Simulation of Polymer Exchange Membrane Fuel Cell Utilizing Empty Fruit Bunch Pyrolysis using Aspen Plus

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Abstract: Indonesia has a large potential of biomass energy which can be used to increase electrification ratio of the country. One the most important biomass resources to be considered as a promising option for fossil fuel substitution and greenhouse effect reduction in the country is waste from palm oil mill plant (POM). This study analysed the possible layout and performance of an integrated biomass pyrolysis with a polymer electrolyte membrane fuel cell (PEMFC) as an alternative for energy system. The PEMFC is considered to be one of a promising conversion technology for clean and efficient power generation in the current situation. The biomass from empty fruit bunch (EFB) sent to pyrolysis unit to produce syngas which can be used as fuel for PEMFC. A Purification processes consisting of a water gas shift reactor and a selective oxidation reactor is necessary in order to reduce the impurity that can harmful fuel cell. It was found that, the PEMFC can generate electricity around 512.5 kW (AC) at 0.22 A.cm^{-2} with the system efficiency of 55.26% (HHV).

1 INTRODUCTION

Fuel cell is a device that converts chemical energy into electrical energy with high efficiency through electrochemical reaction (Guan, 2008). Fuel cell systems have different variables such as type of the electrolyte used in fuel cell, type of the reactants (e.g. primary fuels and oxidants), operating temperature and pressure, type of the exchanged ion through the electrolyte, direct and indirect usage of the primary fuels in fuel cell system. Based on the electrolyte used, fuel cells can be classified into: (1) alkaline fuel cells (AFC), (2) phosphoric acid fuel cells (PAFC), (3) polymer electrolyte membrane fuel cell (PEMFC), (4) molten carbonate fuel cells (MCFC), (5) solid oxide fuel cells (SOFC) (Peighambardoust, 2010). The polymer electrolyte membrane fuel cell (PEMFC), with electrolyte is a solid polymer in which protons are mobile, has received growing attention as an efficient power generation unit due to its low emissions, potentially high energy density, compactness, modularity, light weight, fast start-up and fast response to load changes (Chutichai, 2013; Jo, 2017). The ideal fuel for PEMFC is hydrogen which does not exist in nature and need to be produced from other sources, such as natural gas, water, and biomass. Due to the low temperature, the PEMFC operates only with hydrogen of high purity, and the concentration of carbon monoxide in the gaseous flux should not exceed 10 ppm (Authayanun, 2013).

Biomass possesses a potential source for renewable hydrogen production, and likely will give the fuel cell a sustainable future. Biomass may be divided into two groups according to its physical characteristics: (1) liquid biomass mainly from manure, agriculture and sludge from municipal wastes and (2) solid biomass mainly as forest residues

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from the forest industry (Guan, 2015). Pyrolysis is one of the most promising technologies of biomass utilization, and it is also the first stage of biomass thermochemical conversion, which converts biomass resource to solid char, liquid oil, and hydrogen-rich gas (Yang, 2006).

Palm oil has been one of the success stories of the North Sumatera Province of Indonesian agricultural sector. Following the palm oil extraction procedure, palm oil wastes are obtained as empty fruit bunch (EFB), palm kernel shell (PKS) and palm fibre. Approximately 1 ton of EFB, 0.3 ton of PKS, and 0.7 ton of palm fibre are produced as palm oil mill (POM) wastes from each ton of oil production (Nizamuddin, 2016). Annual production of palm oil in Indonesia during 2016 reached 31.40 million tons which can be used as renewable energy sources to generate electricity (BPS, 2017). This paper presents the thermodynamic analysis of PEMFC fuelled by syngas from empty fruit bunch (EFB) pyrolysis to generate electricity by using Aspen Plus simulation.

2 SYSTEM DESCRIPTION AND MODELLING SIMULATION

The system configuration used in this analysis consists of pyrolysis unit, fuel reforming unit, and PEMFC unit. The process flow diagram (PFD) of biomass pyrolysis unit is shown in Figure 1. The biomass combustion will be simulated at near atmospheric condition. The Aspen Plus block units used to simulate biomass pyrolysis process are RYield, RGibbs, and SSplit (Nur, 2018). The biomass (1BIOMASS) was sent to RYield, labeled with DECOMP, to predict the decomposition of the biomass into the reference components such as C, H_2, S, O_2, N_2, etc. The RGibbs, labelled with PYROLYS, used as pyrolysis reactor with the nitrogen as inert gas.
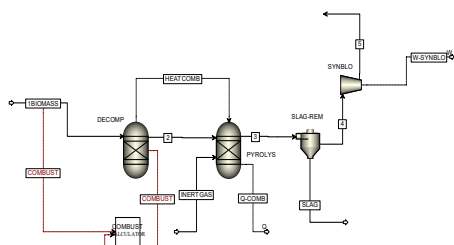

Figure 1: The process flow diagram of biomass pyrolysis unit.

The raw-syngas (stream 5) produced by pyrolysis unit will go to the fuel reforming unit which comprises syngas blower (named with BLOWE3) to increase the pressure of raw-syngas, methane steam reforming with water gas shift reactor (REFORMER), heat exchanger (HEX-02), water pump (WATER-P), and a selective oxidation reactor (SELOX). Since the raw-syngas contains high CO fraction, which will poison the PEMFC catalysts and then degrade the PEMFC performance. Therefore, the system equipped with a CO removal processes as shown in Figure 2. The CH_4 is converted to H_2, CO and CO_2, and the ratio of steam to carbon (S/C) is 3.4:1. The steam obtained by utilizing the heat energy contained in the system during the process takes place that is by using heat exchanger during the process of reducing the syngas temperature to the working temperature of PEMFC. The steam methane reaction process in the reformer reactor is followed by a CO removal process. There are two sub-steps included in the CO removal process, e.g., water shift reactor, and a selective oxidation reactor (SELOX). The involved reactions for the production of hydrogen and CO removal are shown in table 1. remember that all the papers must be in English and without orthographic errors.
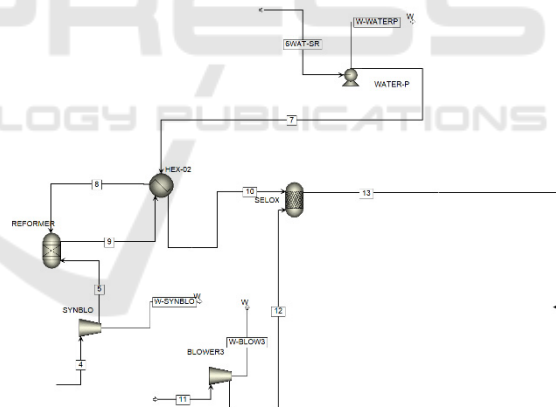

Figure 2: The process flow diagram of fuel reforming unit.

Table 1: Reactions involved in the hydrogen production process and CO removal (Guan, 2015).

Steam reforming:
$CH_4 + H_2O \leftrightarrow CO + 3H_2$ $\Delta H^o_{298} = 206$ kJ mol^{-1}
CO water shift:
$CO + H_2O \leftrightarrow CO_2 + H_2$ $\Delta H^o_{298} = -41$ kJ mol^{-1}
SELOX:
$2CO + O_2 \leftrightarrow 2CO_2$ $\Delta H^o_{298} = -283$ kJ mol^{-1}
Electrochemical:
$H_2 + 1/2O_2 \rightarrow H_2O$

Syngas that are free from contaminants (stream 13) are fed into PEMFC, undergoing electrochemical reactions while producing electrical energy and thermal energy. Syngas out of the PMFC unit goes to the burner sub unit where the remaining gases will be burned completely. The Aspen Plus flowsheet of the PEMFC unit is illustrated in Figure 3. The model is based on the following assumptions: steady state operation, pressure drops are neglected; chemical reactions such as reforming and shift reactions reach chemical equilibrium; the mobile ion cross over through the electrolyte cannot modelled within Aspen Plus, therefore the overall oxidation of H_2 was considered instead of the cell half reaction.

3 METHODOLOGY

3.1 PEMFC Stack

The output voltage of a single cell (V_{cell}) can be obtained by considering the ohmic, activation, and concentration losses from the thermodynamic equilibrium potential, V_{Nernst}, as follow (Jo, 2017):
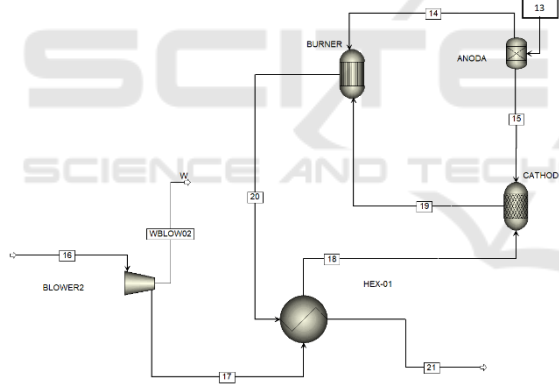

Figure 3: The process flow diagram of PEMFC unit.

$$V_{cell} = V_{Nernst} - V_{ohm} - V_{act} - V_{con} \qquad (1)$$

where V_{ohm}, V_{act}, and V_{con} represent the ohmic, activation, and concentration polarization, respectively. The Nernst Potential, V_{Nernst}, is given by (Jo, 2017):

$$V_{ohm} = i(R_{H^+} + R_{elec}) \qquad (3)$$

where the area specific resistance due to the proton transport, R_(H^+)was obtained by considering the membrane and catalyst layer properties below (Jo, 2017):

$$R_{H^+} = \frac{\delta_{mem}}{k} + \frac{0.5\,\delta_{aCL}}{v_{aCL}^{1.5}\,k} + \frac{0.5\,\delta_{cCL}}{v_{aCL}^{1.5}\,k} \qquad (4)$$

The v_{aCL} and v_{cCL} represent the volume fractions of the electrolyte in the anode and cathode catalyst layers, respectively. The number 0.5 appearing in the numerator of Eq. (4) is due to the assumption that the average proton transport path through the catalyst layer is half of its thickness.

The activation polarization is the voltage over potential required to overcome the activation energy of the electrochemical reaction on the catalytic surface. This type of losses dominates at low current density. The activation polarization, V_{act}, is calculated using the Butler-Volmer equations for hydrogen oxidation reaction in the anode ($V_{act,a}$) and oxygen reduction reaction in the cathode ($V_{act,c}$), as follows (Jo, 2017):

$$V_{act,a} = \frac{i}{i_{0,a}^{ref}} \frac{R_u T}{(\alpha_a + \alpha_c)F} \left(\frac{C_{H_2,ref}}{C_{H_2}}\right)^{1/2} \qquad (5)$$

$$|V_{act,c}| = \frac{R_u T}{\alpha_c F} \ln\left[\left(\frac{C_{O_2,ref}}{C_{O_2}}\right)^{3/4} \frac{i}{i_{0.c}^{ref}}\right] \qquad (6)$$

where C_j and α represent the molar concentration and transfer coefficient, respectively. The exchange current density of hydrogen oxidation reaction, $i_{0,a}^{ref}$, and exchange current density of oxygen reduction reaction, $i_{0.c}^{ref}$, can be calculated by (Jo, 2017; Jiao, 2010):

$$i_{0,a}^{ref}(T) = i_{0,a}^{ref}(353.15\,K).\exp\left[-1400\left(\frac{1}{T} - \frac{1}{353.15}\right)\right] \qquad (7)$$

$$i_{0,c}^{ref}(T) = i_{0,c}^{ref}(353.15\,K).\exp\left[-7900\left(\frac{1}{T} - \frac{1}{353.15}\right)\right] \qquad (8)$$

The concentration polarization, V_{con}, can be calculated by following by (Jo, 2017; Jiao, 2010):

$$V_{con} = \frac{RT}{4F} \ln\left(\frac{i_{lim}}{i_{lim}-i}\right) \qquad (9)$$

where the limiting current density, i_{lim}, determined by:

$$i_{lim} = v_{GDL}^{1.5} D_{O_2} \frac{C_{O_2}}{\delta_{GDL}} \qquad (10)$$

After calculating the voltage losses, the fuel cell power output is the product of the cell voltage and the current. The total current (I) and the direct current (DC) output power of each cell can be calculated as follows (Taufiq, 2015; Zhang, 2005):

$$I_{tot} = \frac{\left(jH_{2,equivalent}\left(\frac{mol}{h}\right)\right)\left(2\,U_f\,F\left(\frac{C}{mol}\right)\right)}{\left(\frac{3600\,s}{h}\right)} = \frac{jH_{2,equivalent}U_f}{0.018655}$$

(11)

$$W_{PEMFC-DC} = V_{cell}\, x\, I_{tot}$$

(12)

The alternating current (AC) power of the cell module can be specified using (Taufiq, 2015; Zhang, 2005):

$$W_{PEMFC-AC} = W_{PEMFC-DC}\, x\, \eta_{inv}$$

(13)

where η_{inv} is the inversion efficiency of direct to alternating current.

The performance of this system is defined by its ability to convert the chemical energy contained in biomass into electrical. The electrical efficiency of the system is defined as follow (Chutichai, 2013):

$$\eta_{System} = Net\ powered\ generated\ (kW)/m_{EFB}\, x\, HHV_{EFB}$$

(14)

3.2 Input Data

EFB were selected as the main fuel in this study because of its abundant availability in Indonesia, especially the province of North Sumatera. The feed composition of the EFB is specified as described in table 2, while the main assumptions for analysis are shown in table 3.

Table 2: Composition of EFB (Wijono, 2014).

Proximate analysis (wt.%)	
Fixed carbon	9.94
Volatile matter	42.20
Moisture content	44.60
Ash content	3.26
Ultimate analysis (wt.%)	
Ash content	3.26
Carbon	26.94
Hydrogen	3.22
Sulphur	0.05
Nitrogen	0.35
Oxygen	21.58
Heating values (MJ/kg)	
Higher heating value (HHV)	10.29

Table 3: Main operational conditions and assumptions for plant calculation.

EFB feed pyrolysis reactor (kg hr^{-1})	250
Nitrogen feed pyrolysis reactor (kg hr^{-1})	25
Pyrolysis working temperature (°C)	650
Pyrolysis working pressure (bar)	1.013
Environment temperature (°C)	25
PEMFC operating temperature (°C)	120
Anode/Cathode inlet pressure (bar)	1.20
Thickness of anode/cathode GDLs, CLs, $\delta_{GDL}, \delta_{GDL}$ (mm) (Jo, 2017)	0.35; 0.015
Thickness of anode/cathode membrane, δ_{MEM} (mm) (Jo, 2017)	0.07
Reference H_2/O_2 molar concentration, $C_{H_2,ref}/C_{O_2,ref}$ (mol/m^{3}) (Jo, 2017)	40.88
Anode/cathode transfer coefficient (Jo, 2017)	0.5; 0.65
Reference exchange current density in anode/cathode, $i_{0,a}^{ref}, i_{0,c}^{ref}$ (A/m^{2}) (Jo, 2017)	1.0×10^9; 1.0×10^4
Porosity of GDL, CL (Jo, 2017)	0.6; 0.4
Volume fraction of ionomers in CL (Jo, 2017)	0.3
Electronic conductivity in CL (S m^{-1}) (Jo, 2017)	300
DC to AC inverter efficiency (%)	95
Electric generator efficiency (%)	98.7
Miscellaneous BOP, % input HHV	13.3

4 RESULTS AND DISCUSSION

The main raw synthesis gas mass and composition leaving the pyrolysis unit (stream 4) are 264.20 kg.hr^{-1} and 13.74% H_2O, 42.92% H_2, 6.68% N_2, 0.04% S, 19.61% CO, 12.88% CO_2, 4.13% CH_4, respectively. This raw synthesis gas from the pyrolysis process is treated to reduce the quantity of CO it contains to an acceptable level for PEMFC operation. The main raw syngas composition leaving the reformer and CO removing are 21.8% H_2O, 1.4 O_2, 31.8% H_2, 24.8% N_2, 0.0143% S, 19.7% CO_2, 0.4394% CH_4. Then, this clean syngas goes to the PEMFC unit.

The performance of the PEMFC is evaluated using a polarization curve showing the relationship between current density, cell potential and power density. The cell potential decreases with increasing current density due to large voltage losses are observed at higher current density as shown in figure

4. It can be seen that the activation polarization is much higher than the other polarizations.

The maximum power density that PEMFC unit can generate in this study is around 0.829 W.cm^{-2} at current density of 1.42 A.cm^{-2} as shown in figure 5. With the total current is 502,932.72 A, the PEMFC unit can produce power of 512.5 kW (AC) at 0.22 A.cm^{-2}.

Based on the analysis, it was observed also the requirement of power during processes within the system and system electrical efficiency. Those internal power consumed are listed in table 4. The system electrical efficiency when PEMFC generate power of 512.5 kW (AC) at 0.22 A.cm^{-2} is 55.26% (HHV).
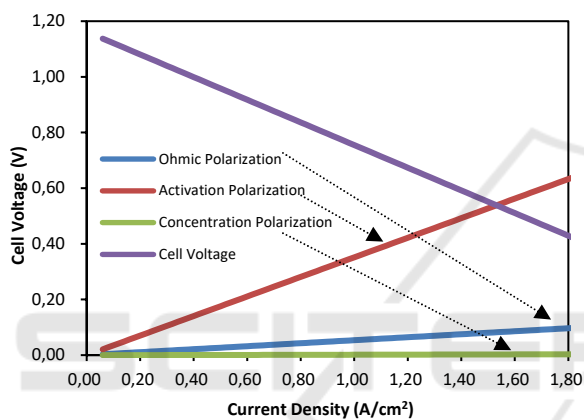

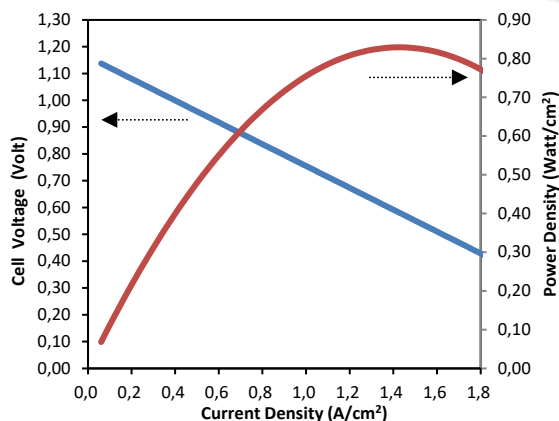Figure 4: PEMFC voltage characteristics versus current density.

Figure 5: Effect of current density of voltage and power density.

Table 4. Energy consumption during processes

Energy consumed by blower to supply air for SELOX reactor (BLOWER3)	1.72 kW
Energy consumed by syngas blower (SYNBLO)	7.04 kW
Energy consumed by air blower for cathode section (BLOWER2)	12.33 kW
Energy consumed by water pump (WATER-P)	0.0035 kW
Miscellaneous BOP	96.47 kW

5 CONCLUSIONS

In this study, the system consists of a biomass pyrolysis to produce syngas as fuel and PEMFC to generate electricity was analysed by using Aspen Plus simulation. It was found that EFB is a potential fuel for PEMFC unit. When this biomass pyrolysis unit operated at 650 °C and atmospheric pressure, it can produce raw syngas which composition of H_2 is 42.92%. Based on the analysis, the PEMFC can generate electricity around 512.5 kW (AC) at 0.22 A.cm^{-2} while the system efficiency can reach up to 55.26% (HHV). More details calculation doing modelling simulation and experimental are needed to improve this analysis.

ACKNOWLEDGEMENTS

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