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Performance Analysis of Single Cell Alkaline Electrolyser Using Mathematical Model

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Abstract. The generation of hydrogen using electrolysis process with integrated renewable energy sources is very important specially in environmental aspects. In this paper, we demonstrate that, the performance of electrolysis process which could be enhanced by decreasing the distance between electrodes while changing the properties of electrodes. At first, two single cell alkaline electrolysers are fabricated using an in-house 3D printer. Thereafter, the best performing cell is selected by considering its performance through different experiments. Finally, the performance of the selected cell is analysed by changing the distance between electrodes and changing the properties of electrodes. Throughout this research study the SolidWorks is used as the design software while using Mathlab Simulink as a modelling tool.

1. Introduction

Today, the generation of hydrogen using electrolysis process has been identified as a very important environmentally friendly method. The renewable energy source, particularly wind, hydro and solar can be integrated to generate hydrogen from electrolysis process by making the whole system as zero emission system. Thus, it is important to enhance the performance of the electrolysis cell in order to generate hydrogen through electrolysis process.

The performance of electrolysis cell is directly proportional to the properties of electrodes and the distance between electrodes. The ohmic loss of alkaline electrolysis cell is mainly induced by the electrical resistance of the electrolytes, which can be reduced by shortening the distance between the anode and cathode. If the distance between the anode and cathode is small, it may enhance the performance of the cell. Thus, there should be an optimum distance between the anode and cathode. Hence, the main aim of this research work is to investigate the optimum parameters to enhance the performance of electrolysis cell.

The manufacturing cost of an alkaline electrolysis cell is comparatively lower than other existing electrolysis process such as Proton Exchange Membrane (PEM) and Solid Oxide Electrolysis (SOE). The working principle of an alkaline electrolysis cell is shown in Fig. 1.

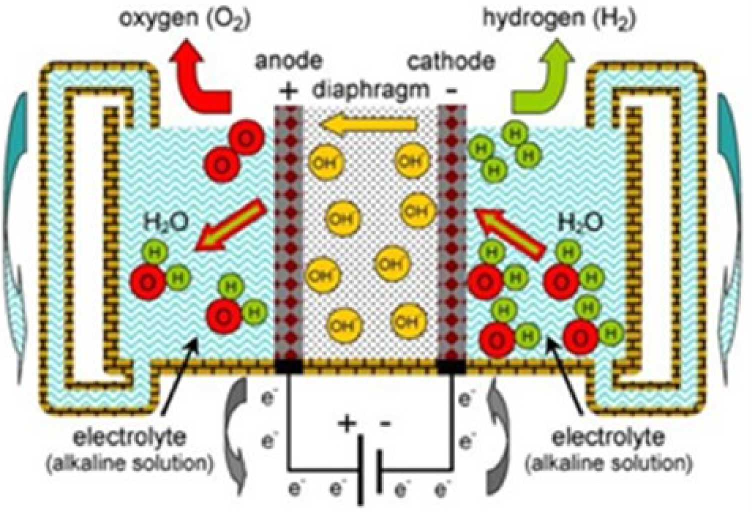

Figure 1. Working principle of single cell alkaline electrolyser [1].

The anode and cathode electrochemical reactions of alkaline electrolyser are illustrated as follows [2],

$$\text{Cathode:} \quad 2H_2O + 2e^- \rightarrow 2OH^- + H_2\uparrow \tag{1}$$

$$\text{Anode:} \quad 2OH^- \rightarrow H_2O + 2e^- + \frac{1}{2}O_2\uparrow \tag{2}$$

$$\text{Total:} \quad 2H_2O \rightarrow H_2 + \frac{1}{2}O_2\uparrow + H_2O \tag{3}$$

The generated hydrogen from the above-mentioned reactions do not require further rectifications since it has a purity level in between 95.5% - 99.9998% [3]. Furthermore, the electrical conductivity value of the feeding water should be below 5µS/cm in order to make sure the purity level of feeding water [4].

Some research studies are presented in the literature on alkaline electrolysers regarding design, modelling and different base materials which are used to enhance the performance of the cell. The different kind of electrolysis processes are integrated with renewable energy sources particularly wind, hydro and solar in Ref [5 – 9] to observe the performance of the system. In Ref [10-12], the static and dynamic model of alkaline electrolysis stacks are explained. Prior to that, the performance of electrolysis process can be enhanced by introducing new materials for electrolysis cell [13, 14]. In Ref [15], the ohmic resistance of alkaline electrolysis cell has been minimized through effective cell design. The zero-gap alkaline electrolysis cell design for renewable energy storage as hydrogen gas is discussed in Ref [16] in detail.

In this paper, we describe the design considerations of complete high-performance finite gap single cell alkaline electrolyser using 3D printed plastic housing since 3D printing technology is able to reduce the manufacturing cost of electrolysis cell by reducing costs for the post machining [17]. At the beginning of this study, two designs of electrolysis cells were fabricated and examined the respective performance, particularly the electrolysis power and efficiency of the cell were examined to select the best performing cell. Prior to that, the purity level and the flow rate of product gas were measured to compare the performance of fabricated cells. Thereafter, the performance of selected cell was enhanced through several experiments by changing the properties of electrodes and varying the distance between electrodes to reduce the ohmic loss of the cell. Throughout this research work, the Solidworks and MATHLAB/SIMULINK were used as design software and modelling tool respectively.

2. Methodology

In this research work, the main task can be classified into two groups as design and modelling of the cell, depending on the components and validation of the observed results as shown in Fig 2.

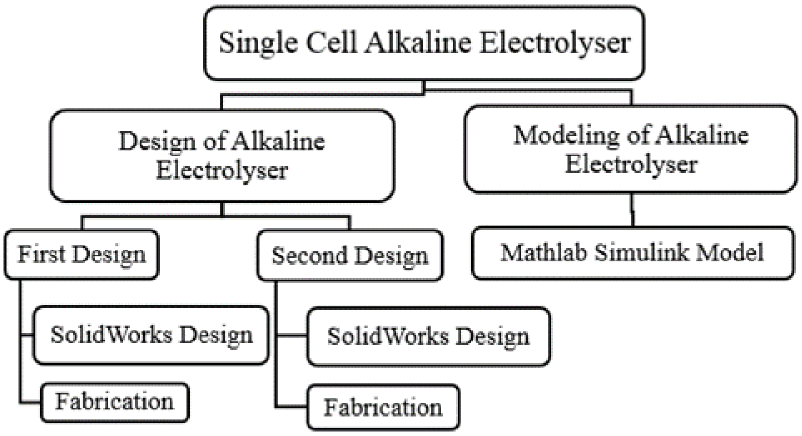

Figure 2. Classification of the design and model

SolidWorks software was used in the design part, to design base plates and the intermediate base plate. Thereafter, the lab-based 3D printer (Project type) was used to create a 3D print of designed cells. The printer is based on fused deposition modelling (FDM) 3D printing technology [18] and utilized a resin that is cured to form a dense plastic part. While fabricating the alkaline electrolyser, a sandwiching of all the inside parts occurs in between the base plates to implement the cell as shown in Fig. 3. At last, the observed results were validated by considering the results of mathematical model which was developed by MATLAB/SIMULINK modelling packages.

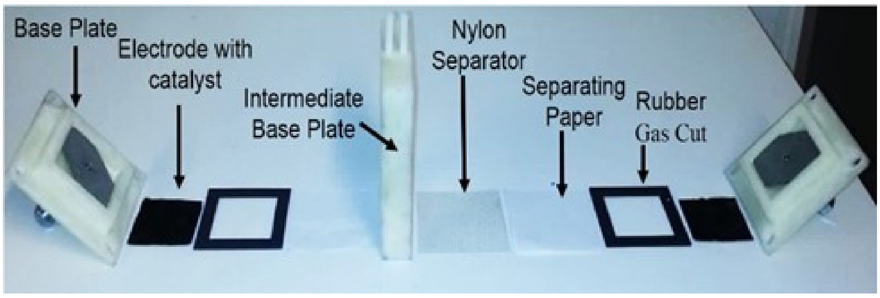

Figure 3. Basic parts of alkaline electrolysis cell

3. Design and fabrication of electrolysis cell

In this research study, two electrolysis cells were designed, and their performance was examined to identify the most suitable design. Figure 4 shows the first design of electrolysis cell and several experiments have been implemented by using first design to examine the performance of the cell. During the experiment with first design, it was observed that the product gasses contain some amount of water vapor by reducing the purity level of product gas. Thus, in order to enhance the purity level of product gas by eliminating this problem, the intermediate storage tank was designed on the intermediate base plate as shown in Figure 5 (second design). That storage tank was able to condense water vapor while increasing the purity level of product gas and the performance of the cell as well. Hence the second design was selected as the best performing electrolysis cell throughout this research study. Figure 6 shows the comparison of performance of the first design and the second design with the mathematical model.

When considering the first and second design, they are almost same in dimensions. Nevertheless, the only difference between first and second design is the intermediate storage tank which is mounted on the middle base plate in the second design.

Once the design process is over, the fabrication process of single cell alkaline electrolyser was started to obtain the required results. All the component parts of the single cell alkaline electrolyser are illustrated in Fig. 3.

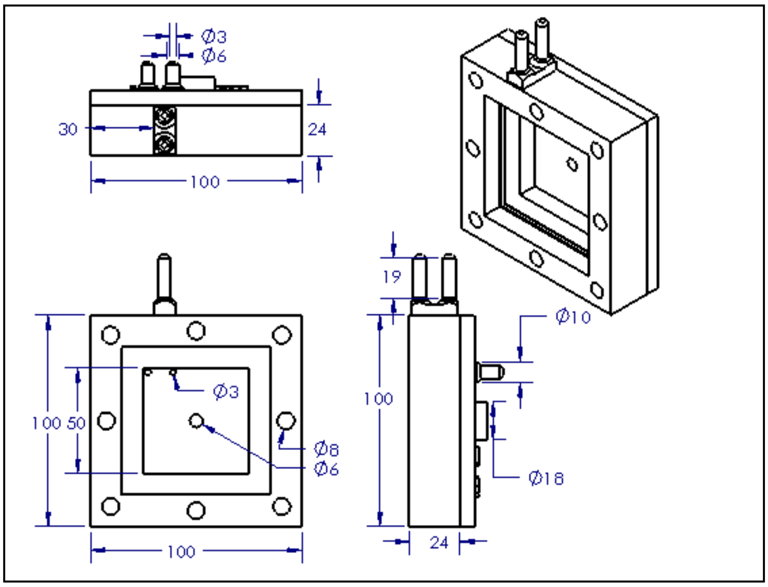

Figure 4. Detailed drawing of first design

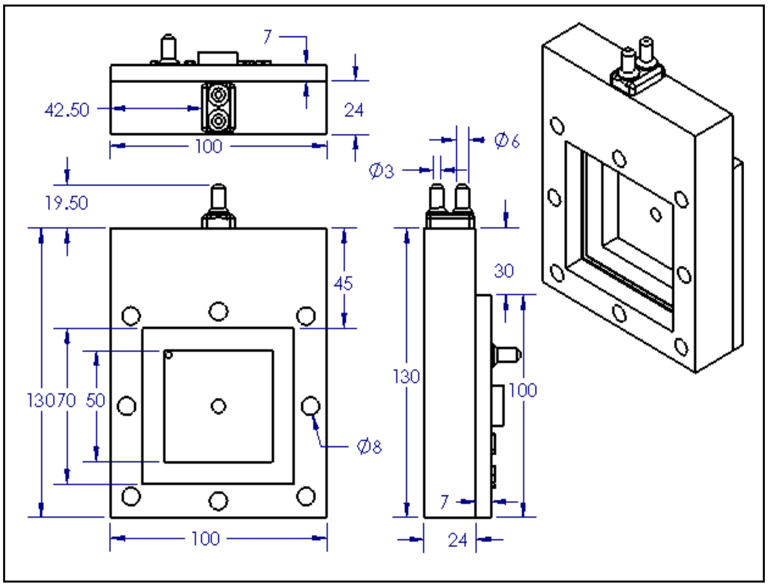

Figure 5. Detailed drawing of second design

According to the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) of the electrolysis process, nickel and its alloy can be used as electrodes of the cell [19], [20]. Thereafter the electrocatalyst was applied to electrodes in order to enhance the efficiency of the electrolysis process by reducing the activation energy for the electrochemical reaction. Furthermore, the catalyst layer consists of a Nafion® perfluorinated solution, 10% platinum on activated charcoal and methanol. The separating diaphragm (separating papers and nylon separator) separates the anode and cathode from each other.

The nylon mesh makes sure that there is no short circuit affects inside the cell. At last, to increase mechanical sealing inside the cell, the rubber was used as a gasket material.

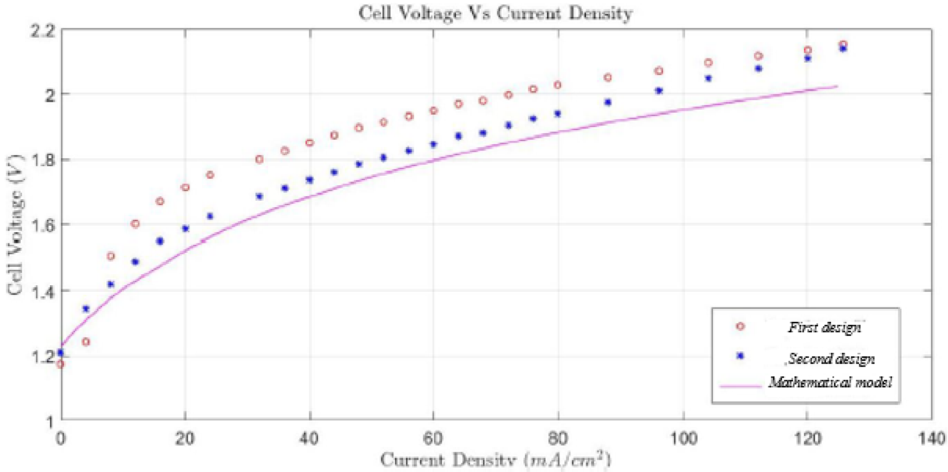

Figure 6. Performance comparison of first and second design with mathematical model

4. Modelling of electrolysis cell

The mathematical model of alkaline electrolysis cell is developed in MATHLAB/SIMULINK environment considering electrochemical equations. Figure 7 shows the V-I characteristic curve (Polarization Curve) of the typical alkaline electrolysis cell where the cell voltage is enhanced by some primary sources that caused to reduce the efficiency of the cell [21]. Hence, the cell voltage is a function of the overvoltages and reversible voltage as defined in (4).

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

Where, V_{rev} = reversible cell voltage, V_{act} = activation overvoltage, V_{ohm} = ohmic losses, V_{con} = concentration overvoltage.

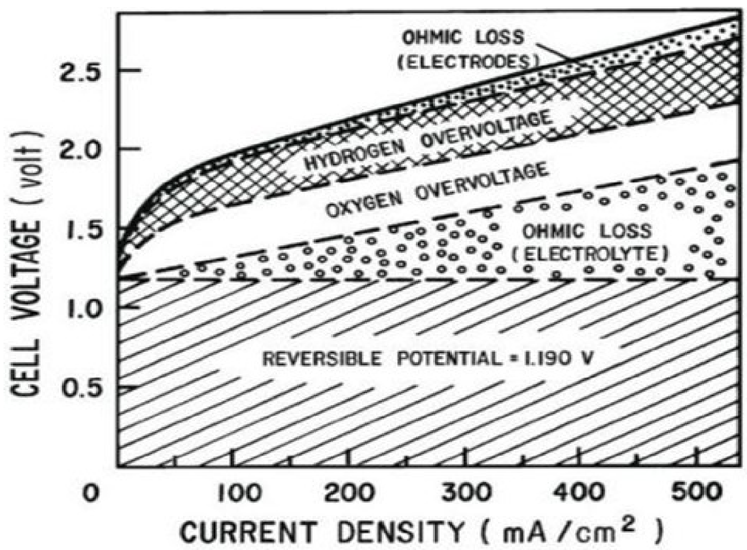

Figure 7. V-I Characteristic curve of typical electrolysis cell [22]

The V_{rev} can be calculated using the Gibbs equation as illustrated in (5) [23].

$$\Delta G = zFV_{rev} \tag{5}$$

Where, ΔG is Gibbs energy (237.2 kJ mol−1) [20] and F is Faraday's Constant (96485 C mol−1) [23]. The analytical value of z equals to 2. Moreover, the V_{act} can be defined by following expression in (6).

$$V_{act} = s\log\left\{\frac{t_1 + \frac{t_2}{T} + \frac{t_3}{T}}{A} I + 1\right\} \tag{6}$$

Where s, t_1, t_2, t_3 are the coefficients for overvoltage on electrodes, I is the current density, T is the temperature of the cell and A is the electrode area respectively [23], [24].

The electrical resistance of the electrolytes causes to generate the ohmic loss (V_{ohm}) which mitigate the performance of the cell by a considerable amount. However, for the optimum anode and cathode distance, the electrolysis cell is able to reduce the ohmic loss by increasing the cell performance. This overvoltage can be determined as in (7) [21].

$$V_{ohm} = \frac{r_1 + r_2 T}{A} I \tag{7}$$

Where r_1, r_2 = ohmic resistance parameters [23], [24]. The V_{con} is neglected in this modelling part since it has extremely low value compared to the V_{act} and V_{ohm}. Hence, the equation (4) can be rewritten as in (8).

$$V_{cell} = V_{rev} + V_{act} + V_{ohm} \tag{8}$$

4.1. Simulation background

Table 1 illustrates the relevant parameters including units which is used in this mathematical modelling study. Reference [23] and [24] are explained in the modelling part of electrolysis cell and most of the data available in the table are taken from that research article.

Table 1. Details of constants for mathematical modelling

Name of Constants	Symbols	Units	Value
Reversible Voltage	V_{rev}	V	1.229
Area of Electrode	A	cm^2	0.25
Faraday's Constant	F	$Cmol^{-1}$	96485
Number of Electrons	Z		2
Coefficient for overvoltage on electrodes	s	V	0.185
	t_1	$A^{-1}m^2$	1.002
Coefficient for overvoltage on electrodes	t_2	$A^{-1}m^{2\,0}C$	8.424
	t_3	$A^{-1}m^{2\,0}C$	247.3
Parameter related to ohmic resistance of electrolyte	r_1	Ωm^2	$8.05e^{-5}$
	r_2	$\Omega m^{2\,0}C^{-1}$	$-2.5e^{--7}$

4.2. Mathematical model of electrolysis cell

A developed mathematical model in MATLAB/SIMULINK environment, is illustrated in Figure 8. The operating temperature (T) and area of the cell (A) are selected as inputs during this modelling study.

The V-I characteristic and P-I characteristic of alkaline electrolyser obtained by mathematical model are shown in Figure 9 and Figure 10 respectively. Furthermore, the cell voltage and overvoltage characteristics are illustrated in Figure 11.

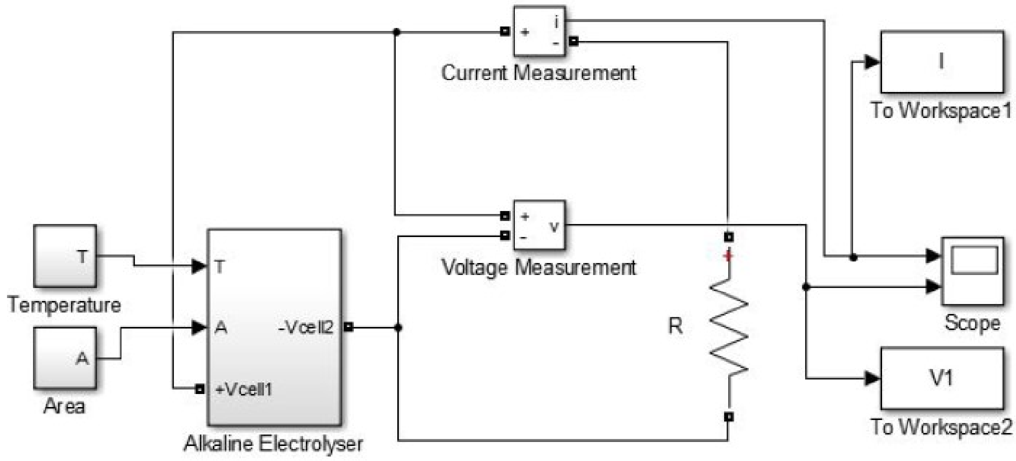

Figure 8. Mathematical model of alkaline electrolysis cell in MATLAB/SIMULINK

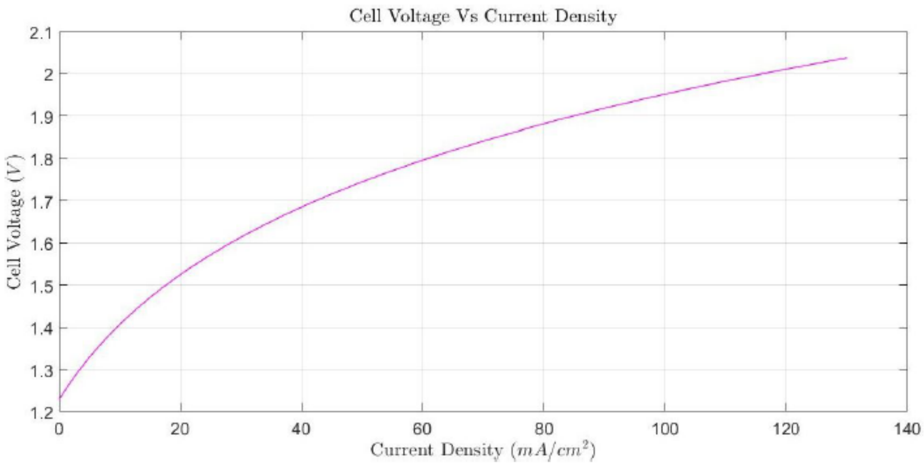

Figure 9. V-I characteristic of alkaline electrolysis cell

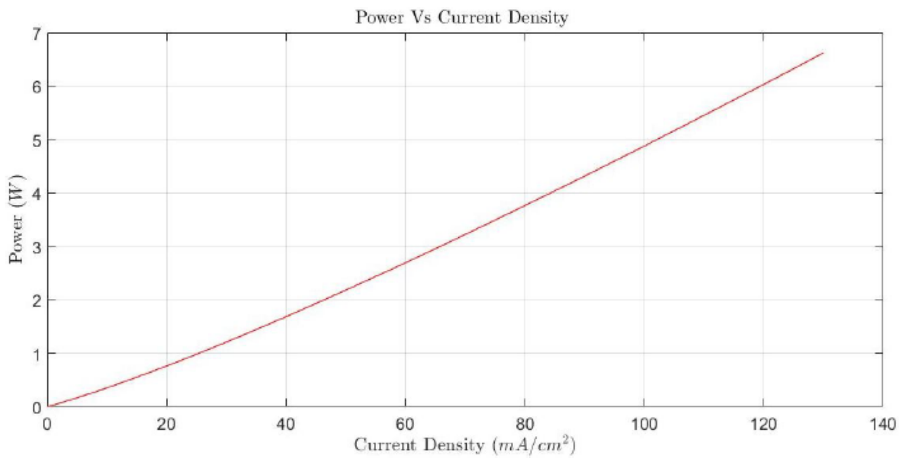

Figure 10. P-I characteristic of alkaline electrolysis cell

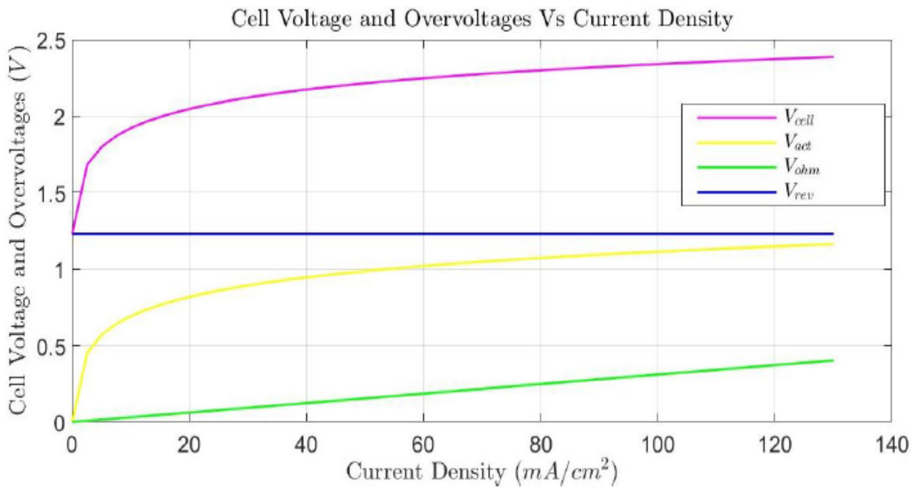

Figure 11. Cell voltage and overvoltages of alkaline electrolysis cell

5. Experiments and results

Different experiments have been done in order to enhance the performance of single cell alkaline electrolyser by changing the properties of Membrane Electrode Assembly (MEA) and electrode distance of the cell.

5.1. Experiment I: Effect of Distance Between Electrodes

The distance between electrodes of electrolysis cell is a critical fact to make deviation of the electrolysis performance, particularly power and efficiency. The performance of electrolysis cell could be increased by keeping optimum distance between the anode and cathode while reducing the ohmic loss inside the cell.

In order to investigate the effect of electrode distance for electrolysis process, three experiments were implemented while varying the distance between electrodes as 2.5mm, 1.9mm and 1.3 mm respectively. Figure 12 shows the bench setup of the Experiment I. The V-I characteristic curves of each experiment were drawn with the mathematical model by considering experimental data to examine the performance of the cell as shown in Figure 13. According to the observation of this experiment, 1.3 mm thick electrode assembly was exhibited better performance compared with other two experiments.

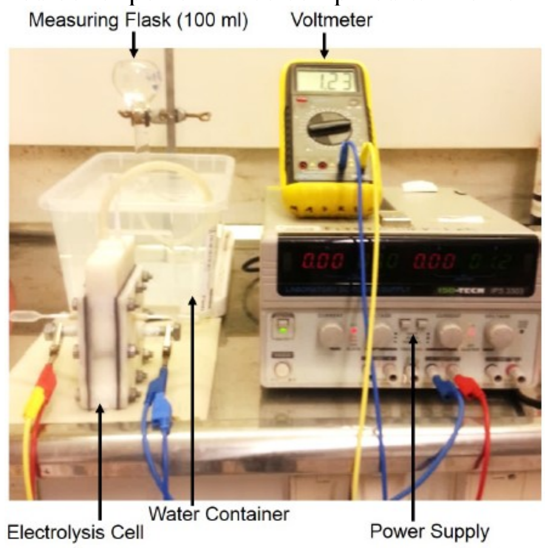

Figure 12. Bench setup of the Experiment I

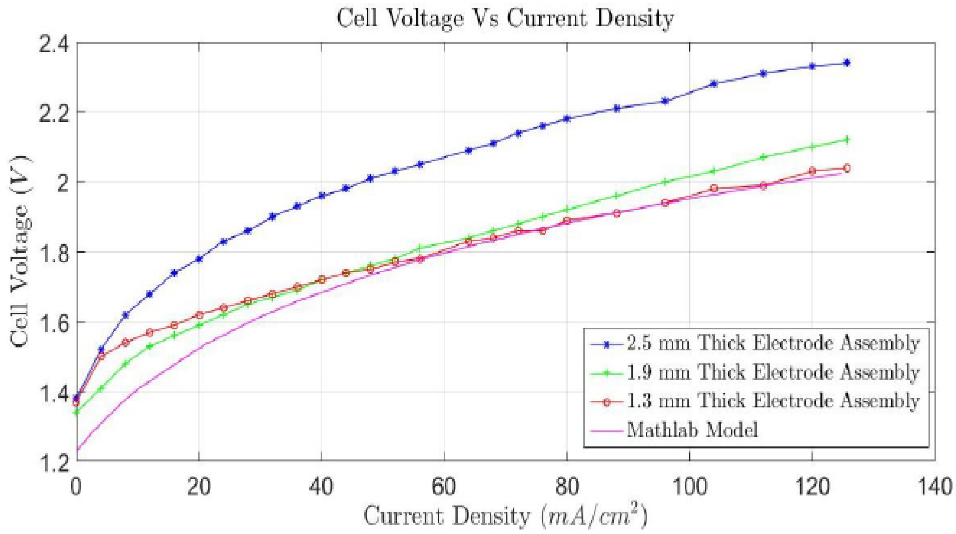

Figure 13. Comparison of the Experiments (Electrode gap 2.5mm, 1.9 mm, 1.3mm) with the mathematical model

5.2. Experiment II: Electrolysis Cell with Fine Nylon Mesh

In this experiment, one nylon mesh and two filter papers were adopted as separating diaphragm and, the same procedure was continued to observe required data by keeping the gap between electrodes as 1.3 mm. Table 2 and 3 shows the observed data and calculated parameters for Experiment II.

Table 2. Flow rate calculation data of the Experiment II

Produced Gases	Cell Current (A)	Voltage of Cell (V)	Time (s)
Hydrogen $(H_2(g))$	2.5	2	334
	3.1	2.05	254
Oxygen $(O_2(g))$	2.5	2	613
	3.14	2.05	551

Table 3. Calculated parameters of the Experiment II

Flow rate calculation		Power and efficiency calculation	
Variable	Value	Variable	Value
Current of the cell (A)	3.1	Voltage of cell (V)	2.05
n_{H_2} (mol/min)	9.6388 x 10^{-4}	P_{Total} (W)	6.355
n_{O_2} (mol/min)	4.8194 x 10^{-4}	R_{Ohmic} (Ω)	0.2
$V_{H_2}(g)$ (Theo)(cm^3/min)	23.71	P_{Ohmic} (W)	1.922
$V_{O_2}(g)$ (Theo)(cm^3/min)	11.86	$P_{electrolysis}$ (W)	4.433
$V_{H_2}(g)$ (Exp)(cm^3/min)	23.62	$\eta_{electrolysis}$ (%)	69.8
$V_{O_2}(g)$ (Exp)(cm^3/min)	10.89	η_{energy} (%)	72.2

5.3. Experiment III: Effect from the Thickness of Electrodes

In this experiment, the thickness of the electrodes was enhanced by adding porous nickel plates to MEA. Same bench setup was deployed as in Experiment 1 and observe the required data for efficiency and power calculations. The performance comparison was done through the V-I characteristic curve which is generated from a mathematical model.

Table 4. Flow rate calculation data of the Experiment III

Produced Gases	Cell Current (A)	Voltage of Cell (V)	Time (s)
Hydrogen ($H_2(g)$)	2.5	2.03	301
	3.14	2.1	260
Oxygen ($O_2(g)$)	2.5	2.06	672
	3.14	2.1	554

Table 5. Calculated parameters of the Experiment III

Flow rate calculation		Power and efficiency calculation	
Variable	Value	Variable	Value
Current of the cell (A)	3.14	Voltage of cell (V)	2.1
n_{H_2} (mol/min)	9.7632 x 10^{-4}	P_{Total} (W)	6.594
n_{o_2} (mol/min)	4.8816 x 10^{-4}	R_{Ohmic} (Ω)	0.207
$V_{H_2}(g)$ (Theo)(cm^3/min)	24.017	P_{Ohmic} (W)	2.0433
$V_{O_2}(g)$ (Theo)(cm^3/min)	12.008	$P_{electrolysis}$ (W)	4.5507
$V_{H_2}(g)$ (Exp)(cm^3/min)	23.077	$\eta_{electrolysis}$ (%)	69.01
$V_{O_2}(g)$ (Exp)(cm^3/min)	10.83	η_{energy} (%)	70.5

5.4. Experiment IV: Electrodes with Porous Stainless-Steel Plates

To reduce the ohmic overvoltage, electrodes of the cell were replaced by porous stainless-steel plates and the relevant data was observed as in previous experiments by keeping the electrode gap as 1.3 mm. The observed data and calculated parameters are illustrated in Table 6 and 7 respectively.

Table 6. Flow rate calculation data of the Experiment IV

Produced Gases	Cell Current (A)	Voltage of Cell (V)	Time (s)
Hydrogen ($H_2(g)$)	2.5	1.98	300
	3.1	2.04	250
Oxygen ($O_2(g)$)	2.5	1.98	588
	3.14	2.04	505

Table 7. Calculated parameters of the Experiment IV

Flow rate calculation		Power and efficiency calculation	
Variable	Value	Variable	Value
Current of the cell (A)	3.14	Voltage of cell (V)	2.05
n_{H_2} (mol/min)	9.7632 x 10^{-4}	P_{Total} (W)	6.4056
n_{o_2} (mol/min)	4.8816 x 10^{-4}	R_{Ohmic} (Ω)	0.194
$V_{H_2}(g)$ (Theo)(cm^3/min)	23.017	P_{Ohmic} (W)	1.914
$V_{O_2}(g)$ (Theo)(cm^3/min)	12.01	$P_{electrolysis}$ (W)	4.4921
$V_{H_2}(g)$ (Exp)(cm^3/min)	24	$\eta_{electrolysis}$ (%)	70.13
$V_{O_2}(g)$ (Exp)(cm^3/min)	11.88	η_{energy} (%)	72.5

Figure 14 is illustrated combinations of V-I characteristic curves of the Experiments II, III and IV with the mathematical model as a comparison of particular experiments.

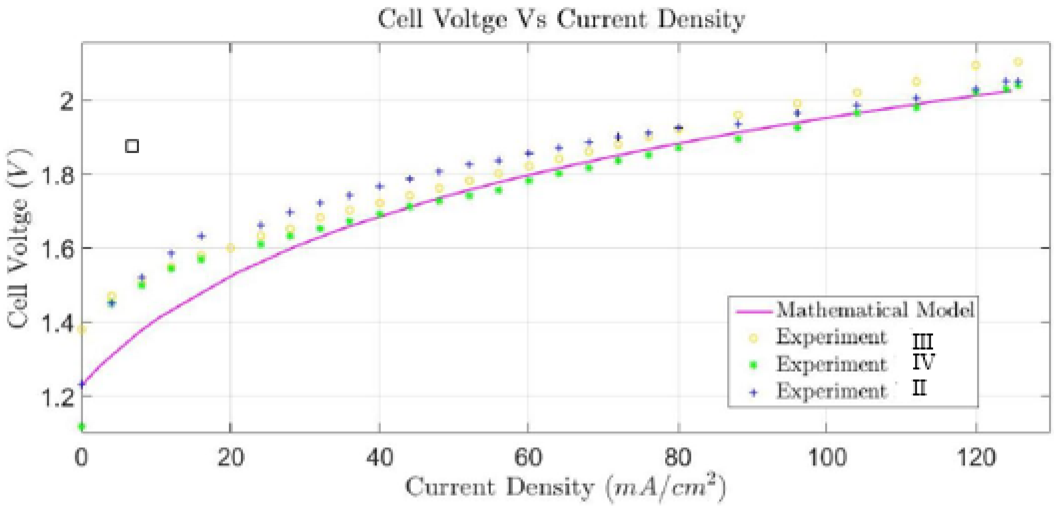

Figure 14. Comparison of the Experiments II, III, IV with the mathematical model

5.5. Experiment V: Electrolysis Cell with Polymeric Membrane Separator

In this experiment Nafion 115 and Nafion 117 polymeric membranes were deployed as a separating diaphragm respectively. According to the observed data, the Nafion 115 was given a good performance compared to the Nafion 117. Nevertheless, the performance of both polymeric membranes is much lower than when compared with other experiments. The performance comparison of both polymeric membranes with a mathematical model is shown in Figure 15.

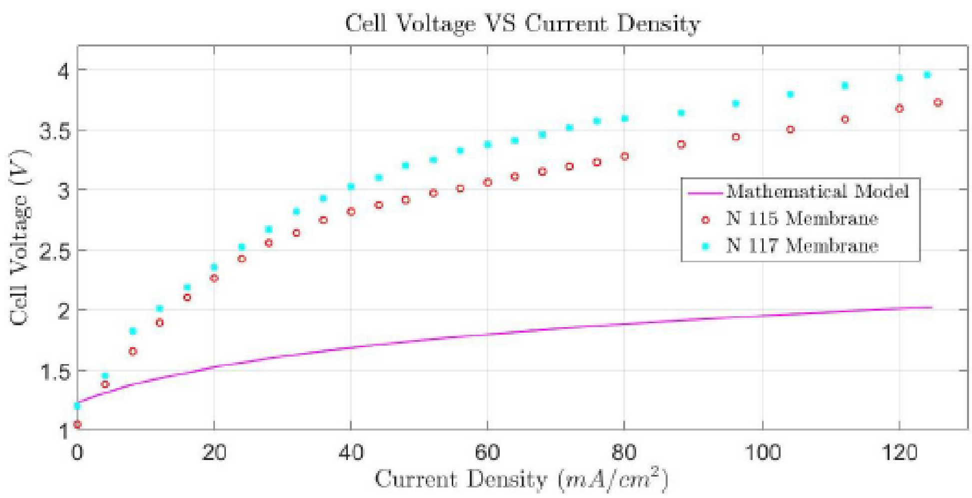

Figure 15. Performance comparison of both polymeric membranes with the mathematical model

6. Conclusion

In this research study, we have enhanced the performance of the electrolysis process by decreasing the distance between the anode and cathode while changing the properties of electrodes. The main aim of this research was to investigate the optimum parameters to enhance the performance of electrolysis cell using mathematical model. Thus, two designs of single cell alkaline electrolysis cell were deployed, and second design was selected as the best performing cell after considering their performance separately. The Experiment IV is selected as the best performing cell among five Experiments after considering the performance comparison graph with the mathematical model. In that experiment the distance between porous electrodes was set to 1.3 mm to reduce the ohmic overvoltage inside the cell by increasing the efficiency and power. According to the observation of Experiment IV, the practical values of hydrogen gas flow rate, oxygen gas flow rate and electrolysis efficiency are calculated as 24 cm3/min, 11.88 cm3/min and 70.13% respectively. The nafion is an acid and react with alkaline solution by reducing the lifetime of the cell. Nevertheless, the life expectancy of the cell is obviously adequate for experimental purposes. In the future, we intend to develop a zero-gap electrolysis cell with different catalyst layers to reduce the ohmic loss furthermore and to integrate optical sensing technology to observe the optimum distance between electrodes quite accurately. During this research study the SolidWorks and MATLAB/Simulink were used as design and modelling tools respectively. As a whole, it is obvious that by shortening the distance between the anode and cathode, the performance of electrolysis cell can be enhanced by a considerable amount in terms of electrolysis efficiency and power.

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