major operating parameters include cell temperature, pressure, reactant stoichiometry, and gas stream composition (Rowe & Li 2001). The objective of this study is to present the stack design of a PEM fuel cell including the model development for the design of the electrodes, the mass and heat balances of the stack. Effect of some important parameters over the performance of the fuel cell system, such as polarization, pressure, temperature, gas stream composition, etc. are also made in this study. Besides that, this study also determines the voltage of single cell, number of cells required, current density, power density, and finally the pattern of current flow in the stack.

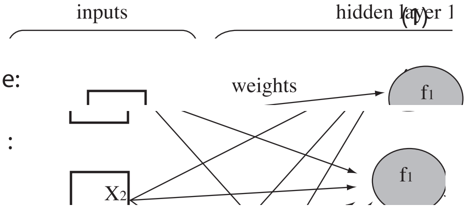
MODEL DEVELOPMENT

Generally the PEM fuel cell consists of three major components: an anode, typically featuring platinum or platinum-contain catalyst, a thin, solid polymeric sheet, which acts as electrolyte, and a cathode platinum-catalysed. The reaction in a hydrogen/oxygen fuel cell can be written as:

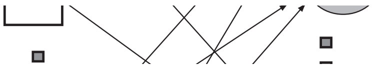
Anode: (1)

Cathode:

Overall :



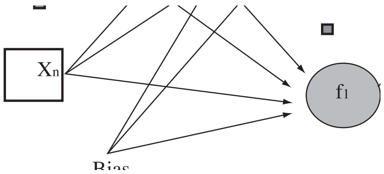
The products of this process are direct current electricity, liquid water and heat. The output voltage for a single cell, considering thermodynamics, mass transport, kinetics, and ohmic resistance are described (Tscuchiya & Kobayashi 2004; Fowler et al. 2002; Amplett et al. 1998; Mann et al. 2000):



(4)

Reversible Cell Voltage, E_r

The reversible cell voltage, E_r, is the cell potential obtained at thermodynamic equilibrium. In this model, E_r is calculated from a modified Nerst equation, with an extra term to account for changes in temperature from the standard reference temperature (Baschuk & Xianguo 2000). This is given by:



(5)

where, ΔG is the change in Gibbs free energy, F is the Faraday constant, ΔS is the change i P_{H_2}, P_{O_2} y, R is the universal gas constant while are the partial pressures (in atm) of hydrogen and oxygen, respectively. The variable T denotes the temperature of the cell, with T_{ref} denoting a reference temperature. Using standard value of ΔG, ΔS and $T_{ref,}$ equation (5) can be simplified to:

(6)

Over-voltage Activation, η_{act}

Activation polarization is a result of the need to affect electron transfer and to break and form chemical bonds in the anode and cathode. The voltage loss due to activation is calculated by (Mann et al. 2000):

(7)

with the value of $c^*_{O_2} = 0.667$ referred to the water effluent from the outlet of cathode

(7a)

(7b)

(7c)

(7d)

Over-voltage Ohmic Resistance, η_{ohm}

Ohmic polarization, η_{ohm}, is caused by electrical resistance losses in the cell. Electrical resistance is found in the electrodes, the membrane (ionic), the fixtures that connect the MEAs (Membrane-Electrode Assemblies), and the interfaces between each component. The total ohmic polarization is defined as (Baschuk & Xianguo 2000):

(8)

where,

and (8a)

(8b)

(8c)

However, the ohmic polarization can be reduced by using components that have high electrical conductivity and by reducing the thickness of the membrane layer, where the actual values of η^{e}_{ohm} and η^{m}_{ohmic} should not be significant in comparison to $\eta^{p}_{ohmic}{}^{\text{Proton}}$ and can be assumed to be insignificant (Amplett et al. 1998; Jain et al. 2003).

Concentration Polarization, $\eta_{concentration}$

Concentration polarization is the result of resistance to mass transport of gases to the reaction sites. This includes transporting of process gases and removing product water and impurities from the reaction site. Equation (9) is an empirical approach to capture the smooth drop-off of the polarization curves at elevated current densities (Francesco & Arato 2002; Chu & Jiang 1999; Laurencella et al. 2001). The parameters m and n are of empirical nature and assumed as 0.000312 and 0.008, respectively.

$$\eta_{concentration} = m \exp [ni], \tag{9}$$

Cell Efficiency

The cell efficiency, η_{FC} is defined as (Bernay et al. 2002):

$$\eta_{FC} = V_{cell}/V_{ref} \tag{10}$$

For hydrogen: $V_{ref} = 1.25V$; while for methanol, $V_{ref} = 1.08V$.

Current Density

The PEM fuel cell model presented here is a comprehensive isothermal and steady state model. In order to determine the value of current density, there are apparently many factors that need to be considered. Therefore, the followings are the assumptions that have been made in the current density model developments:

1) The amount of water produced during the reaction is small and negligible, otherwise the membrane is presumably to be fully humidified;
2) The gases flow continuously in the electrodes and Darcy Law is applicable;
3) The vector of the gas velocity is uniform and
4) Each of the porous electrodes is in contact with a serpentine gas distributor.

For anode, the current density, i_a is defined as:

$$i_a = -K_1 (C_{H_2} - C^{ref}_{H_2} exp(-K_2 (\phi_s - \phi_m - \Delta\phi_{eq,a})))(1 - K_3 \coth K_3) \tag{11}$$

with $$K_1 = \frac{6\delta_l (1 - \varepsilon) F D^{agg}_{H_2}}{(R^{agg})^2} \quad ; \tag{11a}$$

$$K_2 = \frac{2F}{RT} \quad ; \tag{11b}$$

$$K_3 = R^{agg} \sqrt{\frac{i_{o,a} S}{2FC_H^{ref} D_H^{agg}}} \quad ; \tag{11c}$$

and similarly for cathode, $i_{c,}$ the current density is defined as:

$$i_c = K_4 C_{O2} (1 - \sqrt{K_5 \exp(-K_6(\phi_s - \phi_m - \phi_{eq}^c)} \; \coth \sqrt{K_5 \exp(-K_6(\phi_s - \phi_m - \phi_{eq}^c))} \tag{12}$$

$$K_4 = \frac{12\delta_l (1-\varepsilon) F D_{O_2}^{agg}}{(R^{agg})^2} \quad ; \tag{12a}$$

$$K_5 = \frac{i_{O,c} S (R^{agg})^2}{4FC_{O_2}^{ref} D_{O_2}^{agg}} \; ; \tag{12b}$$

$$K_6 = \frac{0.5F}{RT} \tag{12c}$$

In these expressions, C_{H_2,O_2} denotes the molar concentration of hydrogen and oxygen in the electrolyte, while, $C_{H_2,O_2}{}^{ref}$ describes the molar concentration of hydrogen or oxygen at reference state, ϕ_s and ϕ_m are the potentials of electrode and membrane respectively, ϕ_{eq} shows the difference of potential between electrode and membrane, δ_1 is the thickness of the active layer, ϕ , is the dry porosity of the electrode, F is the Faraday's constant, D^{agg} is the diffusion coefficient of the dissolved gas in the electrolyte, R^{agg} is the radius of the electrolyte, i_o describes the changes of current density and S is the specific area of the electrode.

Material and Energy Balance

The basic structure and operation principles of the model considered here are illustrated in Figure 1. The total area, *A* for the gas flow at any point on the electrode is given by:

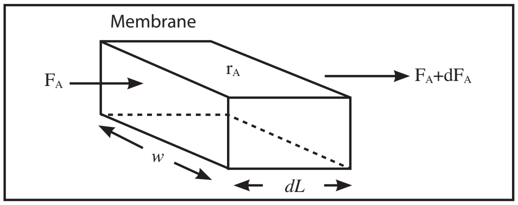


FIGURE 1. The Schematic diagram of a gas distributor channel and gases stream to membrane in single stack PEM fuel cell

$$A = wdL \tag{13}$$

and $$r_A = \frac{i_n wdL}{nF} \tag{14}$$

where w is the width for the gas distributor surface, *dL* is defined as differential element for length and r is the rate of reaction. Assuming the electrode operates as a plug flow reactor, thus for reactant A,

$$F_{A0} C_A = F_A (C_A + dC_A) + (-r_A) \tag{15}$$

and $$dC_A = d\left[C_{Ao}(1 - X_A)\right] = -C_{Ao} dX_A \tag{16}$$

where F_{A0} is the input of A, mole time^{-1}, F_A is the output of A, mole time^{-1}, X_A *is the* conversion of *A*, C_A is concentration of A in molar, C_{A0} is the initial concentration of component A in molar and r is obtained from:

$$r_A = F_A dC_A \tag{17}$$

With that,

$$F_A dC_A = \frac{i_n wdL}{nF} \tag{18}$$

where n = the number of electrons , i_n = current density and *F*= Faraday constant, and equation (18) rearrange as :

$$2H_2 \rightarrow 4e^- + 4H^+ \tag{19}$$

where (19a)

$$2H_2 + O_2 \rightarrow 2H_2O$$

and $$V_{cell} = E_r - (\eta_{act} + \eta_{ohm} + \eta_{concentration}) \tag{19b}$$

with H_i = Henry constant, y_A = molar fraction of gas A and P_A = partial pressure of gas A.

From equation (19):

$$E_r = \frac{\Delta G}{2F} + \frac{\Delta S}{2F}\left(T - T_{ref}\right) + \frac{RT}{2F} \text{ x } \left[1n\left(P_{H_2}\right) + \frac{1}{2} 1n\left(P_{O_2}\right)\right] \tag{20}$$

Upon rearrangement,

$$E_{nerst} = 1.229 - \left(8.5 \times 10^{-4}\right)\left(T - 298.15\right) \tag{21}$$

$$\eta_{act} = \xi_1 + \xi_2 T + \xi_3 T \left[ln\left(c^*_{O_2}\right)\right] + \xi_4 T \left[ln \right. \quad (22)$$

The conversion for A in PEMFC electrodes is calculated from a set of given inlet composition:

$$2F \qquad \alpha_c nF \qquad (23)$$

$$R \qquad \left[\quad (\ ^*\ )^{1-\alpha_c} (\ ^*\ ) \right]$$

Finally the total area, *A,* for gas flow is defined as:

$$+ \frac{\quad}{2F} ln \left\lfloor 4FAk_a^o c^*_{H_2} \right\rfloor \qquad (24)$$

where i_n is referred to current density for anode or cathode.

Assuming other components like, N_2, CO and CO_2 are constants, the overall material balances for fuel cell stack are as follows,

For hydrogen:

$$\alpha_c nF \qquad (25)$$

$$\xi_4 = -\left(\frac{R}{2F} + \frac{R}{\alpha_c nF} \right)$$

For oxygen:

$$\eta_{ohm} = \eta_{ohm} + \eta_{ohm} + = 2iwL\,(\xi_4 + \xi_5) + \xi_6 \qquad (26)$$

$$= 2iwL\,(\xi \quad \xi\ ) \quad \xi \qquad \rho^{eff}$$

For water:

$$\xi_5 = \frac{\quad}{8n_g \delta_e L}(W_c + W_s) \qquad \rho_{R,e} \qquad (1-\phi_e)^{3/2}$$

$$\rho^{eff} = \frac{\rho_{R,e}}{\quad}$$

$$(27)$$

$$\xi_6 = \frac{\rho_{R,p}}{L}\left(\frac{h_p}{W} + \frac{h_c}{W \quad n \quad w} \right)$$

where k_a and k_c are defined as the mass transfer coefficient of anode and cathode, respectively.

For the purpose of energy balance, it was assumed that the anode and cathode gas would enter and leave the stack at a temperature of 70°C. The stack was thermally insulated, therefore heat loss to the surroundings was assumed to be negligible. The overall fuel cell reaction is a formation of water from hydrogen and oxygen, producing electricity and heat. The relation of cell reaction and formation of water from H_2 and O_2 is given by:

$$\xi_7 = \delta_m \frac{\quad}{\left(1 + \quad F^2 K_E C^2_{H^+} \right)} \qquad (28)$$

The energy balance for the fuel cell stack is given by,

$$\left(\qquad H_2O \qquad \right) \qquad (29)$$

The energy conversion efficiency of fuel cell is higher than that of combustion engines or boilers. Yet significant amount of heat is released during the cell reaction. Thus, the heat flux from the cell reaction depends on the hydrogen fraction consumed by the cell reaction and on the current. The heat flux is expressed by using enthalpy of the reaction to be:

$$G(i,\ j) = \max\left\{1, \max_{k=0}^{7}[|\,5S_k - 3T_k\,|]\right\} \qquad (30)$$

where Q_E is the power output of the stack.

$$S_k = A_k + A_{k+1} + A_{k+2}$$

$$T_k = A_{k+3} + A_{k+4} + A_{k+5} + A_{k+6} + A_{k+7} \qquad (31)$$

$$G(i,\ j)_D = max(|5S_0 - 3T_0|, |5S_4 - 3T_4|)$$

The heat flux for each gas that comes in and goes out of the stack is expressed by:

$$G(i,\ j)_T = max(|5S_2 - 3T_2|, |5S_6 - 3T_6|)$$

$$G(i,\ j)_{PKa} = max(|5S_1 - 3T_1|, |5S_5 - 3T_5|) \qquad (32)$$

$$G(i,\ j)_{PKi} = max(|5S_3 - 3T_3|, |5S_7 - 3T_7|)$$

A_0	A_1	A_2
A_7	*(i,j)*	A_3

(33)

The fuel cell electricity cost, *EC*, is given as follows (Kazim 2002):

4 4444
6 6666
E EEEE
G GGGG (34)

with C_F as the fuel cell cost, AEP as the annual fuel cost, η as the average fuel cell efficiency, C_{fix} is the fuel stack cost, C_{cell} is the fuel cell cost, A_{cell} as the active surface area of the cell, i_r as the annual interest, and n_y as the life span of the fuel cell.

RESULTS AND DISCUSSION

The models are solved using the Matlab Version 6.5. Based on equations (5) to (9), the polarization parametric curves are illustrated in Figure 2. The reversible thermodynamic potential, E_r, values remain almost constant along the operation. Meanwhile the activation polarization, η_{act} and concentration polarization, $\eta_{concentration}$, are minimum at the temperature range value of 338-343K. In the activation over potential region, the dominant source loses is due to the resistance to chemical reaction. These losses also referred to as activation loses, which occur when slow electrochemical reactions are driven from equilibrium in order to produce electric current. Besides that, the ohmic polarization, η_{ohm}, also decreases from 0.4 to 0.3 at the temperature range of 338-343K. As such, it is concluded that the optimal operating temperature for the fuel cell stack falls in the range of 338-343 K. Figure 3 shows the trend for the current density and power density. After considering the polarization parameters, the voltage for single cell in this study is determined as 0.68 V with current density and power at 1.0 Acm^{-2} and 0.6 Wcm^{-2}, respectively.

Figure 3 shows the predictions of the consumption of hydrogen and oxygen at anode and cathode, respectively. The hydrogen and oxygen that flow in the gas channel react in the MEA region. From the plot, it is observed that the mole fraction of both gases reduce sharply along and inside the gas diffusion layer. However, the slope decreases as it goes further into the channel. As observed, the reaction for hydrogen terminates at a distance of 0.25m while for oxygen at 0.65m. From this result, it can be concluded that hydrogen is the limiting source for the reaction.

The variation of contribution to current density is plotted in Figure 4 over a range of distance flow in channel for different pressures. The plots show that the current density increase with the increase in the operating pressures. Generally, a higher operating pressure results in high cell efficiency. However, increasing the operating pressure can also affect the performance of the stack in term of the characteristics of single cell performance as shown in Figure 5.

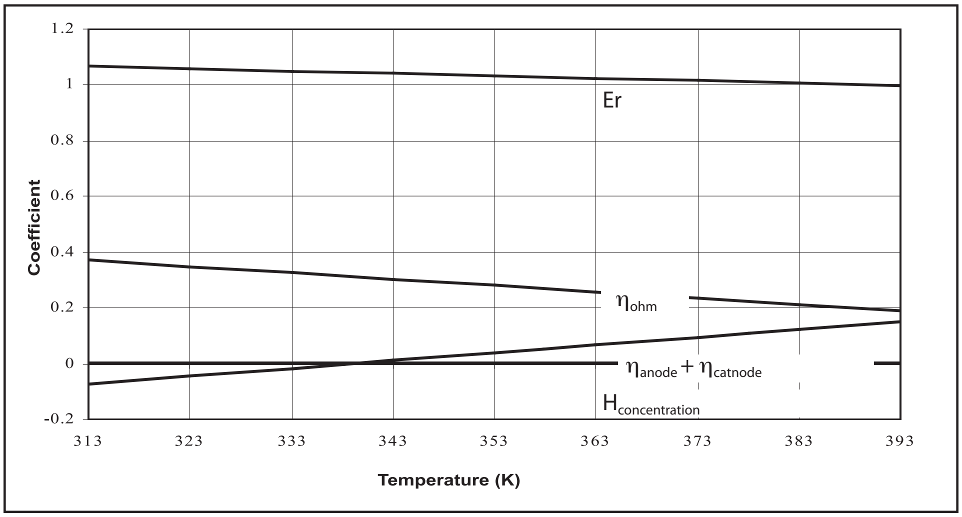


FIGURE 2. Polarization Coefficient versus Temperature

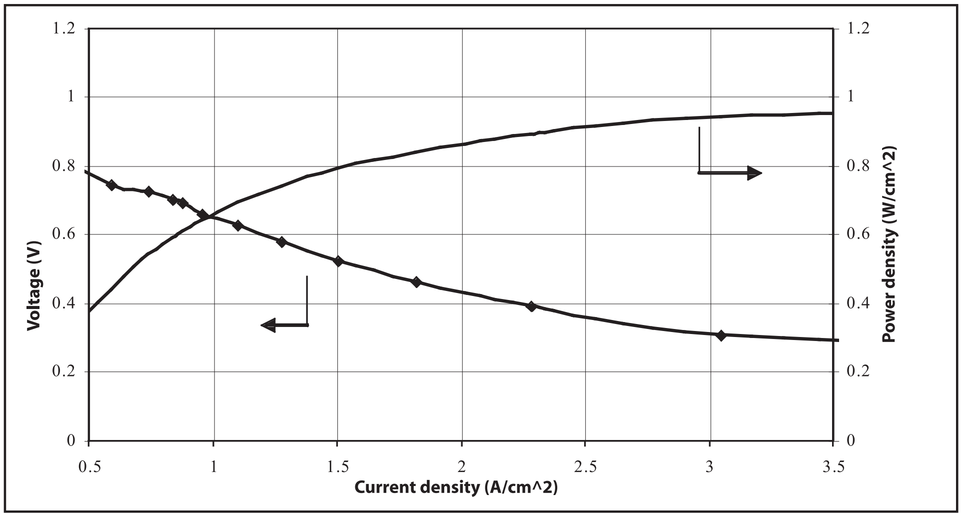


FIGURE 3. The Trends plots for Current Density and Power Density

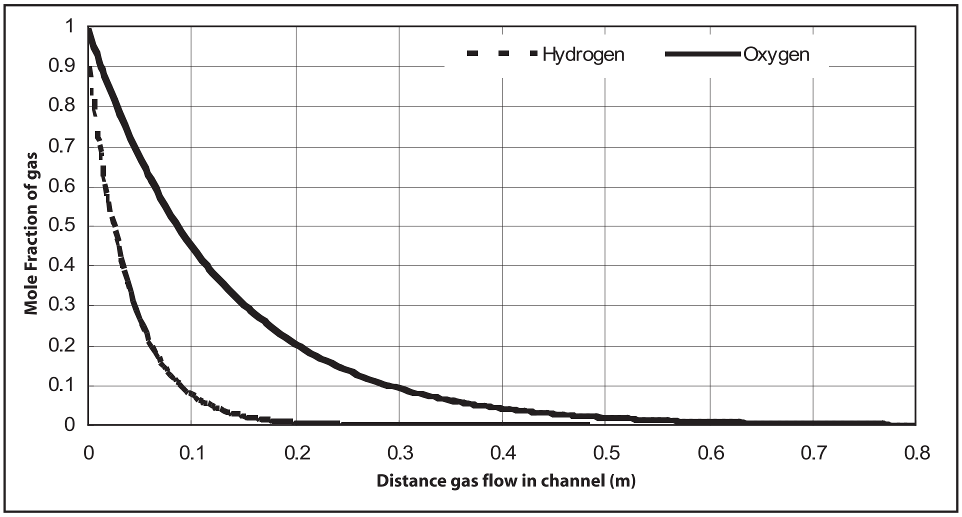


FIGURE 4. Mole Fraction of Hydrogen and Oxygen Profile over distance of gas flow in channel

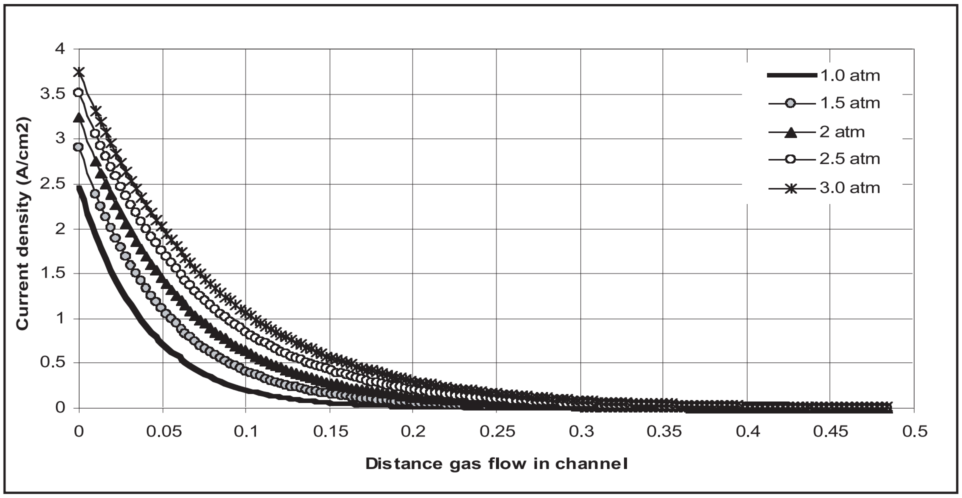


FIGURE 4. Variation of Current density Over Distance Gas Flow in Anode Channel at Different Pressure

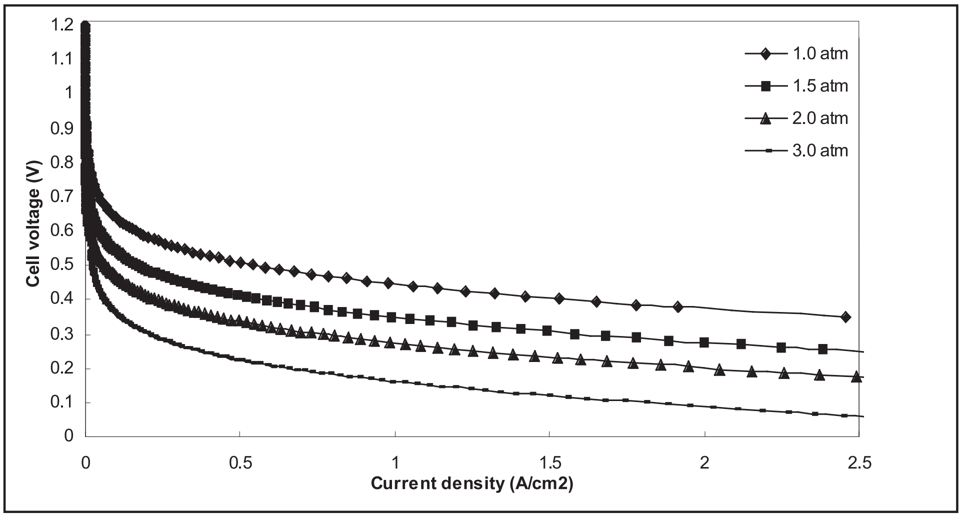


FIGURE 5. The Changes of Current Density at Different Operating Pressure

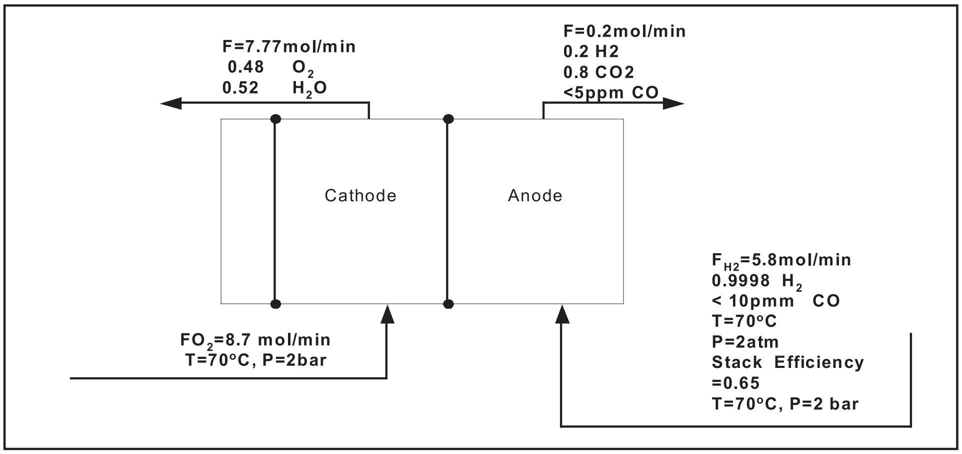


FIGURE 6. Summarized Material Balance across the System

TABLE 1. Design Parameters for Fuel Cell Stack

Parameters	Value
Power Output	5 kW
Voltage per cell	0.7V
Current	260 A
Power Density	660 mWcm^{-2}
Current Density	1000 mAcm^{-2}
Cell Efficiency	64.8%
Temperature	343K
Pressure	2 bar
Excess Air	100%
Membrane type	ETEK MEA Nafion 117
Membrane Thickness	200μm
Active area	250 cm^2 per cell
Length X Width	15.7 cm x 15.7 cm
Number of Cells	32

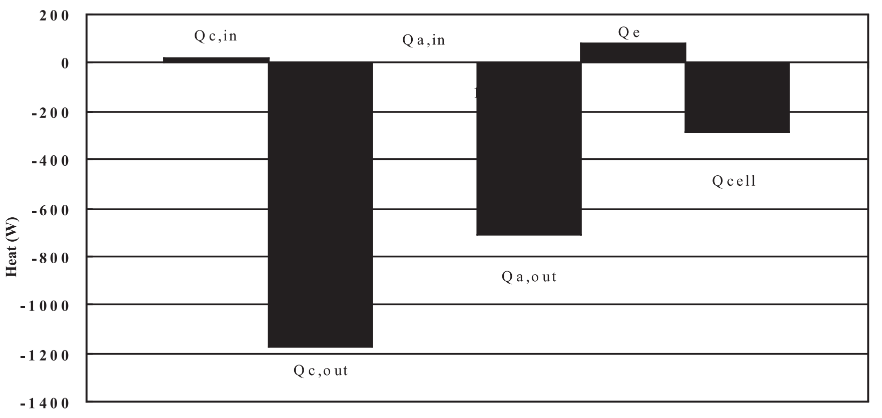


FIGURE 7. Summarized Heat Flux across the System

TABLE 2. Comparison with other Design Parameters

	This study	Amplett et al. 1998	Laurencella et al. 2001	Lin 2001
Power Output (kW)	5.0	5.0	5.0	5.9
Current Density (A cm^{-2})	1.0	1.2	1.3	1.0
Voltage for single cell (V)	0.7	0.6	0.53	0.61
Active area for single cell (cm^2)	250	232	232	168
Number Of Cell	32	35	36	56

TABLE 3. Data For Electricity Cost Estimation

Parameter	Value
Power Output	5 kW
Hydrogen Cost	\$10 GJ^{-1}
Capacity Factor Of Fuel	0.9
Life time	5 years
Annual rate	7%

TABLE 4. Comparison Of Electricity Cost With Other Studies

References	kWh (RM)
Dufour 1998	0.152-0.912
Sammer & Boersma 2000	0.266
Kazim 2005	0.152
Kwak et al. 2004	0.152
This Study	0.152

Taking the hydrogen consumption in the fuel cell stack as 1000 Lh^{-1} for a power output of 1 kW_e, the total hydrogen required at the stack for a power output of 5kW is calculated as 3.74 $molmin^{-1}$ (0.084 m^3min^{-1}). However, the total feed flow rate of hydrogen into the anode, F_{H_2} is taken as 5.8 $molmin^{-1}$ (0.13 m^3min^{-1}) after considering the cell efficiency as 65% based on equation (10). Figure 6 summarizes the overall material balance in mole percentage, while Figure 7 presents a summary of the heat balance across the system. Neglecting the lost of heat through thermal radiation from the stack, the waste heat generated in the fuel cell stack is calculated as 1.4 kW. As the overall result, Table 1 presents the design parameters for the direct hydrogen PEM Fuel Cell system in this study as base case simulations, while Table 2 shows the design outputs obtained in this study in comparison with other previous studies.

Lastly, the electricity cost in this study is estimated at RM 0.152 kWh^{-1} based on Equation (34) and Table 3. The cost value is found to be almost the same as the values found by other studies (Table 4).

NOMENCLATURE

A	Cell Active Area
C_{H_2,O_2}	Molar concentration of H_2/O_2 in electrolyte
$C_{H_2,O_2}{}^{ref}$	Molar concentration of H_2/O_2 in electrolyte at standard condition
c	Concentration in gas phase
c^*	Equilibrium concentration
D^{agg}	Gas diffusivity in electrolyte
D	Diffusivity
D_L	Axial dispersion
F	Faraday Constant (96,487 C)

CONCLUSION

A shortcut design method using a mathematical model of PEM fuel cell stack is presented by taking into consideration the entire polarization factors, current density and mole fraction of gases and polarization behaviour along the gas surface area. Several assumptions and considerations are used in order to develop the model of serpentine distributor. The mole fraction of hydrogen and oxygen, and the current density decrease noticeably along the channel and inside the gas diffusion layer. Finally, the electricity cost is determined as RM 0.152 kWh.

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i_o	Changes of current density
i	Current Flow
P	Pressure
$p^*_{H_2}, p_{H_2O}$	Partial pressure for hydrogen at anode
$p^*_{O_2}$	Partial pressure for oxygen at anode
P_{H_2}	Partial pressure of H_2
P_{H_2O}	Partial pressure of water
P_{O_2}	Partial pressure of O_2
$Q_{cooling\_water}$	Total heat released to the cooling water
Q_c, Q_a	Sensible heat for the anode and cathode streams
Q_{cell}	Energy released by the reaction

$Q_{electrical}$	Output Heat from the system
V_F	Volumetric flow rate of feed
R	Ideal gas constant
R^{agg}	Radius of electrolyte
S	Specific surface area of electrode
T	Temperature
V_{cell}	Voltage of single cell (V)
G	Greek symbols
ΔG	Standards Gibbs activation energy
ϕ_S	Potential of electrodes
ϕ_M	Potential of membrane
$\Delta\phi_{eq}$	Potential different between the electrodes and membrane at equilibrium
δ_l	Electrodes thickness on active area

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