Volume 5 Issue 1 (March 2025)
DOI 10.24191/jaeds.v5i1.98
eISSN 2805-5756

Journal of Applied Engineering Design & Simulation

Modelling and Simulation Analysis of a PEM Water Electrolyser for Hydrogen Production

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ABSTRACT

Hydrogen energy is a renewable energy that can substitute fossil fuels in a wide application range. One of the efforts is producing hydrogen gas using a system called a Polymer Electrolyte Membrane (PEM) Electrolyser. Several efforts have been made in designing and improving a PEM electrolyser system to achieve optimum efficiency. This paper aims to develop a computational model for analysing the performance of a PEM water electrolyser, focusing on voltage losses, hydrogen production efficiency, and system optimization. This performance can be improved by analysing the effect of electrode potential on polarisation based on electrochemical and thermodynamics concepts. A MATLAB coding simulation was used in this paper to analyse the performance using combinations of Fick's Law and Darcy's Law. The first model, Model A, specifies the number of voltage losses in a PEM electrolyser with an open-circuit voltage and the three overpotentials of activation, ohmic and diffusion. Meanwhile, the second model, Model B, is known as the number of voltage and hydrogen losses due to convection and diffusion. The performance of the PEM electrolyser can be influenced by a variety of factors. This performance assessment focuses on the following relative humidity on the anode side, pressure and temperature. The results showed that Model B has a lower operating voltage than Model A, which only considered reversible voltage and voltage losses. The findings highlight the crucial role of anode relative humidity, where higher humidity lowers the operating voltage. Meanwhile, higher cathode pressure increases hydrogen crossover, raising the operating voltage but improving voltage efficiency. Model B accurately predicted output across various current densities, proving its reliability. This study underscores the importance of modelling in PEM electrolyser performance analysis. Future work should explore mass transport effects on hydrogen production using these models.

Keywords: PEM Electrolyser, Fick's Law, Overpotential, relative humidity, temperature, pressure.

Nomenclature (Greek symbols towards the end)

μ	Viscosity
λ	Water content of the membrane
η	Overpotential
β	Symmetry factor
β	Symmetry factor
α	Charge transfer coefficient
z	Stoichiometric coefficient of electron
z	Stoichiometric coefficient
n	Number of electron
i	Current density
R	Universal gas constant
F	Faraday's constant
Δp	Absolute pressure
σ_m	Membrane conductivity
δ_m	Thickness of the membrane
α_c	Charge transfer coefficients for cathode
α_a	Charge transfer coefficients for anode
i_o	Exchange current density

Received on 09.03.2025
Accepted on 27.03.2025
Published on 30.03.2025

R_{ion}	Ioniv resistivity (Ωm)
R_{elec}	Electronic resistivity (Ωm)
D_w	Diffusion coefficient
$C_{H_2O,mem}^{cat}$	Concentration of water at the cathode
$C_{H_2O,mem}^{an}$	Concentration of water at the anode

Abbreviations

PEM	Polymer electrolyte membrane
MATLAB	Matrix laboratory
DC	Direct current

1.0 INTRODUCTION

Renewable technology is being used more extensively around the world. Natural sources of renewable energy may be the ultimate resolution in combating climate change. The long-term decline of fossil fuels has resulted in the introduction of a clean ‘Green Energy' system based on hydrogen, which has been regarded as a potential fuel since the 1970’s [1]. Hydrogen is a highly reactive gas that is able to augment fossil fuels in broad applications, from cars to factories to homes, and its energy produces no carbon emissions.

In recent years, Proton Exchange Membrane (PEM) fuel cells have gained attention as an efficient and clean energy conversion technology, particularly in transportation and stationary power applications [2]. However, the operation of PEM fuel cells requires a continuous supply of high-purity hydrogen gas, further emphasizing the importance of efficient and sustainable hydrogen production methods such as water electrolysis.

Although hydrogen is not readily available in our environment, it can be generated through water electrolysis method which splits water molecules into hydrogen and oxygen [3]. Through this dissociation of water molecules, hydrogen is stored, while oxygen is directly released into the environment. As carbon is not involved in the electrolysis process, it is referred to as a renewable energy source [4].

Water electrolysis technologies can be classified into four types: polymer electrolyte membrane electrolysers, alkaline electrolysers, solid oxide electrolysers and anion-exchange membrane electrolysers [5]. The Polymer Electrolyte Membrane (PEM) electrolyser is a form of water electrolysis technology that has piqued the interest of the present researchers. PEM electrolyser is one of the water electrolysis methods used to produce hydrogen on a wide scale so that it can be processed and used in the future [6]. The PEM electrolyser device uses electricity to initiate the water-splitting process. These systems operate on similar principles, with two compartments called anode and cathode. Electrodes and electrolytes are present in each compartment. For the chemical reaction to take place, an electric current is applied from a DC power supply. The current flowing through the PEM electrolyser device creates a potential difference, which breaks the water molecule and ultimately builds an overvoltage. Due to the potential difference between the anode and the cathode, a gas crossover occurs. The system's output would be affected by the occurrences of overvoltage and gas crossover.

To enhance the efficiency and performance of PEM water electrolysers, researchers have employed modelling and simulation analysis to gain deeper insights into system behaviour and optimization strategies. Various computational models, including electrochemical, thermal, and fluid dynamics models, have been developed to analyse key parameters such as current density, temperature distribution, membrane hydration, and gas crossover effects [7]. Computational Fluid Dynamics (CFD) simulations have been widely used to study the impact of flow field designs and electrode configurations on hydrogen production efficiency. Moreover, multiphysics models integrating electrochemical kinetics and transport phenomena have been implemented to predict performance under different operating conditions [8]. These modelling efforts allow researchers to identify critical performance limitations, optimize system components, and propose advanced control strategies to enhance hydrogen yield and overall system durability. By leveraging modelling and simulation, PEM electrolysers can be systematically improved, contributing to the large-scale deployment of green hydrogen production technologies [9].

This study aims to develop a computational model for analysing the performance of a PEM water electrolyser, focusing on voltage losses, hydrogen production efficiency, and system optimization. The research specifically seeks to: (i) investigate the effects of key operating parameters, such as temperature, pressure, and relative humidity, on the electrolyser’s performance; (ii) develop a mathematical model to simulate the electrochemical behaviour of the system, integrating concepts such as overpotential losses and gas crossover; and (iii) validate the computational model against existing experimental data to assess its accuracy and applicability for real-world hydrogen production scenarios. Through this work, the study contributes to the advancement of green hydrogen technology, supporting its integration into renewable energy systems.

1.1. PEM Electrolyser principle

Anode and cathode are the two compartments that make up a PEM electrolyser. These two compartments are divided by a polymer membrane, with an electrocatalyst in each compartment. All components are sandwiched together to form a compact PEM electrolyser, as shown in Figure 1.

At the start of the electrolysis process, water is pumped into the anode side. Once the power supply's current is applied, the water molecule receives enough energy to dissociate into hydrogen ions and oxygen gas. Then, the hydrogen ions diffuse from the anode to the cathode compartment while the oxygen gas escapes into the atmosphere. The polymer membrane's high conductivity allows hydrogen ions to diffuse to the cathode side and combine with electrons to create hydrogen gas. Next, the hydrogen gas is stored. The electrochemical reactions of this particular process are described by the following equations:

$$Anode: H_2O \rightarrow 2H^+ + 0.5O_2 + 2e^- \tag{1}$$

$$Cathode: 2H^+ + 2e^- \rightarrow H_2 \tag{2}$$

$$Overall: 2H_2O \rightarrow 2H_2 + O_2 \tag{3}$$

Some amount of energy is required to initiate the occurrence of the dissociation of water, and the minimum amount of potential under a reversible condition is about 1.23V. This process is called reversible voltage, $V_{rev.}$

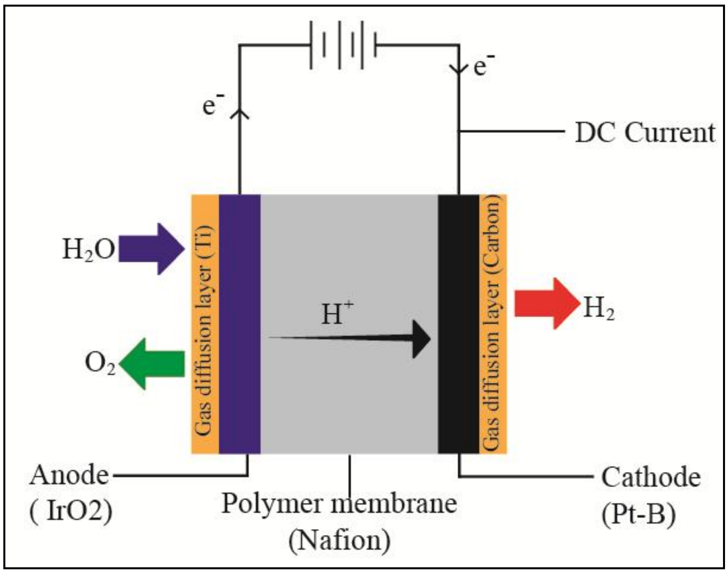

Figure 1. Polymer Electrolyte Membrane (PEM) electrolyser

2.0 METHODOLOGY

2.1 Mathematical modeling

A coding simulation is applied using MATLAB software to determine the cell performance of the PEM electrolyser. By using MATLAB software, the trends are illustrated in two-dimensional polarisation. The simulation analysis of the PEM electrolyser is performed in MATLAB using mathematical modelling. In PEM electrolyser, the different voltage losses in the operating cell voltage, also known as Model A, are calculated based on Equation (4):

$$V_{cell} = V_{rev} + \eta_{act} + \eta_{ohm} + \eta_{diff} \tag{4}$$

where V_{rev} is reversible voltage, η_{act} is activation overpotential, η_{ohm} is ohmic overpotential and η_{diff} is diffusion overpotential.

Activation overpotential

In this study, the activation overpotential is the difference between the reversible quantities of the electric current needed for the occurrence of the water-splitting process. This energy is required to initiate the movement of the electrons. The activation overpotential is calculated using the Butler-Volmer equation:

$$i = i_0 \left[e^{\alpha_1 (\frac{F}{RT}) \Delta\eta_{act}} - e^{-\alpha_2 (\frac{F}{RT}) \Delta\eta_{act}} \right] \tag{5}$$

$$\eta_{act} = \frac{RT}{\alpha n F} \ln \left(\frac{i}{i_0}\right) \tag{6}$$

Ohmic overpotential

The voltage losses caused by charge transport are defined as the ohmic overpotential. In this study, the PEM electrolyser is composed of several specific components, namely a polymer membrane, a catalyst layer, a gas diffusion layer and a bipolar plate. Each of these components contributes to electrical resistance, resulting in voltage losses. Given that the ohmic voltage [10]:

$$V = iR \tag{7}$$

Therefore, the equation for the ohmic overpotential is given by:

$$\eta_{ohm} = iR_{ohm} = i(R_{elec} + R_{ionic}) \tag{8}$$

The relationship between resistance and the electrodes is given as :

$$\eta_{ohm} = \delta_m \frac{i}{\sigma_m} \tag{9}$$

where δ_m is the thickness of the membrane and σ_m is the conductivity of the electrolyte and the ionic conductivity. Given the membrane conductivity, σ_m [11] is expressed by the following equation:

$$\sigma_m = (0.005139\lambda_m - 0.003260) exp \left(1268 \left[\frac{1}{303} - \frac{1}{T}\right]\right) \tag{10}$$

The value of water content in the membrane is:

$$\lambda_m 0.048 + 17.81RH - 39.83RH^2 + 39.85RH^3 \tag{11}$$

where *RH* is relative humidity in the PEM electrolyser stack.

Diffusion overpotential

Diffusion overpotential, also known as concentration overpotential, is the number of voltage losses due to mass transport. In this study, when the electrochemical reaction occurs rapidly, the mass transport of the hydrogen flow occurs slowly. This results in a high diffusion overpotential. The amount of diffusion overpotential is determined using the Nernst equation [12]:

$$\eta_{diff} = \eta_{diff,a} + \eta_{diff,c} \tag{12}$$

$$\eta_{diff,a} = \left(\frac{RT_a}{4F} ln \frac{C_{O_2 m}}{C_{O_2 m0}}\right) \tag{13}$$

$$\eta_{diff,c} = \left(\frac{RT_c}{4F} ln \frac{C_{H_2 m}}{C_{H_2 m0}}\right) \tag{14}$$

where $C_{O_2 m0}$ and $C_{H_2 m0}$ are the oxygen and hydrogen concentrations under a reference operating conditions, respectively, while $C_{O_2 m}$ and $C_{H_2 m}$ are the oxygen and hydrogen concentrations at the membrane-electrode interface, respectively.

Hydrogen losses due to diffusion and convection

The different concentration gradient of gas dissolved between the anode and the cathode causes a diffusion mechanism for gas crossover. According to Fick's Law, the rate of gas crossover moves from a higher concentration gradient to a lower concentration gradient. As a result, the hydrogen crossover flux due to the diffusion is calculated as follows [13]:

$$N_{H_2}^{diff} = -D_{H_2} S_{H_2} \frac{\Delta p_{H_2}}{d} \qquad (15)$$

where D_{H_2} is the hydrogen diffusion coefficient, S_{H_2} is hydrogen solubility, and p Δp_{H_2} is the hydrogen differential pressure between the anode and cathode compartments. In comparison to the anode compartment, the pressure of hydrogen gas in the cathode compartment is usually higher. Part of the hydrogen gas produced at the cathode can be a significant disadvantage.

Convection is one of the mechanisms involved in PEM electrolyser mass transfer. The differential pressure gradient of hydrogen between the anode and the cathode drives convection transport, causing the hydrogen to cross the membrane. With the difference in pressure between the anode and cathode compartments, dissolved hydrogen gas is carried from the anode to the cathode. Darcy's Law is used to determine hydrogen crossover flux in a PEM electrolyser due to the convection [13].

$$N_{H_2}^{conv} = -\frac{K}{\mu} S_{H_2} p_{H_2}^{cat} \frac{\Delta p}{d} \qquad (16)$$

where K is membrane permeability, μ is viscosity, and Δp is the absolute pressure between the anode and the cathode. According to Henry's Law, the partial pressure of hydrogen gas at the cathode compartment affects the hydrogen crossover flux, which is responsible for the concentration of dissolved hydrogen. So, the equivalent of cell voltage can be expressed as Model B. Thus, Model B is written as:

$$V_{cell} = V_{rev} + \eta_{act} + \eta_{ohm} + \eta_{diff} + N_{H_2}^{diff} + N_{H_2}^{conv} \qquad (17)$$

2.2 Analysis of PEM electrolyser performance

A MATLAB programme is used to obtain polarisation by analysing the output of the PEM electrolyser. Prior to that, the reversible voltage is calculated to obtain the polarisation of a PEM electrolyser. Hydrogen partial pressure at the cathode, anode partial pressure and water partial pressure are all used as parameters.

The output graphs are cell voltage against current density to complete the polarisation of the PEM electrolyser efficiency. Two types of models, Model A (Equation 4) and Model B (Equation 16), are used to measure the cell voltage. The reversible voltage, activation overpotential, ohmic overpotential and diffusion overpotential are calculated in Model A. In Model B, the activation overpotential, ohmic overpotential, diffusion overpotential, hydrogen losses due to convection and hydrogen losses due to diffusion are considered. The output of Model A and Model B are compared, and all data are measured in 2D coding using MATLAB software. Several parameters are considered in this study to obtain the polarisations, namely the relative humidity, temperature, pressure and current density. These parameters are tabulated in Table 1.

Table 1: Parameters and operating conditions

Parameter	Unit	Symbol	Value	Reference
Temperature	°C	T	50	[14]
Anode Pressure	Bar	P,an	1	[14]
Cathode Pressure	Bar	P,cat	30	[14]
Water flow rate	l/min	$\dot{\eta}$	5.5	[14]
Exchange current density, Pt based catalyst	$A\ cm^{-2}$	$i_{0,cat}$	10^{-3}	[15]
Exchange current density, Pt-Ir based catalyst	$A\ cm^{-2}$	$i_{0,an}$	10^{-12}	[15]

3.0 RESULTS AND DISCUSSION

3.1 Mathematical modeling

The electrochemical modeling is validated by comparing the simulation model with the experimental data to estimate the characteristic values in this analysis. As a consequence, the model simulation findings are corroborated by the data provided in Table 1 from the literature. The PEM electrolyser polarisation curve of current density (A/cm^{-2}) – voltage (V) is plotted with current ranging from 0 A/cm^{-2} to 2 A/cm^{-2}. With a 178mm membrane thickness, 1 bar anode pressure and 30 bar cathode pressure, the operating temperature is set to 50°C.

Validation of Model A against Model B

Model A (Equation 4), the Nernst Equation, is used to characterise the efficiency of the PEM electrolyser, where the reversible voltage, activation overpotential, ohmic overpotential and diffusion overpotential are included, as discussed in the previous section. In Model B (Equation 16), all voltage losses and losses due to hydrogen crossover are taken into consideration, which include the reversible voltage, activation overpotential, ohmic overpotential, diffusion overpotential, hydrogen losses due to diffusion and hydrogen losses due to convection. Figure 2 shows the validation of the cell voltage in the PEM electrolyser using Model A and Model B. The effects of the cell voltage using Model A and Model B are tabulated and shown in Table 2. It can be observed that at every current density parameter, the cell voltage value of Model B decreases slightly from the cell voltage of Model A. At a specific point, when the cell voltage of Model A is 1.693 V, the corresponding voltage for Model B is 1.690 V, resulting in a percentage difference of approximately 0.18%. This is due to the effect of hydrogen crossover as the diffusion and convection are considered when evaluating the output of the PEM electrolyser. Even though the values are insignificantly small, it indicates that measuring hydrogen crossover due to the diffusion and convection can have an impact on the PEM electrolyser's operating characteristics.

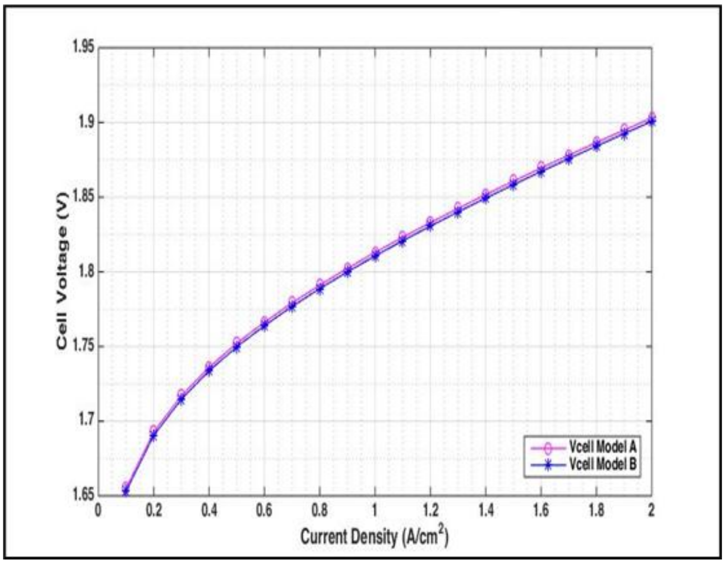

Figure 2. Validation of Cell Voltage in PEM Electrolyser using Model A and Model B

Table 2: Results of Cell Voltage using Model A and Model B

Current Density (A/cm^2)	Cell Voltage (V)	
	Model A	**Model B**
0.2	1.693	1.690
0.4	1.736	1.734
0.6	1.766	1.764
0.8	1.791	1.789
1.0	1.813	1.811
1.2	1.833	1.831
1.4	1.852	1.849
1.6	1.869	1.867
1.8	1.887	1.884
2.0	1.903	1.901

Effects of Relative Humidity on the Cell Voltage using Model A and Model B

The polarisation in the PEM electrolyser is greatly influenced by the relative humidity (RH) in the anode compartment. Figure 3 reveals that when the RH increases from 50% to 90%, the output cell voltage in both Model A and Model B decreases. Additionally, as current density increases, cell voltage also increases for all RH levels. Higher RH values lead to higher cell voltage, showing better cell performance. The results showed that when the device is completely humidified to allow ionic movements, the lower output cell voltage improves the efficiency of the PEM electrolyser.

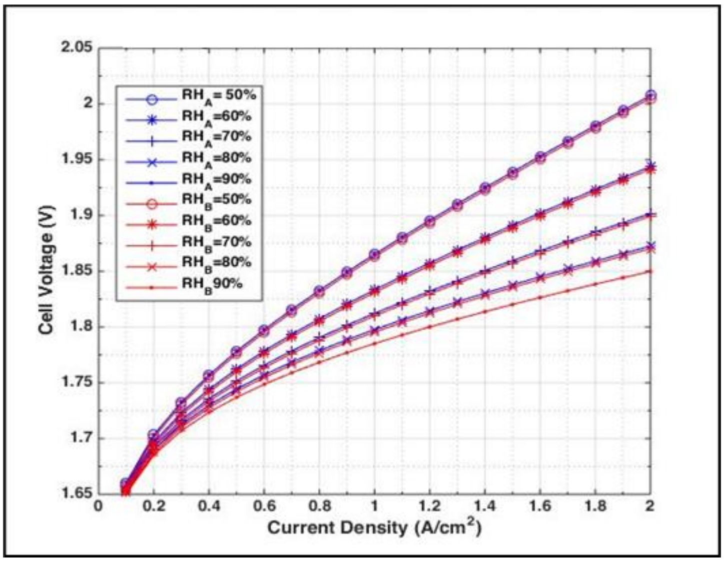

Figure 3. Effects of Relative Humidity on the Cell Voltage (V) using Model A and Model B. RH_A denotes as Effect of RH on the Cell Voltage (V) using Model A and RH_B denotes as Effect of RH on the Cell Voltage (V) using Model B

Effects of Operating Pressure on the Cell Voltage using Model A and Model B

Figure 4 indicates that the pressure at the anode is maintained at 1 bar, while the pressure at the cathode varies between 1 and 30 bar. The results showed that the cell voltage rises in tandem with the pressure at the cathode, and a higher operating pressure affects the PEM electrolyser performance. The process creates a high concentration gradient at the cathode and promotes high hydrogen crossover that affects the power demand for the operating system. Interestingly, the graph showed that Model B has lower cell voltage output as current density increases in comparison to Model A. This indicates that as the pressure at the cathode rises, the hydrogen crossover to the anode increases as well. This is due to the significant pressure gap between the anode and the cathode.

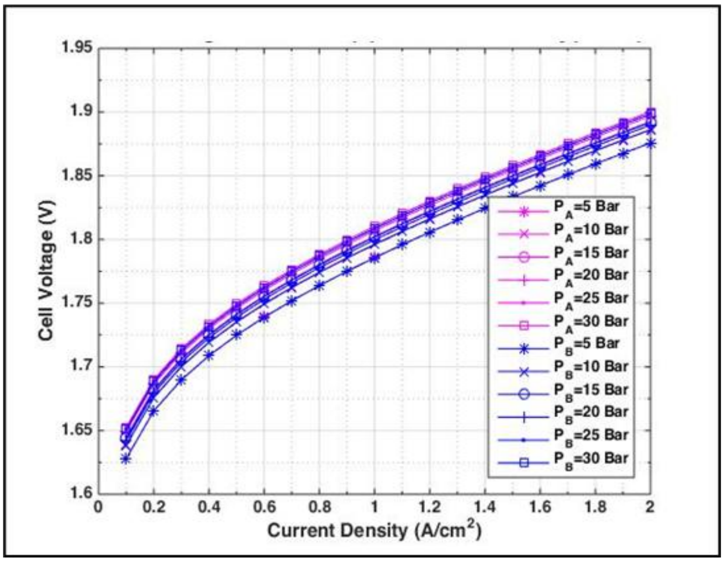

Figure 4. Effects of Operating Pressure on the Cell Voltage using Model A and Model B

Effects of Operating Temperature on the Cell Voltage using Model A and Model B

The effects of different operating temperatures on the cell voltage in both Model A and Model B are shown in Figure 5. It can be seen that higher operating temperature reduces the output cell voltage of PEM electrolyser systems. At the highest operating temperature, which is 80°C, the cell voltage in both Model A and Model B decreases eventually. In comparison, Model B exhibits a lower cell voltage of 1.85 V, while Model A achieves 1.88 V, resulting in a 1.6% difference. This variation may be attributed to the model used, which enhances cell performance.

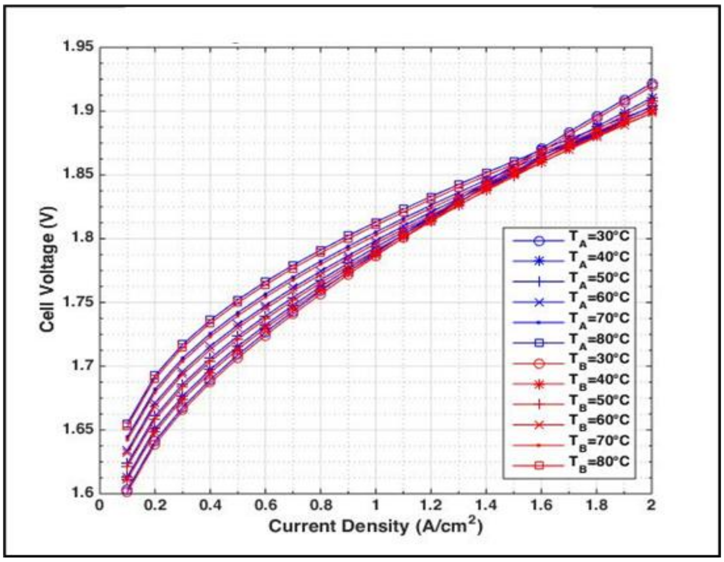

Figure 5. Effects of Temperature on the cell voltage in Model A and Model B

Effects of Relative Humidity on the voltage efficiency of PEM electrolyser

Figure 6 illustrates the effects of relative humidity of both voltage efficiency using Model A and Model B. The results showed that voltage efficiency increases as relative humidity (RH) rises. Specifically, as RH increases from 50% to 90%, the voltage efficiency improves for both models, representing an approximate 8.2% increase in voltage efficiency. This observation is suitable with the operating condition in the PEM electrolyser as water is fed into the anode of the system before the dissociation of the water process takes place. Nevertheless, in comparison, the voltage efficiency in Model B, which considers hydrogen losses due to convection and diffusion in cell voltage, showed higher efficiency than Model A.

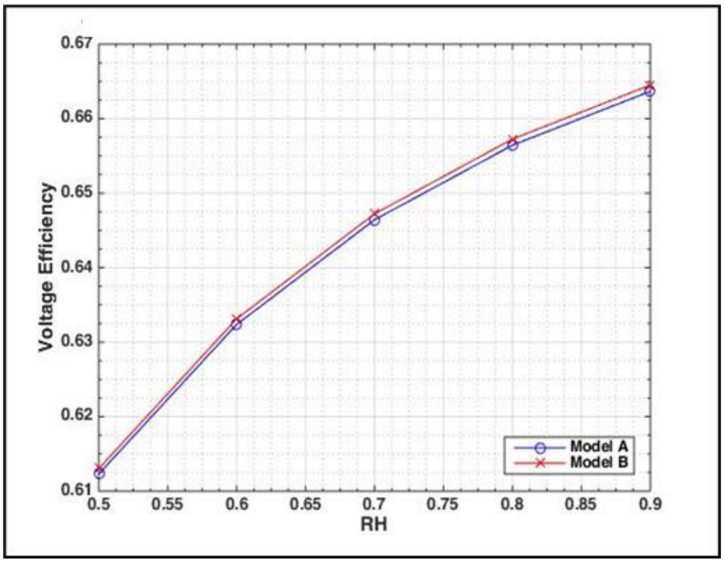

Figure 6. Effects of Relative Humidity on the Voltage Efficiency using Model A and Model B

4.0 CONCLUSION

As a conclusion, this study has successfully computed the cell voltage using Model B which includes the reversible voltage, voltage losses and the hydrogen losses due to convection and diffusion. In comparison, the results showed that Model B has a lower cell operating voltage than Model A, which only considers the reversible voltage and voltage losses. Specifically, at a given current density, Model B exhibits a cell voltage approximately 1.6% lower than Model A. An implication of the findings is that the relative humidity at the anode is very crucial as the higher the relative humidity, the lower the cell operating voltage. The results indicated that increasing RH from 50% to 90% leads to an 8.2% improvement in voltage efficiency. Meanwhile, the pressure at the cathode remains higher due to the high saturation of hydrogen compared to the anode, creating a higher hydrogen crossover rate. Consequently, the operating voltage of the PEM electrolyser also increases. The most significant finding that emerged from this study indicates that once Models A and B are validated, Model B can accurately predict the output at various current densities. The anode's relative humidity indicates that the more humidified the anode, the lower the operating voltage in both Model A and Model B. The cell voltage of the PEM electrolyser is affected by increasing cathode pressure because more hydrogen flux needs more power to work more efficiently. Therefore, this paper shows a development and significance of different models used in calculations for PEM electrolyser performance. Future work needs to be carried out using these two models to investigate the effects of mass transport on the hydrogen production in PEM electrolyser.

ACKNOWLEDGEMENT

The authors gratefully acknowledge financial support for this work from Universiti Teknologi MARA and Ministry of Higher Education (MOHE) Malaysia through Grant No. FRGS/1/2019/TK10/UITM/02/10.

AUTHORS CONTRIBUTION

Abdul Hadi Abdol Rahim: Formal analysis, Investigation, writing original draft
Suhadiyana Hanapi: Conceptualization, Methodology, writing - Review and editing
Fatin Athirah Mazlan: Formal analysis, Investigation
Raja Muhammad Aslam Raja Arif: Introduction and Literature review
Hazim Sharudin: Validation
Azizan As'arry: Conceptualization

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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