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Improving the Performance of Single Cells in the Design of Proton Exchange Membrane Fuel Cell (PEMFC) when Using Hydrogen

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Abstract— A proton Exchange Membrane Fuel Cell (PEMFC) was developed as a potential solution in power supply applications. In this study, the parameter values such as the relative humidity, the temperature, the pressure, the stoichiometric ratio of hydrogen to oxygen and the mass of catalyst used were varied to determine their effects on the single cell performance of PEMFC. The investigation showed that an increase in the temperature from 353 to 363 K resulted in a modest improvement in the single-cell performance. The single cell performance was more affected by an increase in relative humidity at the cathode (RHC) in comparison with an increase in relative humidity at the anode (RHA). The best performance when the cell was operated at relative humidity values were 75% for the RHA and 90% for the RHC, the optimal operating temperature was 353 K, and the amount of Pt catalyst required was 0.2 mg.

Keywords—PEMFC; modelling; single cell; performance; design system

I. INTRODUCTION

Fuel cells are electrochemical devices that convert chemical energy from fuel (hydrogen) and oxidant (oxygen or air) directly into electrical energy and thermal energy, producing water as a byproduct. One type of fuel cell is the PEMFC, which can be operated at low temperatures to produce electrical energy. Developing the system performance of PEMFC requires a suitable design and appropriate technology. The main purpose is to achieve optimal performance and obtain a low-cost PEMFC system.

Some parameters in the PEMFC system are associated with other parameters in the system. These parameters consist of the operating conditions, the design of the membrane electrolyte assembly (MEA) and the stack PEMFC [1]. The performance of the PEMFC is evaluated in the form of the voltage generated, the power density and the efficiency. The optimal performance of the cells is influenced by many internal and external factors, such as the fuel cell design and assembly, the degradation of materials, the operating conditions and the impurities or the contaminants [2]. Other parameters such as the pressure, temperature, composition and utilization of the fuel, and composition and the utilization of oxidant can be varied simultaneously to achieve the desired operating point. Much research has been conducted to develop the operating conditions in the design of PEMFC. Mulyazmi [3] studied

the performance of PEMFC which are influenced by the operating temperature, pressure, and humidity of the reactant gas to the effects of mass transport in membranes and the transportation of the water produced at the stack fuel cell. Ozen et al.[4] Investigated the effects of operating conditions such as humidification, stack temperature, and flow gas on the individual cells and a stack of PEMFC. The operating parameters that facilitated better water removal rates by a temperature, stoichiometric and pressure resulted in the generation of a higher net current [5]. The use of a system design for PEM fuel cells allows for the manipulation of parameters to obtain the best combination of system variables. Abdin et al. [6] and Salva et al. [7] investigated the optimal conditions PEMFC based on temperature, pressure, and humidity on cell and ratio stoichiometry. The PEMFC central system must be supported by providing an oxidant supply (oxygen or air), a fuel supply (hydrogen), heat and water management, process control, equipment and supervision [8], [9]. The many failures in PEMFC systems include flooding, the diffusion of water in stack fuel cell and poor of integration heat and mass during the operation [10]. Mulyazmi et al [3] conducted a study on water balance in PEMFC stack. Then get to know the effect of various operating conditions of optimum performance PEMFC system. The focus of this research was to develop a fundamental thermodynamic basis for developing a modelling system to optimize the performance of PEMFC systems. The next focus was to determine the

influence of system parameters such as the temperature, operating pressure, relative humidity and stoichiometry of the reactants entering the PEMFC cell stack on the voltage and the current density that was produced by the resulting fuel cell system.

II. MATERIAL AND METHOD

The model was developed based on several assumptions:

- There are negligible pressure drops in the PEMFC stack.
- The reactant gases in the system possess ideal gas behaviors.
- The PEMFC system operates at steady state.
- The water flowing into the stack is in the gas phase.
- The operation of the PEMFC stack is an isothermal process.

The voltage value of each cell in a PEMFC stack is determined by the maximum value of the voltage cells and the loss of voltage. The loss of voltage in fuel cells includes activation loss, ohmic resistance loss, concentration loss and the loss of internal currents. The cell voltage value V_{oper} on in the operation of a PEMFC is:

$$V_{oper} = V_{rev} - V_{irrev} \tag{1}$$

$$V_{irrev} = V_{act} - V_{ohm} - V_{con} \tag{2}$$

A. Reversible Voltage (View)

The reversible cell voltage is the maximum theoretical potential of a fuel cell and is independent of the loading in a fuel cell. The free energy change is a measure of the maximum electrical work that can be obtained from a system at a fixed reaction temperature and pressure. The reversible voltage in a PEMFC is:

$$V_{ref} = E_T + \frac{RT}{Fn} ln \left[\frac{P_{H_2} \times (P_{O_2}^{0.5})}{P_{H_2} o} \right]$$
 (3)

 P_i is the partial pressure (atm). The electrical potential at standard conditions is: $E^{(0)} = -\frac{\Delta G_f^{(0)}}{nF}$. The electrical potential E_{m} is:

$$E_T = 1.229V - 0.85 \times 10^{-3} (T - T_{ref}) \frac{V}{R} \tag{4}$$

The reversible voltage in the PEMFC can be obtained by substituting equation (3) into equation (4), with the assumption that the partial pressure of water is 1 atm because it exists as a liquid [11]:

$$V_{rev} = 1.229V - 0.85 \times 10^{-3} (T - T_{ref}) + 4.31 \times (5)$$

$$10^{-5} \times T \times \ln (P_{H_2} \times (P_{O_2}^{0.5}))$$

B. Activation Voltage (Vact)

The current density can then be written as:

$$i = nF \left(k_f C_{O_2} - k_b C_{H_2} \right) \tag{6}$$

Equation (6), which is also known as the Volmer Butler equation, the reaction concentration becomes [12]:

$$i = nF \left(k_{f,0} \exp\left(\frac{-\alpha FE}{RT}\right) C_{O_2} - k_{D,0} \exp\left(\frac{(1-\alpha)FE}{RT}\right) C_{H_2}\right)$$
 (7)

The change in the current density is:

$$i_0 = i_{0,ref} \left(\frac{c_{\theta_2}}{c_{\theta_2,ref}} \right)^{(1-\alpha)} \left(\frac{c_{H_2}}{c_{H_2,ref}} \right)^{\alpha} exp \frac{z_c}{z_T} \left(1 - \frac{T}{T_{ref}} \right)$$
(8)

The i_0 value influenced by the reaction surface area per unit volume of the catalyst layer (a) is

$$i_0 = a i_{0, \text{ref}} \left(\frac{p_{\text{R}}}{p_{\text{Rref}}} \right) exp \frac{E_{\text{F}}}{RT} \left(1 - \frac{T}{T_{\text{ref}}} \right)$$
 (9)

R = reactant (H₂ and O₂) and E_{r} = activation energy (76.5 kJ/mol) . Song [13] defined the value of α as:

$$a = a_0 \frac{m_{pr}}{L} \tag{10}$$

The value of a_0 was determine by Song [14] to be:

$$a_0 = 10^8 (4.4198Y^9 - 27.691Y^8 + 74.206Y^7 - 111.06Y^6 + 101.43Y^5 - 57.841Y^4 + 20.231Y^3 - 4.089Y^2 + 0.39451Y)$$
(11)

Where Y= % Pt. According to Inoue [15], the reference current density is:

$$i_{0,ref} = 10^{\left(3.057 - \frac{4001}{T}\right)} \tag{12}$$

If **t** is compared with **t** is:

$$\begin{split} \frac{i}{i_{0}} &= \frac{c_{\mathcal{Q}_{2}}}{c_{\mathcal{Q}_{2}}} \bigg(\exp \bigg(\frac{-\alpha F E}{RT} \bigg) + \bigg(\frac{\alpha F E_{T}}{RT} \bigg) \bigg) - \bigg(\exp \bigg(\frac{-\alpha F E}{RT} \bigg) + \bigg(\frac{\alpha F E_{T}}{RT} \bigg) \bigg) \end{split}$$

 $\mathbf{E} - \mathbf{E}_{\mathbf{r}} = \eta_{\text{act}}, \frac{\mathbf{f}}{\mathbf{f}_{\text{in}}}$ value became:

$$V_{\text{set}} = \frac{RT}{2\pi F} \sin h^{-1} \left(\frac{i}{t_0}\right)$$
 (14)

The voltage activation [16] is

$$V_{act} = \frac{RT}{naF} \ln \left(\frac{i}{t_0} \right) \quad \text{where } i > i_0$$
(15)

From equation (15) the Tafel constant can be obtained:

$$b = \frac{MT}{naF} \tag{16}$$

Where b = the Tafel constant. According Mann [17]:

$$b = 0.1937 e^{-2.197(\alpha)}$$
 (17)

The value of the exchange coefficient value α was obtained from Zhang [18]:

$$\alpha = (0.001552RH_{c,in} + 0.000139)T$$
 (18)

 $RH_{\sigma,in}$ is the relative humidity of the reactants that flow into the cathode side of the stack of PEMFC.

C. Ohmic Voltage (Vohm)

The ohmic voltage that is lost was presented:

$$V_{ohm} = i R_{ohm} \tag{19}$$

where the R_{ohm} value is

$$R_{ghm} = \frac{t_m}{\sigma_m} \tag{20}$$

The membrane proton conductivity can be written as [19]:

$$\sigma_{m} = (0.005139 \, \lambda_{m} - 0.003260) \, \exp \left[1268 \left(\frac{1}{303} - \frac{1}{T} \right) \right]$$
(21)

where λ_{m} is the water content in the membrane:

$$\lambda_m = 0.048 + 17.81RH - 39.83\alpha RH^2 + 39.85RH^3$$
 (22)

where **RH** is the average relative humidity in the stack of PEM fuel cells.

D. Concentration Voltage (V_{conc})

The concentration voltage was presented by Shaker [20] as:

$$V_{conc} = c \ln \left(\frac{t_{L}}{i_{L-1}} \right)$$
 (23)

Where ε is the concentration loss constant. The value of ε is:

$$c = \frac{RT}{n\pi} \tag{24}$$

The concentration voltage value is:

$$V_{conc} = \frac{RT}{nE} \ln \left(\frac{i_L}{i_{c-1}} \right)$$
 (25)

 t_L is the limiting current density $\left(\frac{A}{cm^2}\right)$. The limiting current density is [21]

$$i_L = nFh_m \left(\frac{c_{D_2,\text{ivs}} - c_{D_2,\text{out}}}{\ln \frac{c_{D_2,\text{ivs}}}{c_{D_2,\text{out}}}} \right)$$
(26)

 $e_{\mathcal{O}_{2,in} \text{ and out}}$ is the concentration of oxygen entering and exiting a PEMFC stack (mol), and h_{in} is the convective mass

transfer coefficient (m s⁻¹). The convective mass transfer coefficient can be written as [22]:

$$h_m = \frac{\operatorname{sa}_f b_{ij}}{H_c} \tag{27}$$

III. RESULTS AND DISCUSSION

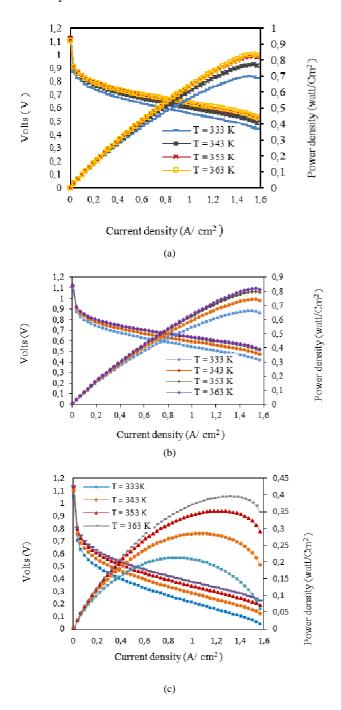
In this study, several parameters that affect the performance of single cell PEMFC have been discussed, such as the operating temperature, the relative humidity, the operating pressure, the stoichiometric ratio of the hydrogen and oxygen reactants, and the influence of the mass of catalyst that was added to the cells. The operating parameters for the base case are listed in Table 1.

TABLE I BASE CASE MODEL PARAMETER

Parameter	Value
Cell temperature	333K to 363K
Reference temperature	298.15 K
Dry membrane thickness	0.0051 cm for Nafion 112
Catalyst load	0.0002 g cm ⁻²
Thickness of the catalyst	0.0005 cm
Anode side pressure	1 atm
Cathode side pressure	1 atm
Relative humidity at the anode	0.5 to 0.9
Relative humidity at the anode	0.5 to 0.9
Universal gas constant	8.314 J/mol K
Faraday constant	96,485 C/mol electrons
Stoichiometric ratio for hydrogen	1.2
Stoichiometric ratio for oxygen	2

A. The Influence of the Operating Temperature

Fig. 1a shows the increase in the single cell performance when the operating temperature was increased from 333K to 353 K. However, a subsequent increase in the temperature from 353K to 363 K had little effect on the single cell performance. A current density of less than 0.3 Acm⁻² showed that a temperature difference did not affect the power density that was produced, but current densities that exceeded 0.3 Acm⁻² affected the power density hat was produced when the temperature was increased 333 K to 353 K; however, increasing the temperature from 353K to 363 K did not affect the power density that was produced. Fig. 1b shows an increase in the temperature also improved the performance of the PEMFC. However, an increase in the temperature from 353 K to 363 K did not significantly affect the single cell performance. At current densities that were greater than 1 Acm⁻², an increase in the temperature from 353 K to 363 K did not affect the current density significantly. Figs. 1c, 1d, and 1e show that an increase in temperature from 333 K to 363 K at different operating conditions resulted in an increase in the single cell performance because there was an increased voltage and an increased power density that was generated by the PEMFC. The result of this study was an increase in the power density when the current density was greater than 0.25 A cm⁻² under the operating conditions shown in Fig.1c, when the current density was greater than 0.4 A cm⁻² under the operating conditions shown in Fig.1d, and when the current density was greater than 0.6 A cm⁻² in the conditions shown in Fig. 1e. The results of this study followed the trends observed by Shamardinaetal [23], who found that an increase in operating temperature cause and improvement in the performance of PEMFC systems.



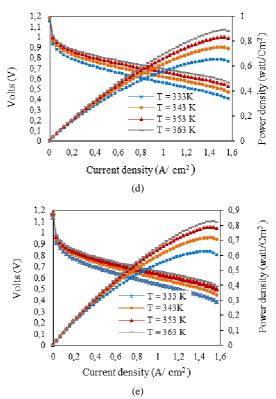
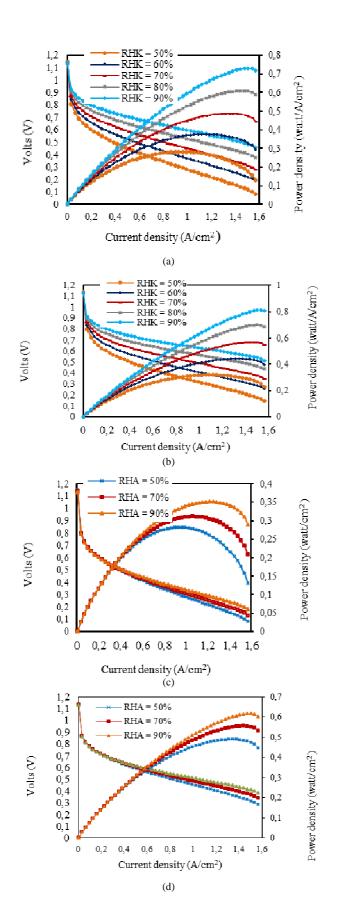


Fig. 1 Effect of operating temperature on single cell performance of PEMFC at the stoichiometric ratio of H_2 is 1.2 and O_2 is 2. Other operating conditions are: (a) RHA and RHC are 90%, PA and PC are 1 atm (b) RHA and RHC was 50% and 90%, PA and PC are 1 atm (c) RHA and RHC are 90% and 50%, PA and PC are 1 atm (d) RHA and RHC are 50% and 90%, PA and PC are 1 atm and 2 atm (e) RHA and RHC are 50% and 90%, PA and PK are 2 atm and 1 atm

B. The Effect of Relative Humidity on the Reactants

Figs. 2a and 2c show the effects of varying the relative humidity while all the other conditions are kept constant. The RHA in Fig. 2a was maintained at 50% while the RHC was varied from 50% to 90%. In Fig. 2c, the RHC was maintained at 50% while the RHA was varied from50% to 90%. Fig. 2a shows the improvement in the single cell performance with an increase in the RHA. Fig. 2c shows that the increase in RHA causes an insignificant improvement in the single-cell performance. Increasing the RHC was more effective than increasing the RHA with regard to improving the single cell performance. The increases in the RHA and the RHC resulted in an increased voltage and an increased power density. Specifically, an increased RHC significantly improved single cell performance. Figs. 2c, 2d and 2e show the effect of RHA on the single cell performance; improved performance occurs beyond a voltage of 0.6 V. Figs. 2a and 2b show the effect of maintaining the RHA at 50% and 70% while the value of RHC was kept constant from 50% to 90%.



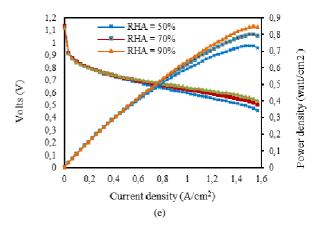


Fig. 2 Effect of relative humidity on single cell performance of PEMFC at temperatures of 353K, the operating pressure of 1 atm, the stoichiometric ratio is 1.2 for H2 and O2 are 2: (a) RHA is 50% and RHC are 50%, 60%, 70%, 80% and 90%. (b) RHA is 75% and RHA are 50%, 60%, 70%, 80% and 90%. (c) RHA is 50%, 70% and 90%, RHC is 50%. (d) RHA are 50%, 70% and 90%, RHC is 70 %.(e) RHA are 50%, 70% and 90%, RHC is 90%

C. The Effect of Operating Pressures

Figs. 3a and 3b show the performance of the single cells when the cathode and the anode pressures were varied from 1 atm to 2.5 atm. An increase in anode pressure resulted in improved performance of the single cell. Increasing the cathode pressure from 2 atm to 2.5 atm did not significantly affect the single cell performance. An increased anode pressure from 1 atm to 2.5 atm improved the single cell performance significantly. The increase in current density at a voltage of 0.6 V was caused by an increased pressure on the cathode side, as shown in table 5. An increase in anode pressure from 1atm to 2.5 atm also resulted in an increase in the fuel cell current density. An operating anode pressure of 2.5 atm and an operating cathode pressure that was greater than 2atm produced an above-average current density of 1.6 A cm⁻² at a voltage of 0.6 V. A study by You and Liu [24] showed that the operating pressure affects the performance of the fuel cell system. The study was conducted at an operating temperature of 353 K, the cathode inlet velocity was 0.6 ms⁻¹, and the anode pressure was 1atm while the cathode pressure was 1.2 atm or 3 atm. The results showed that an increasing cathode pressure resulted in the generation of an increased current density. Figs. 3c and 3d show the performance of single cells by varying the anode pressure from 1 atm to 2.5 atm, while the pressure at the cathode was either 1 atm or 2.5 atm, showing that an increased anode pressure improved the single cell performance. The current density at a voltage of 0.6 V is shown in table 6. An increase in the anode pressure from 1 atm to 2.5 atm while the cathode pressure was maintained at 1 atm resulted in a slight increase in the current density. At a cathode pressure of 2.5 atm, there was a significant increase in the current density.

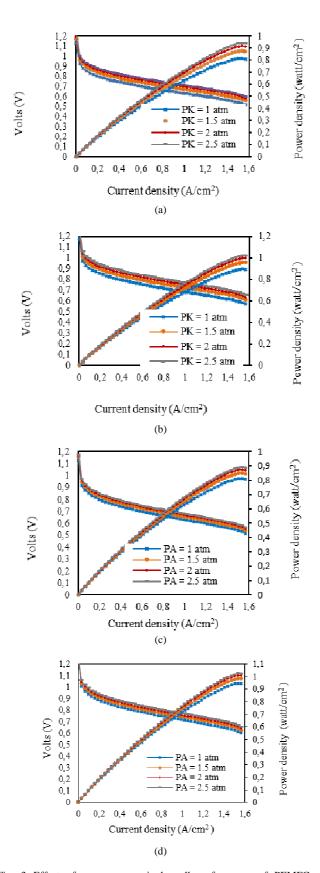


Fig. 3 Effect of pressure on single cell performance of PEMFC at temperatures of 353K, RHA is 75% and RHC is 90%, the stoichiometric ratio is 1.2 for H2 and O2 are 2: (a) PA is 1 atm and PC are 1, 1.5, 2, 2.5 atm. (b) PA is 2.5 atm and PC are 1, 1.5, 2, 2.5 atm and PC is 1 atm. (d) PA are 1, 1.5, 2, 2.5 atm and PC is 2.5 atm

D. Effect of the Stoichiometric Ratio of Reactants

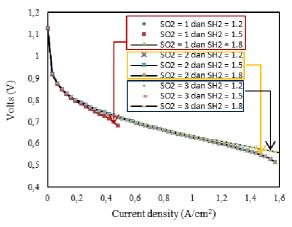


Fig. 4 Effect of stoichiometric ratio on single cell performance of PEMFC at temperatures of 353K, RHA and RHC is 75% and 90%, PA and PC is 1 atm. The stoichiometric ratio of H2 is 1.2 to 1.5 and 1.8, for O2 is 1, 1.5, 2, 2.5 and 3

Fig. 4 shows the single cell performance at an oxygen stoichiometric ratio of 1, 2 and 3, while the hydrogen stoichiometric ratio was varied from 1.2 to 1.8. The results of this study show that an increased hydrogen stoichiometric ratio did not influence the single cell performance significantly [25]. The oxygen stoichiometric ratio that is greater than 2 can achieve the maximum current density while the hydrogen stoichiometric ratio is maintained between 1.2 and 1.8.

E. Comparison of Single Cell Performance

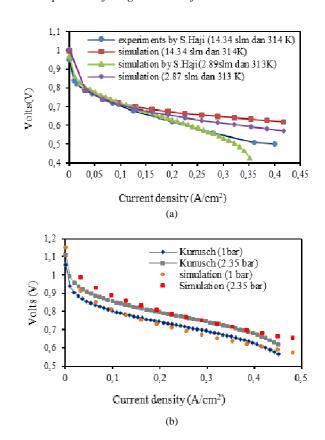


Fig. 5 Comparison of single cell performance of PEMFC with the investigation results of the investigation has been made: (a) comparison

with the results of the investigation S.Haji 2011. (b) comparison with the results of the investigation Kunusch 2010

The results of this study were compared with an experimental and a simulation study conducted by S. Haji [20]. Experiments were conducted data flow rate of 14.34 slm and a temperature of 314K, while the simulations were conducted at a flow rate of 2.89 slm and a temperature of 313K. Fig. 5a shows that the simulation study conducted by Haji showed a similar trend with their experimental data, while the simulation in this study showed a better performance than the simulation generated by Haji. At a flow rate of 2.87slm and a temperature of 313K, the simulation performance in this study was better than the simulation performance reported by Haji. Fig. 5b shows the comparison of the simulation results with the simulation study by Kunush [26]. The operating pressures for simulating the performance were 1bar and 2.35 bar. The simulation results showed a trend similar to the performance of the single cell. However, the simulation results in this study showed no significant performance decrease beyond a current density of 0.45 Acm⁻², while the simulation results provided by Khunush showed a significant decrease.

IV. CONCLUSIONS

The conclusions that can be drawn from this study, which conducted to determine the effect of several parameters on the performance of single-cell PEM fuel cells, are as follows:

- An increase in the temperature from 333K to 353K resulted in a significant improvement in the performance of a single PEM fuel cell. However, a subsequent increase in the temperature from 353K to 363K only resulted in a small improvement in the single cell performance.
- At the same relative humidity conditions on one side
 of the stack PEM fuel cell, an increase in the RHC
 exerted more influence on the single cell performance
 than an increase in the RHA. The best performance of
 the cell was 0.6 volts at an RHC from 70% to 90%
 and an RHA of 70%.
- An increase in the cathode pressure improved the cell performance more significantly than an increase in the anode pressure. The maximum voltage achieved at an anode pressure of 1atm and a cathode pressure 2.5atm was 0.6 volts.
- An increase in the load mass of Pt from 0.2 mg to 0.6 mg improved the performance of single cells, but a subsequent increase from 0.6 mg to 1 mg did not affect the performance significantly.

NOMENCLATURE

æ	The surface area to unit volume ratio of	cm ² /cm ²
	the catalyst layer	
a_{a}	The total surface area of the catalyst	cm/g
	per unit mass of catalyst	
b	The Tafel constant	
C	Concentration	mol

D_{ij}	Binary diffusion coefficient of O_2 in N_2	cm/s
E	Electrical potential	V
E ^O	Electrical potential at standard	V
_	conditions	•
E _T .	Electrical potential of PEM fuel cells	V
_	Faraday constant	96,485
F	raraday constant	90,483 C/mol
		electrons
G	Gibbs free energy	J/mol
H	Enthalpy	J
H_{c}	Hydraulic diameter	cm
h_{m}	Convective mass transfer coefficient	m s ⁻¹
i	Current density	A cm ⁻²
i,	Exchange current density	A cm ⁻²
i,	Limiting current density	A cm ⁻²
love	Reference current density	A cm ⁻²
k	Reaction rate constant	
L	Thickness of catalyst	cm
m _{mt}	Catalyst load	gr/cm ²
_	The number of electrons per hydrogen	gi/Ciii
92	molecule	
_		
P	Pressure	atm
P_{k}	Partial pressure	atm
Q	Charge	Coulombs
		/ mol
R	Universal gas constant	J/mol K
r	Reaction rate	mol/cm ² s
RH	Average relative humidity	
RH_{ci}	Relative humidity of the reactants flow	
	into the cathode side	
R	Resistance in the cell	Ω
S	Entropy	J/g K
Sh_f	Sherwood number	3/5 11
T	Temperature	K
_	•	
t _{ee}	Dry membrane thickness	cm
	Reference temperature	K
V	Voltage	V
W_{-1}		J/mol
Y	Pt percentage	%
Gree	ek letters	
α	Exchange coefficient	
σ_{m}	Membrane proton conductivity	S cm ⁻¹
Δ	Delta	
Subs	ecripts	
act	Activation	
con	Concentration	
f	Forward	
b	Backward	
irret	T '1.1.	
_	Ohmic	
ohm oner		
oper	Operation Payorsible	
rev	Reversible	

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