

## Study to development of the passive direct ethanol fuel cell by mathematical model

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**Abstract:** Ethanol is the interested fuel because it is low toxic and has higher energy density and it can produce from biomass. Direct ethanol fuel cell (DEFC) is the alternative fuel cell that is the sustainable energy for the portable electronic device. Now it is not easy to control the level of energy because the oxidation and reduction reactions are very slow and the crossover of water and ethanol. So this research studies the performance of the direct ethanol fuel cell especially on the passive type DEFC and interests to study three mixtures of ethanol consist of ethanol mixed with tap water, ethanol mixed with drinking water and ethanol mixed with pure distilled water. Also study about the effect of fuel cell working temperature. From which the researcher conducted the experiment to analyze the optimization of the performance of the passive direct ethanol fuel cell for the portable electronic device. This research will predict a trend of electrical potential (DEFC cell voltage) when it is out of the condition of the experiment. By using a knowledge of engineering to make a mathematical model and find out the suitable condition and compare with the results of experiment and predict a trend of electrical properly.

**Keywords:** alternative; ethanol; fuel cell; mathematical model; water crossover; performance

### 1. Introduction

Fuel cell is an electrochemical device that can produce electricity continuously for as long as fuel and oxidizing agent is supplied. There are many types of fuel cells, but they all consist of an anode, a cathode and an electrolyte (Larminie and Dick,2003; Wongyao et al, 2011). As the main difference among fuel cell types is the electrolyte, fuel cells are classified by the type of electrolyte they use and by the difference in start-up time ranging from one second for proton exchange membrane fuel cell (PEMFC) to 10 minutes for solid oxide fuel cell (SOFC). The fuel cell that using hydrogen as fuel that its performance is high but need to use the purity of hydrogen and the electrodes made from platinum. So, it is rather expensive. Fuel cells are divided into two types of alcohol fuel cell that are direct methanol fuel cell (DMFC) and direct ethanol fuel cell (DEFC). Previously a lot of research focuses on the study and development of DMFC. There is downside and many other problems in reaction kinetics for the slowly oxidation of methanol fuel and across the water from one electrode to the one electrode (crossover) (Xu et al, 2011; Roelofs et al, 2011). (Matsuoka et al, 2005). Matsuoka et al [5] reported that DMFC electrodes are slowly reaction kinetics because obstruct of carbon monoxide (CO) catalyst platinum (Pt) at low temperatures and high surface quality of the catalysts for membrane. Interested ethanol fuel which

is good choice for fuel cell also address the issue of methanol fuel, also ethanol is less toxic and has higher energy density. Ethanol can produced from biological processes in agriculture which is great energy (Song et al, 2005). Ethanol is a hydrogen-rich liquid and it has a higher specific energy (8.0 kWh/kg) compared to methanol (6.1 kWh/kg). The use of ethanol would also overcome both the storage and infrastructure challenge of hydrogen for fuel cell applications.

The direct ethanol fuel cells (DEFCs) have many challenges that need to be addressed. Many improvements have been made to increase the performance of DEFCs, and there are great expectations for their potential. Concerning the different concepts of fuel delivery and handling, the DEFCs can be categorized as passive and active. Active systems need moving parts to feed oxidant and fuel to the cell requiring power to operate. This type of system supply has greater costs and lower system energy density and thus is better suited for large fuel cells. Passive systems use natural capillary forces, diffusion, convection (air breathing) and evaporation to achieve all processes without any additional power consumption. Therefore a passive system is more suitable for portable power sources (Kamarudin et al, 2009; Shimizu et al, 2004). Like the active ones, the passive systems suffer from ethanol crossover, when the cell is operated with high ethanol

concentrations. This leads to a fuel cell performance loss since ethanol diffuses through the membrane generating heat but no power (Andreadis et al , 2006; Andreadis et al, 2008). The solution is to use low ethanol concentrations on the anode side. As already mentioned, in passive systems, ethanol is delivered to the catalyst layer by a passive diffusion mechanism, so if ethanol is not supplied adequately and timely, polarization of the cell voltage may occur due to a lack of ethanol. Also, the output of a passive DEFC operating with low ethanol concentrations is not acceptable for real applications. Therefore, low ethanol crossover is essential for using high ethanol concentrations in portable power applications. Different approaches including improving and changing the fuel cell structure have been proposed in the last years for an active feed DEFC (Chu and Shul, 2012).

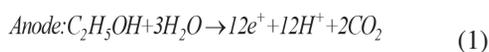
However, as the author is aware, less work on passive DEFC systems was performed. Based on that, Penyarat Saisirirat (Saisirirat, 2018) has conducted experiments to study the passive ethanol-fed fuel cells. The effect of ethanol concentration was investigated. The experimental performance testing were studied about the cell performance by measuring the cell voltage and cell current production at ambient conditions and the effect of fuel cell operating temperature change on the cell performance is also study. (Nandeha and Spinacé, 2014) have studied the effects of ethanol concentrations on the performance of the passive DEFC. The experiment is done at 80 °C with the use of Pt3Sn/C as a catalyst and use ethanol concentration between 0.1 to 2.0 mole per liter to be used in the experiment. The experiment results indicate that the power density increases when the concentration of ethanol increases. As a result of the factors of motion coexistence with diffusion. However, the effect of increasing the concentration when increased by more than 1 mole per liter also results in reduced fuel cell performance and increase the polarity of the ethanol.

Based on that, in this study, the effect of ethanol concentration on the performance of the passive DEFC for the portable electronic device was investigated. In this work that the power is limited not more than 10 watts for suitable with application to the portable electronic devices. This work conducted the experiment to analyze the performance of the passive DEFC. This research will predict a trend of electrical potential when it is out of the condition of the experiment. By using a knowledge of engineering to make a mathematical model and find out the suitable condition and compare with the results of experiment.

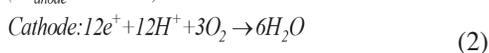
## 2. Theoretical calculation

### 2.1 Calculation of the cell voltage

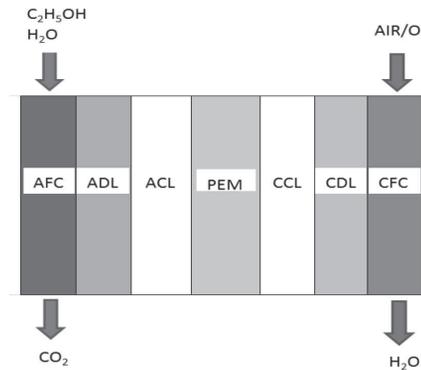
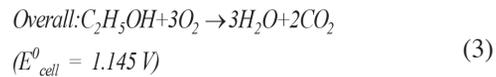
The voltage of single cell DEFC theory at feeding ethanol at 25 C° and 1 atm by the chemical reaction show as the following equation below (Abdullah and Kamarudin, 2015).



$$(E^0_{anode} = 0.084 V)$$



$$(E^0_{cathode} = 1.229 V)$$



**Fig. 1** The system of the passive DEFC

From Fig. 1. that the letters are PEM : Membrane , CDL: Cathode gas diffusion layer , ADL : Anode gas diffusion layer , CCL : Cathode catalyst layer , ACL : Anode catalyst layer , CFC : Splice plate cathode , AFC : Splice plate anode.

Calculate the voltage (V) in single cell DEFC [10] that show in Eq.(4) below

$$E_{cell} = E^0_{cell} - \eta_{conc} - \eta_{ohmic} - \eta_{act} \quad (4)$$

$E_{cell}$  = Voltage of fuel cell (V) ,  $E^0_{cell}$  = Voltage of fuel cell follow theory (V),  $\eta_{conc}$  = Concentration of voltage loss related to kinetics of reaction,  $\eta_{ohmic}$  = Resistance loss ( $\Omega$ ),  $\eta_{act}$  = Reaction of voltage loss involved to kinetics

### 2.2 Calculation of the concentration losses of the voltage related to kinetics of reaction

The move of substrate on anode and cathode catalyst layer resulting loss concentration inside cell, calculate by Eq.(5).

$$\eta_{conc} = (RT/zF) \ln(I_{lim}/(I_{lim} - i)) \quad (5)$$

Where R = Universal gas constant as 8.314 (J/g mol k) and Z = Number electrons in system. While limitation of flow electric current show following Eq. (6) [10].

$$I_{lim} = Z_a F D_b^{eff} (C_b/L_b) \quad (6)$$

Where  $D_b^{eff}$  = Spread efficiency coefficient ethanol at anode ,  $C_b$  = Concentration of ethanol at anode (molar, M) and  $L_b$  = The width of flow channel anode (mm).

### 2.3 Calculation of the resistance loss

The resistance losses are followed the equations below.

$$\eta = iR_{total} \quad (7)$$

$$R_{total} = \eta_{membr} + \eta_{contaci} \quad (8)$$

$$\eta_{membr} = (l_m / K_m^o) i \quad \eta_{contat} = (l_m + 2l_c) / K_s \quad (9)$$

**2.4 Calculation of the reaction of voltage loss involved to reaction kinetics**

Calculation of the reaction of voltage loss involved to reaction kinetics show following equations (10) and (11).

$$\eta_{act,anode} = (RT / \alpha_a z_a F) \ln(i / i_o) \quad (10)$$

$$\eta_{act,cathode} = (RT / \alpha_c z_c F) \ln(i / i_o) \quad (11)$$

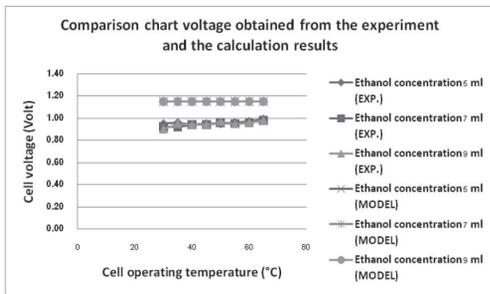
From Eq.(4) so we can calculate the voltage (V) in DEFC single cell following

$$E_{cell} = E_{cell}^0 - \eta_{conc} - \eta_{ohmic} - \eta_{act}$$

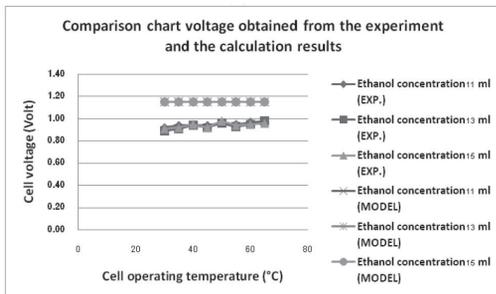
$$E_{cell} = E_{cell}^0 - ((RT / z_a F) \ln(i_{lim} / (i_{lim} - i))) - (i(l_m / K_m + l_m + 2l_c / K_s) / \alpha_a z_a F) \ln(i / i_o) + (RT / \alpha_c z_c F) \ln(i / i_o) \quad (12)$$

**3. Results and Discussion**

It is very important to evaluate the performance effects on passive DEFCs, and the present work accomplish that. In this study, the effect of ethanol concentration on the performance of the passive DEFC for the portable electronic device was investigated by experiment and compare with the results from the mathematical model. Study about the impact of ethanol volume and the impact of temperature on the DEFC voltage that the results are as follow as shown in Figs. 2- 10.

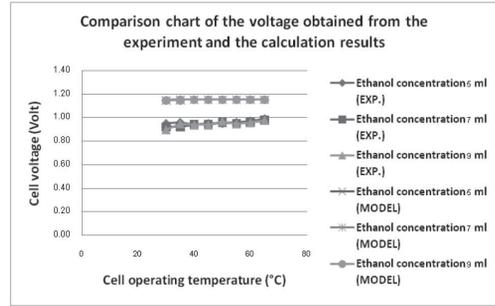


(a)

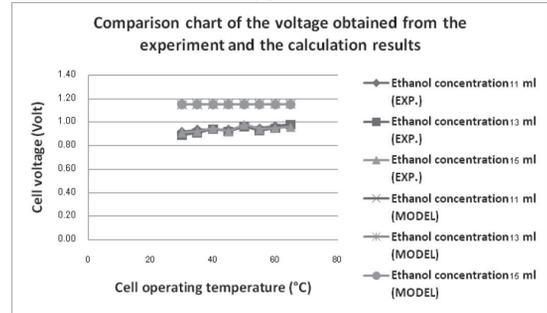


(b)

**Fig. 2** Show passive DEFC voltage results of the experiments compared with the results of the calculation at each ethanol volume mixed with 60 ml. of pure distilled water

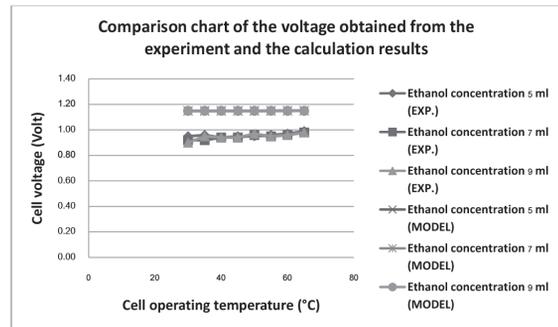


(a)

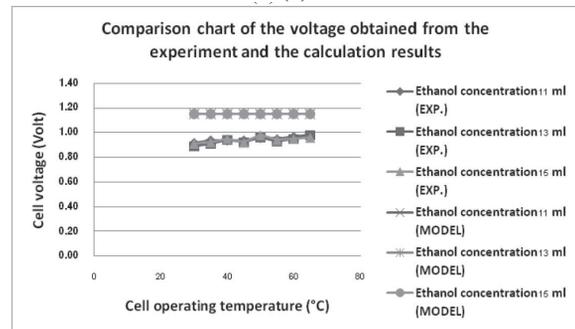


(b)

**Fig. 3** Show passive DEFC voltage results of the experiments compared with the results of the calculation at each ethanol volume mixed with 60 ml of general drinking water



(a)



(b)

**Fig. 4** Show passive DEFC voltage results of the experiments compared with the results of the calculation at each ethanol volume mixed with 60 ml of tap water

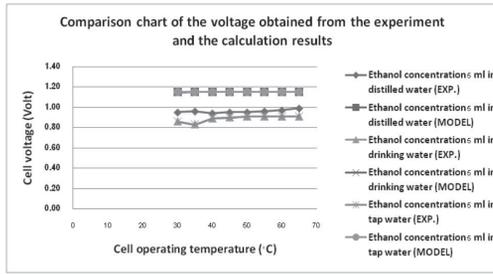


Fig. 5 Show passive DEFC voltage results of the experiments compared with the results of the calculation at 5 ml. ethanol mixed with 60 ml of all sample water

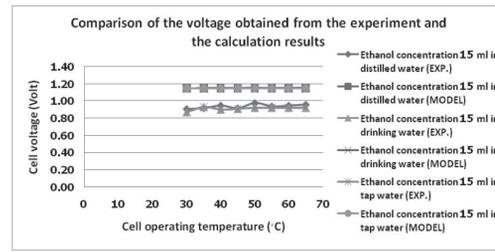


Fig. 10 Show passive DEFC voltage results of the experiments compared with the results of the calculation at 15 ml. ethanol volume mixed with 60 ml of all sample water

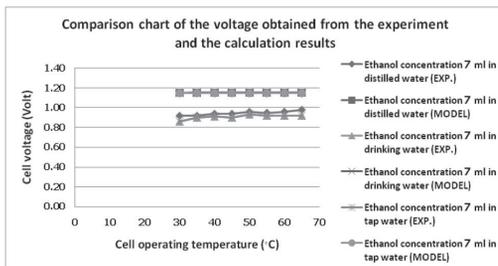


Fig. 6 Show passive DEFC voltage results of the experiments compared with the results of the calculation at 7 ml. ethanol mixed with 60 ml of all sample water

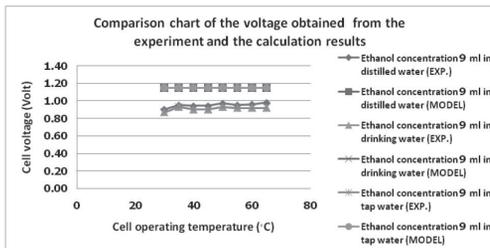


Fig. 7 Show passive DEFC voltage results of the experiments compared with the results of the calculation at 9 ml. ethanol mixed with 60 ml of all sample water

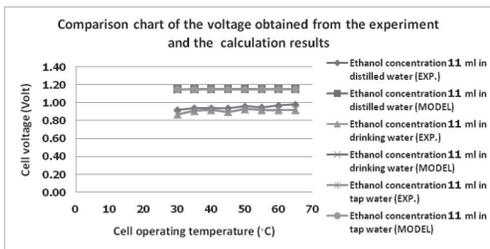


Fig. 8 Show passive DEFC voltage results of the experiments compared with the results of the calculation at 11 ml. ethanol volume mixed with 60 ml of all sample water

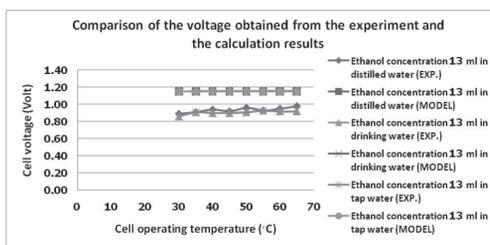


Fig. 9 Show passive DEFC voltage results of the experiments compared with the results of the calculation at 13 ml. ethanol volume mixed with 60 ml of all sample water

Consider the comparison results of the passive DEFC voltage obtained from the experiment and the calculation, it was found that when the working temperature of the passive DEFC increases so the voltage from the experiment increases. While the voltage obtained from the calculation increases as well. At the same time, when increasing the concentration of ethanol, the trend of changing the DEFC voltage obtained from the experiment continues to increase and the DEFC voltage from the calculation when increasing the ethanol concentration increase as well.

The trend of the calculated voltage of ethanol mixed with tap water increase about 0.20%. When considering the trend of the DEFC voltage from the calculation of ethanol mixed with pure distilled water increase by 0.30% and when considering the trend of the DEFC voltage from the calculation of ethanol mixed with general drinking water increase by 0.60%. The viewed from the trend of the DEFC voltage from the experiment, it is found that when increasing the concentration of ethanol 5 ml - 15 ml according to the increased temperature, the DEFC voltage increases as well. The total reaction of water from one electrode to one electrode of ethanol is minimal. So the production efficiency of the fuel cell set fully efficient. The production of electricity gradually decrease when increase the concentration of ethanol more than 13 ml. The production of the electrical charge decreases due to the combined reaction of water from one electrode to one electrode of the ethanol fuel, the production of the electrical charge of the fuel cell set is not effective.

The passive systems suffer from ethanol crossover, when the cell is operated with high ethanol concentrations. This leads to a fuel cell performance loss since ethanol diffuses through the membrane generating heat but no power. The solution is to use low ethanol concentrations on the anode side. As already mentioned, in passive systems, ethanol is delivered to the catalyst layer by a passive diffusion mechanism, so if ethanol is not supplied adequately and timely, polarization of the cell voltage may occur due to a lack of ethanol. Also, the output of a passive DEFC operating with low ethanol concentrations is not acceptable for real applications. Therefore, low ethanol crossover is essential for using high ethanol concentrations in portable power applications.

#### 4. Conclusions

This research studies the performance of the passive direct ethanol fuel cell by experiment and mathematical model and interests to study about three mixtures of ethanol

consist of ethanol mixed with tap water, ethanol mixed with drinking water and ethanol mixed with pure distilled water. Also study about the effect of fuel cell working temperature. When comparing the voltage obtained from the calculation, it is found that the higher the concentration of ethanol and the operating temperature of the fuel cell gives the cell voltage trends to increase. And from the experiment found that when increase the concentration of ethanol and temperature so the production of the cell voltage of the fuel cell varies according to the increase in ethanol concentration and temperature. By which the cell voltage trends to increase as well. By increasing the concentration of ethanol and temperature so the fuel cell set will gradually react to produce electrical cell voltage by increasing to a maximum of one point, then decreasing until all the fuel is empty. In addition, it was found that the cell voltage obtained from the calculation is greater than the value obtained from the experiment. On average about 13%, 20% and 23% in the case of ethanol fuel mixed with pure distilled water, general drinking water and tap water, respectively. However, the factors that have resulted in the calculated values are quite different from the values obtained from the experiment because the production efficiency, the electrical values of the fuel cell sets used in the experiment have limited capabilities. In addition, the factors that result from cross-polarization of water in the fuel cell set affect the measured potential difference.

## 6. Acknowledgement

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## 7. References

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