Design of Direct Coupling Advanced Alkaline Electrolysis and Fuel Cells System

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ABSTRACT

Proton exchange membrane fuel cell (PEMFC) is regarded as the most competitive candidate to replace the traditional forms of power conversion because of its prominent characters. Hydrogen is used as a fuel in the fuel cells and it can be produced by water splitting process or known as electrolysis. A green system containing an integrated system of photovoltaic panels, a water electrolyzer, and fuel cell is presented. Therefore, a validated model for design and optimization of direct coupling advanced alkaline electrolysis and PEMFC system (DCS) is introduced. The focus of this work is to study the performance of the direct coupling system (DCS). So several parameters (such as the voltage of the system, the hydrogen and water flow rates production from the system) concerning the (DCS) are studied. The simulations result show that, the voltage of alkaline electrolysis is higher than the fuel cell. The water management process in the whole system is considered satisfactory as a result of the lack of quantity losses. Thus, the electrolysis cell does not need to inject more water; only the water generated from the fuel cell and is injected to electrolysis.

Keywords: (PEMFC) fuel cells; Alkaline electrolysis; parameters performance of full system.

1. Introduction

Continued use of hydrocarbon fuels for generating heat and power has caused environmental problems such as air pollution and global climate change. In this regard, fuel cells are attracting much research attention these days as promising alternative power sources. Fuel cells generate electricity by direct electrochemical combination of hydrogen and oxygen. Fuel cells have higher efficiencies and less environmental impacts compared to the conventional heat engines. Currently, fuel cells are researched in various applications such as portable electronic devices, automotive power sources, and distributed heat and power generations. A polymer electrolyte membrane fuel cell (PEMFC) is one of the most advanced fuel cell technologies. PEMFCs can operate at relatively low temperatures below 100 C due to the high ionic conductivities of polymer membranes electrolytes (PEMs) [1].
Hydrogen is used as a fuel in the fuel cells, but is not freely available in nature. As a result, hydrogen is produced from fossil fuels or water. Please note that, one of the useful renewable energy technology used these days is the production of hydrogen from water electrolysis or known as electrolysis system. Water splitting process requires electricity to flow through electrode and water in order to break their molecule into hydrogen and oxygen. During the past decade, several methods have been utilized to harvest the hydrogen. However, the only state-of-the-art technique is the advanced water electrolysis. The application of hydrogen as fuel had been made practical since water electrolysis is a mature and commercially available technology

which is widely being used for generating hydrogen capacities ranging from few cm^3/min to thousands m^3/h [2].

Research and development of fuel cell systems for various applications has increased dramatically in recent years. In this paper, thermodynamic model for design and optimization of direct coupling advanced alkaline electrolysis and PEMFC system (DCS) is presented. Therefore, the performances of the DCS are evaluated using numerical model that are built in Engineering Equations solver software. So several parameters concerning the DCS such as the current density and temperature are studied to determine their effect on hydrogen and water production rate. The aim of this work is to study the performance of the whole system (DCS).

2. Materials and Methods

The integrated power supply system contains several devices that are connected to each other, As these devices complement each other. The layout in Fig. 1 illustrates the generation path of this system, Point 1 is a renewable energy source (Wind or solar energy) that provides electricity to feed alkaline electrolysis, the electrical energy taken from this source is as required in the alkaline electrolysis. Point 2 is an alkaline electrolysis that production hydrogen gas, which is the fuel of fuel cell by direct current (DC) from point 1. Point 3 is the hydrogen gas storage cylinder, these cylinders store hydrogen gas at a particular pressure to be used as needed and at different times where renewable energy in point 1 is not available. As a result of the disadvantages of renewable energies because the interruption or not available for several days. then discharging the hydrogen gas from storage cylinders and used for electric power generation and reparation the loss of energy production. Point 4 is a PEM fuel cell that uses hydrogen gas as fuel for electric power generation and produce a water and heat by a chemical reaction.

2.1. Alkaline electrolysis

A device that splitting a water molecule to hydrogen gas (H2) and oxygen gas (O2) by passing (DC) current. The electrolysis consists two electrodes anode and cathode, electrolyte, separating diaphragm [1]. The electrodes are metal sheets on both sides of the alkaline electrolysis It is responsible for separating hydrogen and oxygen from water, these metal panels provide area for the flow of electrical charges on their surface. The metal used in the manufacture of cathode can be divided into three class: high overpotentials type (Cd, Ti, Hg, Pd etc.), middle overpotentials type (Fe, Co, Ni, Cu, Au, etc.) and low overpotentials type (Pt, Pd, etc.). Common metals for the manufacture of anode nickel (Ni), nickel-plated steels or alloys. Electrolyte is a water solution used in an electrolysis to provide good electrical conductivity, due to poor electrical conductivity of pure water, this solution contains either potassium hydroxide (KOH) or sodium hydroxide (NaOH) with a typical concentration (20-40wt%) to increase hydrogen production and production efficiency add sodium chloride (NaCl) into electrolyte solution [2]. The diaphragm works to keep the produced gases separated in each chamber, so as not to allow the mixing of produced gases that could allow for re-formation of gases or contamination for the electrolysis. The most important criteria to be considered when choosing a diaphragm is to allow the penetration of hydroxide ions and water and does not allow the penetration of gases, has a mechanical resistance to corrosion and resistance to chemical damage is undesirable which result from chemical reactions and low ohm resistance [3]. As shown in Fig.1. When (DC) current passing into electrodes of electrolysis the electrical energy splitting water molecule. The hydrogen gas bubbles are formed on the negative electrode, and the oxygen gas bubbles are formed on the positive electrode [4].

2.2. PEM fuel cell

An electrochemical device that generates electrical power by chemical reactions of hydrogen and oxygen and produces heat and pure water [5]. The fuel cell block consists of two electrodes (anode & cathode) and electrolyte layer [6]. The electrodes are on both sides of the fuel cell and the anode is the negative electrode of the fuel cell. The function of the anode to deliver electrons released from the hydrogen molecule to the electric circuit fuel cell (electric load) is also its function to provide a path for the diffusion of hydrogen gas on the surface of the catalyst, the cathode is the positive electrode of the cell. This electrode provides a stream for the diffusion of oxygen gas on the catalyst surface. Also the function of this electrode receives electrons from the electric load To combine with oxygen molecules and hydrogen ions to form water [7]. The electrolyte it is a material that allows the passage of positively charged ions which separated from the hydrogen gas to move from the anode to the cathode to unite with the oxygen to form water, the electrolyte does not allow the passage of electrons to be move to an electric load [8] As shown in Fig.1. when hydrogen gas is pumped into the fuel cell, hydrogen gas is oxidized at the anode into protons and electrons, the protons pass through the proton exchange membrane to the cathode. The electrons pass to the electric load because the proton exchange membrane is not conductive [9]

3. Theory and Calculation

The mathematical model describes the system, In terms of many variables (internal and external). The mathematical model helps predict how the system works and behaves in several ways, including the state of thermodynamics and electrochemically, and the effect of operating parameters on system performance such as changes in operating temperature and operational pressure [10].

3.1 Mathematical Expressions and Symbols

A. Alkaline electrolysis model description:

To describe the behaviour of the system mathematically, the processes that occur for the system must be described, including the electrochemical side. The following chemical reactions show the chemical process that occurs at the electrolysis [4]:

1. The general electrochemical reaction of electrolysis:

$$H_2O_{(l)} + DC\ current \rightarrow H_{2_{(g)}} + \frac{1}{2}O_{2_{(g)}} \tag{1}$$

2. Hydrogen evolution reaction (HER):

$$H_2O_{(l)} + 2e^- \rightarrow H_{2_{(g)}} + 2OH^- \tag{2}$$

3. Oxygen evolution reaction (OER):

$$2OH^- \rightarrow \frac{1}{2}O_{2_{(g)}} + H_2O + 2e^- \tag{3}$$

The reversible voltage It can be said that the maximum possible useful work of the electrolysis (reversible work) [12], and can be calculated by following formula [11]

$$V_{rev} = V_{rev}(T) + \frac{R \cdot T}{z \cdot F} \ln \frac{(P-P_{KOH})^{1.5} \cdot P_w}{P_{KOH}} \quad (4)$$

$$V_{rev}(T) = 1.5184 - 1.5421 \cdot 10^{-3} \cdot T + 9.523 \cdot 10^{-5} \cdot T \cdot \ln T + 9.84 \cdot 10^{-8} \cdot T^2 \quad (5)$$

where P_W is the vapour pressure of a purified water, P_{KOH} the vapour pressure of the electrolyte solution in the (atm) unit.

The voltage of alkaline water electrolysis cell can be expressed in the following relationship [11]:

$$V_{cell} = V_{rev} + V_{act} + V_{ohm} \quad (6)$$

Activation voltage required for the electrochemical reaction, it is also a measure of the extent of the electrode activity of the electrolysis cell [13], Can be calculated by the following formula:

$$V_{act} = 2.3026 \frac{R \cdot T}{z \cdot F \cdot \alpha_{a/c}} \log(\frac{i}{i_o}) \quad (7)$$

Where the $\alpha_{a/c}$ is the charge transfer coefficient of the electrodes and i_o the exchange current density [A/cm^2]

And ohm voltage corresponds to the ohm losses, ohm losses are produced in cell elements, such as the resistance generated by the electrodes of an electrolysis cell [2].

$$V_{ohm} = r \cdot i \quad (8)$$

$$r = \frac{\delta}{\sigma_\varepsilon} \quad (9)$$

$$\sigma_\varepsilon = \sigma_o (1-\varepsilon)^{1.5} \quad (10)$$

δ the electrolyte thickness (cm), σ_o the conductivity of KOH solution (S/cm), σ_ε the electrical conductivity in the presence of bubbles and ε the void fraction of the electrolyte.

The rate of hydrogen gas produced is related to the current (*I*) of the number of cells (n_c), Divided by Faradays constant (*F*) multiplied by the number of electrons (*z*), As shown in the following equation[1]:

$$n_{H_2} = n_f \frac{n_c I}{n_e F} \quad (11)$$

The rate of oxygen gas production and water consumption can be calculated by this relationship:

$$n_{H_2o} = n_{H_2} = 2n_{o_2} \quad (12)$$

B. PEM fuel cell model description:

One of the most important steps for understanding fuel cells is to make a mathematical model that describes cell behaviour. It is very important in the mathematical model to apply mathematical equations for the thermodynamic state of the cell for understand the mechanism of electrochemical reactions for show the performance of fuel cell [7]. The PEM fuel cell process can be expressed chemically in the following reactions [5]:

1. The general electrochemical reaction of fuel cell:

$$H_{2(g)} + \frac{1}{2} O_{2(g)} \rightarrow H_2O_{(liquid)} + Electric\ power + \quad (13)$$

2. Anode side:

$$H_2 \rightarrow 2H^+ + 2e^- \quad (14)$$

3. Cathode side:

$$\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O \quad (15)$$

The voltage in the fuel cell is divided into two parts, the first part is the reversible voltage (E) and can be predicted by thermodynamics, because this reversible volt (E) depends on Gibbs's free function of chemical reactions that are affected by the operating temperature and pressure. The other part is a several of losses, these losses reduce the cell's voltage such (Activation voltage, ohm voltage and concentration voltage) The cell voltage can be calculated by the following relationship [15]:

$$V_{cell} = E + V_{act} + V_{ohmic} + V_{conc} \quad (16)$$

It is possible to estimate the reversible voltage in a linear equation, as a function of the temperature and partial pressure of the reaction gases (P_{H_2}& P_{O_2}) [15].

$$E = 1.229 - 8.5 \cdot 10^{-4}(T_{cell} - 298.15) + 4.308 \cdot 10^{-5}(\ln(P_{H_2}) + \frac{1}{2} \cdot \ln(P_{O_2})) \quad (17)$$

$$P_{H_2} = 0.5 \cdot P_{H_2O}^{sat} \cdot [exp\left(-\frac{1.635 \cdot J}{T_{cell}{}^{1.334}}\right)\left(\frac{P_a}{P_{H_2O}^{sat}}\right) - 1] \quad (18)$$

$$P_{O_2} = P_{H_2O}^{sat}.[exp\left(-\frac{4.192 \cdot J}{T_{cell}{}^{1.334}}\right)\left(\frac{P_c}{P_{H_2O}^{sat}}\right) - 1] \quad (19)$$

$$log_{10}P_{H_2O}^{sat} = -2.18 + 2.95 \cdot 10^{-2} \cdot T_c - 9.18 \cdot 10^{-5} \cdot T_c^2 + 1.44 \cdot 10^{-7} \cdot T_c^3 \quad (20)$$

Where:

J = Current density.

$P_{a,c}$ = partial pressure of electrodes.

$P_{H_2O}^{sat}$ = Saturation pressure of water.

The activation voltage is the result of the activation losses due to resistance to the electrodes of the fuel cell and can be calculated by the following mathematical expression [15]:

$$V_{act} = -0.9514 + 3.12 \cdot 10^{-3} \cdot T_{cell} - 1.87 \cdot 10^{-4} \cdot T_{cell} \cdot \ln(I) + 7.4 \cdot 10^{-5} \cdot T_{cell} \cdot \ln(C_{O_2}) \quad (21)$$

Where C_{O_2} the concentration of oxygen gas can be found in the following equation [15]:

$$C_{O_2} = \frac{P_{O_2}}{5.08 \cdot 10^6 \cdot e^{(-\frac{498}{T_{cell}})}} \quad (22)$$

Ohm voltage represents the ohm losses that occur as a result of the resistance to transfer electrons through the electrodes and the transfer of protons through the membrane and can be expressed in the following relationship [16]:

$$V_{ohmic} = -I \cdot R_{int} \quad (23)$$

Internal cell resistance can be calculated using the following formula

$$R_{int} = 1.605 \cdot 10^{-2} - 3.5 \cdot 10^{-5} \cdot T_{cell} + 8 \cdot 10^{-5} \cdot I \quad (24)$$

The concentration voltage of the cell occurs as a result of the excess reactive concentration near the catalyst surfaces, Where B is parameter that depends on the type of fuel cell [16].

$$V_{conc} = B \cdot ln(1 - \frac{I}{I_{\lim}}) \quad (25)$$

$$POWER_{cell} = I \cdot V_{cell} \quad (26)$$

4. Results and Discussion

When the DCS system is operated at different current density values from the renewable source, note the difference values of several parameters, this affects the performance of the system.

Among these variables voltage differentials for devices which Component of the system. As shown in Fig. 2. The voltage difference of the fuel cell is clearly reduced, After the reversible voltage occurs. This decrease is result of several losses which occurs in three stages of operation such as (activation, ohmic and concentration). As for alkaline electrolysis the voltage differential increases with the increase of the current density after the occurrence of the reversible voltage. As a result of the associated voltages of the operation of the alkaline electrolysis it is an activation and ohmic voltages.

As shown in Fig. 3. Note that the activation voltage of the devices increases with increasing current density, As the activation voltage of the fuel cell decreases significantly in the operation of the cell. This voltage results from activation losses when the chemical reaction occurs at the start of operation. Because this chemical reaction needs sufficient energy to occur, the activation voltage of the electrolysis is higher than the activation voltage of the fuel cell, because alkaline electrolysis needs enough energy to reaction. The process of splitting the water molecule requires a higher voltage than the water-forming voltage.

Also among the variables that affect the system voltage is the ohmic voltage, as shown in Fig. 3. the relationship between the ohmic voltage of the system and the direct current is linear, the ohmic voltage is increase by increasing the direct current. The ohmic voltage of the fuel cell occurs as a result of the ohmic loss, because of the internal resistance of the cell, When the ions cross the electrolyte membrane and the electrical resistance of the cell components and manufacturing materials. As for the ohmic voltage of the electrolysis occurs due to electrical resistance of materials also the distance between electrodes and electrolytes.

The relationship between the flow rate of hydrogen production and current density is linear, increasing the current density of the alkaline electrolysis works to increase the voltage and therefore the flow rate of hydrogen produced increases Because the splitting process needs a lot of volt to be done. As shown in Fig. 4.

The amount of water produced from a fuel cell is the same as the amount of hydrogen consumed, That the hydrogen flowing to the cell is the holder of electrons are used in the electric load and then return to the hydrogen atom with oxygen at cathode side to form a pure water molecule. That is mean we do not need to inject a new mass flow rate of water into the alkaline electrolysis. The mass of water produced from the cell is injecting to alkaline electrolysis, that is mean will be a close cycle with mass balance, as shown in Fig. 4. In this case, we do not need to inject more water. Unlike other types of power generation systems such as steam power plant that consume water and there are losses in them, especially in the cooling water

Fig. 5. shows the current density curve and the power produced of the alkaline electrolysis and fuel cell, as the power produced from the both devices increases with increasing electrical current to reach the highest point of power produced (Peak of power) then the power decreases as a result of increased cell polarization. At current density 0.3 A/cm^2 the power of electrolysis is $W_{ele} = 0.5738\ W/cm^2$ and the power of fuel cell is $W_{F.C} = 0.2\ W/cm^2$ that's mean the efficiency of the full system is $\eta_{system} = 34.85\%$. This efficiency is considered close to the efficiency of power plants or internal combustion engines. However, this efficiency is considered clean, environmentally friendly and does not produce environmental pollutants, Also, the fuel used to produce this efficiency is renewable and does not cause continuous losses and injections of fuel quantities during the generation stages such as other systems. It is just a

reverse process between the electrolysis and the fuel cell to use fuel to generate energy and thus provide the source of fuel, which is pure water.

4.1 Figures and Tables

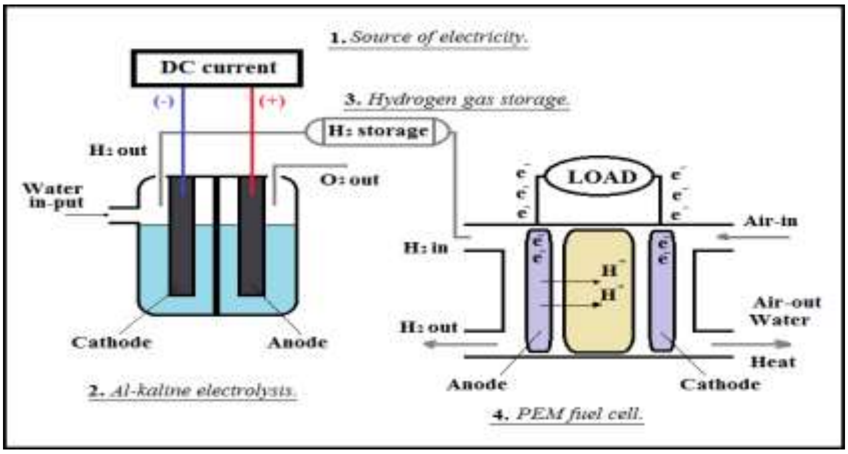

Fig. 1. Layout for DCS system.

Table 1. *Setting parameters of alkaline electrolysis.*

Constant parameter	Symbol	Value
Area of electrodes	A	50 cm^2
Faraday's constant	F	96485 C/mole
Number of cells	n_c	36
Number of electrons	z	2
Gas constant	R	8.314 J/mole·K
exchange current density	i_o	30 A/cm^2

Table 2. *Setting parameters of the PEM fuel cell.*

Constant parameter	Symbol	Value
Area of cell	A	50 cm^2
Faraday's constant	B	0.016V
Number of cells	n_c	36
Number of electrons	n_e	2
Current limit	i_{lim}	25 A

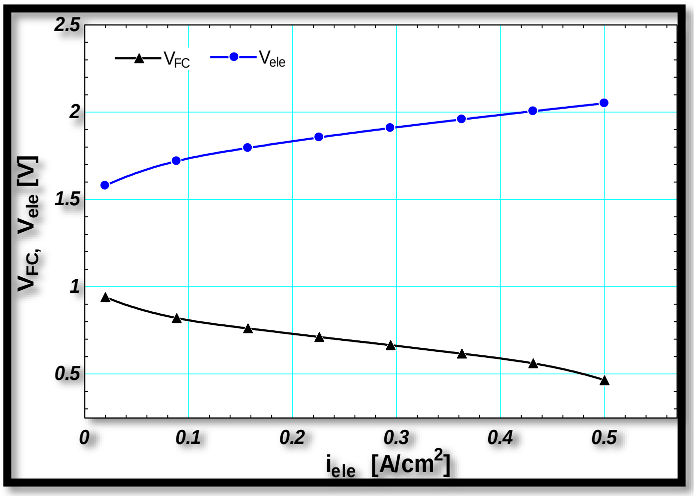

Fig. 2. The change in the voltage of alkaline electrolysis and PEM fuel cell by changing in current density.

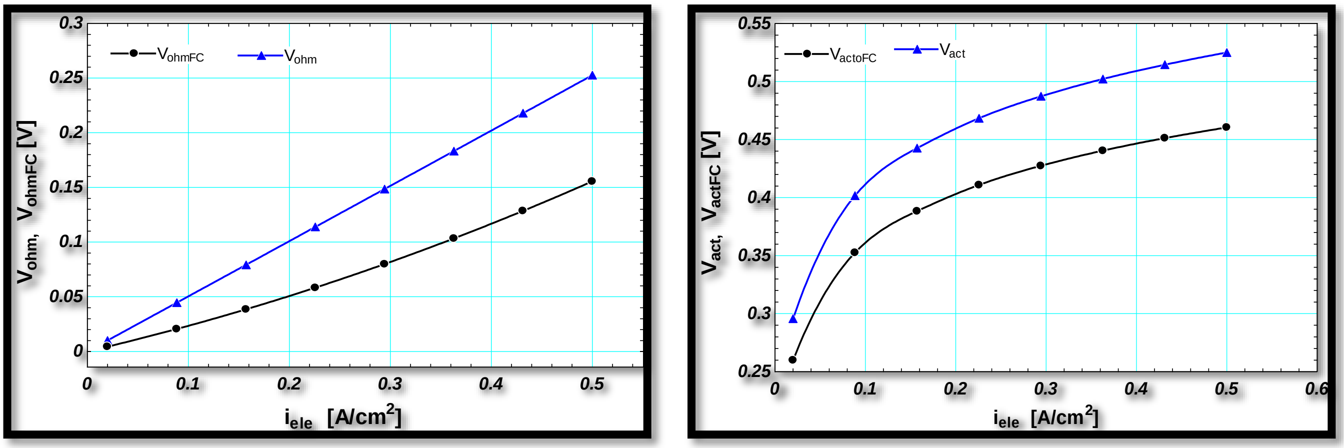

Fig. 3. The change in the activation and ohmic voltage of electrolysis and cell with change of electrolysis current.

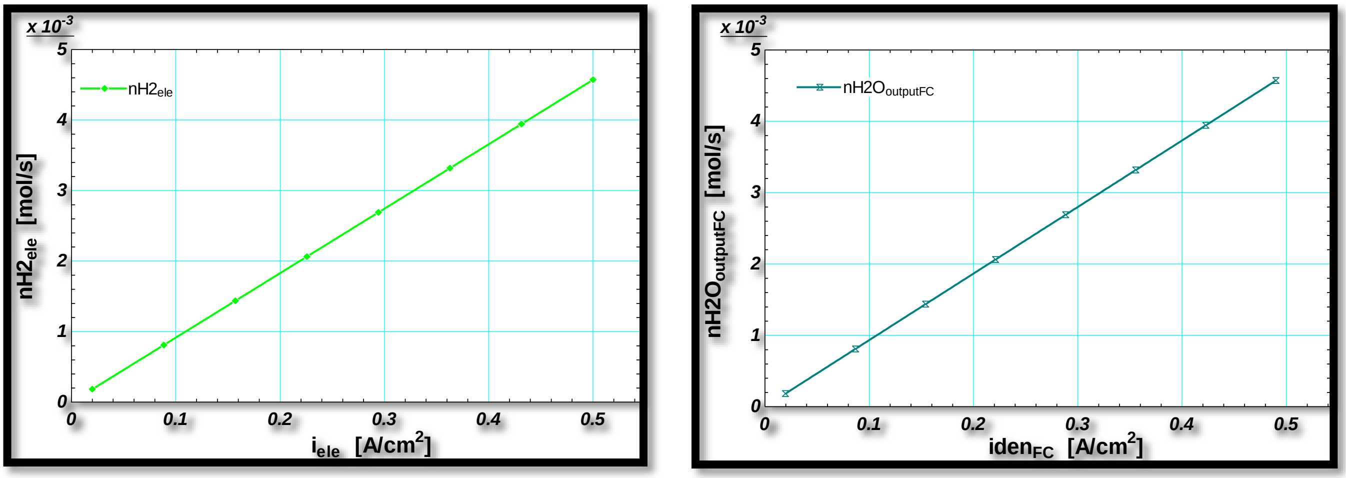

Fig. 4. The change in the Hydrogen production from the alkaline electrolysis and PEM fuel cell by changing in current density.

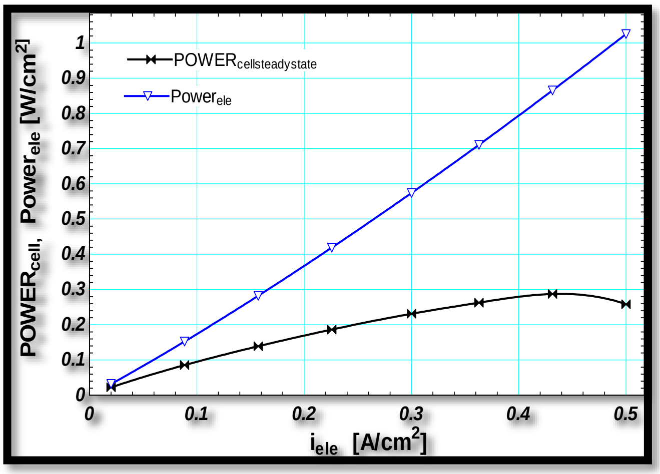

Fig. 5. The change in the power of alkaline electrolysis and PEM fuel cell by changing in current density.

5. Conclusions

Proton exchange membrane fuel cell (PEMFC) is regarded as the most competitive candidate to replace the traditional forms of power conversion because of its prominent characters than other types. This type of fuel cell depended on the pure hydrogen (H_2) as a basic fuel that's make this types cleanest than other types. The pure hydrogen can be produced by electrolysis cell from water (H_2O) using splitting process by direct current, which known as electrolyzer . In this paper, a validated model of direct coupling advanced alkaline electrolysis and PEMFC system (DCS) is presented and introduced. So the performance of the three losses (activation, concentration and ohmic), voltage and power of the system have been evaluated. The simulations result show that, the voltage of electrolysis cell is higher than fuel cell, because the splitting process needs a lot energy for split water element to two gases atom. The water flow rate production from the fuel cell it's the same flow rate which electrolysis cell using to produce hydrogen fuel that's makes the whole system in the mass balance state. This means the electrolysis cell does not need to inject more water; only the water generated from the fuel cell is injected to electrolysis. the advantages of the power generation from this system is obtained from clean and pure hydrogen.

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