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Single stage dimethyl ether plant model based on gasification of palm empty fruit bunch

R Heryadi[1*], A S Uyun[1], E Yandri[1,2], S M Nur[1,2], K Abdullah[2]

[1] Graduate School of Renewable Energy, Darma Persada University, Jalan Taman
Malaka Selatan, Pondok Kelapa, Jakarta 13450, Indonesia
[2] Center of Renewable Energy Studies, Darma Persada University, Jalan Taman
Malaka Selatan, Pondok Kelapa, Jakarta 13450, Indonesia

[*]E-mail: rudy.heryadi@live.com

Abstract. Biomass from empty fruit bunch (EFB) is considered as potential renewable energy
sources to be developed in Indonesia. EFB can be efficiently converted into valuable and useful
fuel products through gasification. Gasification is a process of biomass conversion into syngas.
Syngas is a raw material for most other chemical products, such as Methanol, Ammonia, and
DME. One of the biomasses that has big potential to be utilized is palm EFB waste. Research
about DME synthesis from various biomass has been done, though little research about DME
production based on EFB gasification. The aim of this research is to simulate single stage DME
Plant Model based on gasification of EFB by assuming that the gasification reaction and DME
synthesis reaction are under equilibrium condition. Method encompasses step to perform
simulation of the model and DME plant design. The model predicts yield of DME product in
agreement with published real DME plant operation. The result shows flow rate of DME
produced is 50% of EFB feed flowrate and 73% energy efficiency obtained for pre-treated EFB.
Electric power requirement has been investigated at 4096 kW and can be fulfilled by DME Plant
through steam generation cycle and internal combustion engine fuelled by DME product. The
model developed will be used as a basis for techno-economic analysis of DME plant based on
EFB gasification.

Keywords: Empty Fruit Bunch, Dimethyl Ether, Gasification, Model, Simulation

1. Introduction

A The need for renewable energy in Indonesia is a necessity. From various renewable energy alternatives
available, renewable energy from biomass has great potential to be developed in Indonesia. The biomass
potential in Indonesia is about 32 GWe, and recent utilization was only around 1,740.40 GWe or 5.4%
of the total potential [1]. It was estimated that biomass potential in Indonesia at 146.7 million tons per
year equivalent to 470 GJ/y [2].

Utilization of biomass as one of energy source can be done through gasification process. Gasification
is a thermochemical process that converts biomass into a gas called a producer gas or synthetic gas
(syngas). Syngas is a fuel-based mixture consisting mainly of Hydrogen (H_2), Carbon Monoxide (CO),
and Methane (CH_4) [3]. Syngas is a raw material for most other chemical products, such as Methanol,
Ammonia, and Dimethyl Ether (DME). One of the biomass sources which have big potential to be
utilized is palm empty fruit bunch (EFB) waste. The total EFB waste generated in Indonesia was 17.43
and 30.6 million tons for the year 2014 [4] and 2015 [5], respectively.

Some research on DME production using biomass through gasification process has been widely performed, such as research conducted by [6]–[10]. In addition to research on the process of producing DME from biomass, research done by [7] also examines the technical analysis and feasibility of DME plant investment by utilizing wood pellets that have undergone a torrefaction process. The wood pellets have similar characteristics to coal; therefore, the gasifier used was the same with gasifier built for coal gasification.

Specific study on simulation of gasification process based on EFB gasification to DME had been done by [11] which discussed the parametric analysis of DME production. Another research on DME plant modelling was conducted by [12], which one of the paper was discussing about zero-dimension DME plant model based on torrefied biomass gasification and low CO_2. From those studies which already mentioned above, yet no model developed for DME plant based on gasification of EFB. Hence, this study originated to provide a model of DME plant based on EFB gasification and simulate DME Plant model developed by using Aspen Hysys. In this paper, the model developed was simulated to obtain DME yield, energy efficiency, power consumption, and power generation.

2. Theory of gasification and DME synthesis

2.1. Gasification
Gasification is a process that converts biomass into a gaseous fuel called producer gas (CO, H_2, CH_4, etc.) using a little air or oxygen/steam. The reaction is occurred as incomplete combustion. According to the reference [13], gasification reactions involve several series of chemical reactions such as: drying, pyrolysis, combustion, gasification, and auxiliary processes such as gas and water phase displacement reactions.

2.2. DME synthesis
The process of producing DME using biomass as raw material was divided into 4 stages: gasification, water-gas shift, gas purification, and DME synthesis [11]. In general, two-stage DME is produced by methanol dehydration reaction in (1).

$$2\ CH_3OH \rightarrow (CH_3)_2O + H_2O \tag{1}$$

DME can be produced by single-stage (SS-DME) synthesis and two-stage (TS-DME) synthesis process. The TS-DME two-stage process passes through two different process units, one process with a special catalyst to produce Methanol, and another one for the methanol dehydration reaction as main reaction to produce DME [14]. The basic reaction for single-stage DME synthesis consists of several reaction steps shown in Table 1.

According to [15], there are two routes of the overall reaction of SS-DME synthesis from syngas, those are reactions (a) and (b) as shown in Table 1. The reaction (a) which is the overall reaction consists of 3 reaction steps that is, methanol synthesis reaction (c), dehydration reaction (d), and water-gas shift (WGS) reaction (e). The overall reaction (b) consists of reaction step (c) and (d). The single-stage DME synthesis reaction of JFE technology follows the overall reaction (a), while the Haldor Topsoe A/S technology and other technologies follow the overall reaction (b).

In this study, the simulation was performed using SS-DME synthesis process route. SS-DME synthesis process is considered more economical. In addition, it can overcome the problems associated with equilibrium on synthesis of methanol when synthesis is done through a two-stages synthesis process [11].

The technology used for simulation purposes on the model developed was adopting JFE technology combined with research results done by [7] about the techno-economic analysis of torrefied biomass and process configuration described on [16], which described the potential of DME as an alternative to conventional fossil fuel. Reference [16] was made by EPCM consultant based on South Africa. The description of the process and reaction between [7][16] were quite similar with reference from [15] with topic about pilot plant 5 tons/day DME production through single-stage synthesis route. Those

references based on the technology developed by JFE, and transparently provides detail information about the process.

Table 1. Reaction of single stage DME synthesis

Reaction	Heat of reaction (kJ/mol)
(a) $3CO+3H_2 \rightarrow CH_3OCH_3+CO_2$	-246
(b) $2CO+4H_2 \rightarrow CH_3OCH_3+H_2O$	-205
(c) $2CO+4H_2 \rightarrow 2CH_3OH$	-182
(d) $2CH_3OH \rightarrow CH_3OCH_3+H_2O$	-23
(e) $CO+H_2O \rightarrow CO_2+H_2$	-41

3. Method and DME plant design

The following steps are undertaken to perform the modelling.

    i) Collect information on existing or model of DME plant that was available.

    ii) Perform the simulation by utilizing process engineering simulation tools. In this study, Aspen Hysys was utilized.

    iii) Prepare material stream and energy stream to find DME yield, process efficiency, and energy recovery.

The Process Flow Diagram (PFD) of DME synthesis was developed and shown on Fig.1, included some important parameters. DME plant design process was described in 10 steps as follow.

3.1 Simulation tools

The simulation was done by using Aspen Hysys process simulator. Aspen Hysys has been used in several studies to simulate biomass gasification [12][18] and DME production [11]. The various components that comprise Aspen Hysys provide an extremely powerful approach to steady state process modelling. The user describes the process in terms of pieces of equipment interconnected by process stream, and the program solves all the mass/energy/equilibrium equations, taking into consideration the specified design for the units [19]. Since feedstock EFB is not a default component in Aspen Hysys, hence it must be put manually as Solid Hypothetical component. The input of EFB as hypothetical solid component was based on ultimate analysis of EFB measured feedstock. Base for simulation is dry ash free (daf), from weight percentage of components C, H, O, N, S

3.2 Biomass feedstock

Feedstock used was EFB. The composition of the EFB was based on dry ash free base (daf) taken from [20]. Based on ultimate analysis chemical formula can be determined [18]. In 100 grams of biomass, there is 51.67 grams of carbon. Mass in grams divided by carbon molecular weight (12 g/mol) will give result of 4.306 mol of carbon. The same is applied to other elements which lead to the following chemical formula for EFB biomass: $C_{4.306} H_{6.176} O_{2.587} N_{0.048} S_{0.003}$, and this chemical formula is used as an input to Aspen Hysys as hypothetical solid component. The input of EFB is at 6.16 tonnes per hour, based on [21].

3.3 Biomass pre-treatment.

Before the gasification process, raw biomass in any form needs to go through pre-treatment process. The pre-treatment process was consisting of several parts; such as granulator, dryer, hammermill, and pelletizer. As pellets, EFB has a greater energy density, reducing the bridging problem in gasifiers that use biomass with non-uniform sizes [20]. According to [22], with pelletizing, bulk density of EFB increases almost three times after the pellet-making process. Energy required for granulator, hammermill, and pelletizer were 1.1 %, 2.2% and 2.5% of LHV (low heating value), respectively [20].

3.4 Gasification.

The process of gasification occurs in Circulating Fluidized Bed (CFB) gasifier. Gasifier used Steam–Oxygen as an oxidant. The Oxygen was supplied by cryogenic air separation process. The purity of oxygen was assumed at 100%. The electricity consumption of air separation unit was based on [7] at 1.0 MWe/ kg O_2/s. The composition of the syngas as result of gasification was calculated based on equilibrium reaction at 900 ^{o}C. The process was assumed isothermal during the gasification reaction [23]. The waste heat from reactor was used as heat for steam generation, since reactor was cooled using water, and water will turn into steam (steam generator I) for gasification oxidant supply. From the CFB gasifier, syngas outlet were cooled to 400 ^{o}C, before entering Water Gas Shift (WGS) reactor to adjust for the H_2 to CO ratio (H_2/CO) equal 1 for DME synthesis requirement [24]. Raw syngas outlet was filtered using bag house filter to remove particulates.

3.5 Water gas shift.

Water gas shift reaction takes place to adjust for the composition of H_2/CO equal 1. Temperature of the reaction is at 400 ^{o}C and pressure 1000 kPa based on [18]. Prior to acid gas removal process, syngas was cooled to 25 ^{o}C [12]. Gibbs reactor was used to simulate the reaction and 130 kg/h steam was supplied to WGS reactor to get H2/CO = 1. Type of WGS used is high temperature WGS, because it favors WGS reaction with a greater reaction rate [18].

3.6 Water removal and syngas cleaning.

Water removal was modelled using separator as a dryer and acid gas was removed by MEA scrubber. The removal process was modeled by water separator that removes water content less than 1 % mol as acceptable level [18]. After water removed, syngas entering Acid removal modelled as component splitter. Assumed, CO_2 and H_2S were removed at 90% and 100% [18].

3.7 DME synthesis.

Sweet syngas is compressed into 5000 kPa, according to the operating pressure of JFK process [15]. The reactor used is Gibbs reactor to simulate the synthesis of DME and reactions involved is equilibrium reaction based on [25]. The operating temperature of the reactor was based on JFK process [15] at 260 ^{o}C. The temperature was maintained at 260 ^{o}C throughout the reaction. Water jacketed cooler is used to maintain temperature of DME reactor, and water as a cooler will turn into saturated steam by absorbing heat of DME synthesis reaction. Steam produced was a part of steam integration at steam generator II. Product gas was cooled to 15 ^{o}C [7], then separated by gas–liquid separator where unconverted syngas recycled back to DME synthesis reactor. On this simulation, 95% of unconverted is recycled and 5% is sent to steam boiler to generate electricity [7]. Liquid outlet of gas-liquid separator flows to purification section which consist of three distillation towers

3.8 Distillation.

The distillation process occurred in the first tower was mainly to separate CO_2 and other light gasses with DME, Methanol (MeOH) and water. The tower has 9 stages and feed stage located on stage number 1 from condenser at the top. The gas as a top product mixed with the outlet gas from Gas – Liquid separator and sent as a fuel for steam as part of steam generator II system. Bottom product contains DME, methanol, and water entering DME Tower. The distillation in DME tower is to separate DME as top product with Methanol and water as bottom product. DME recovered from DME tower is 99.6% purity according to [14, 15].
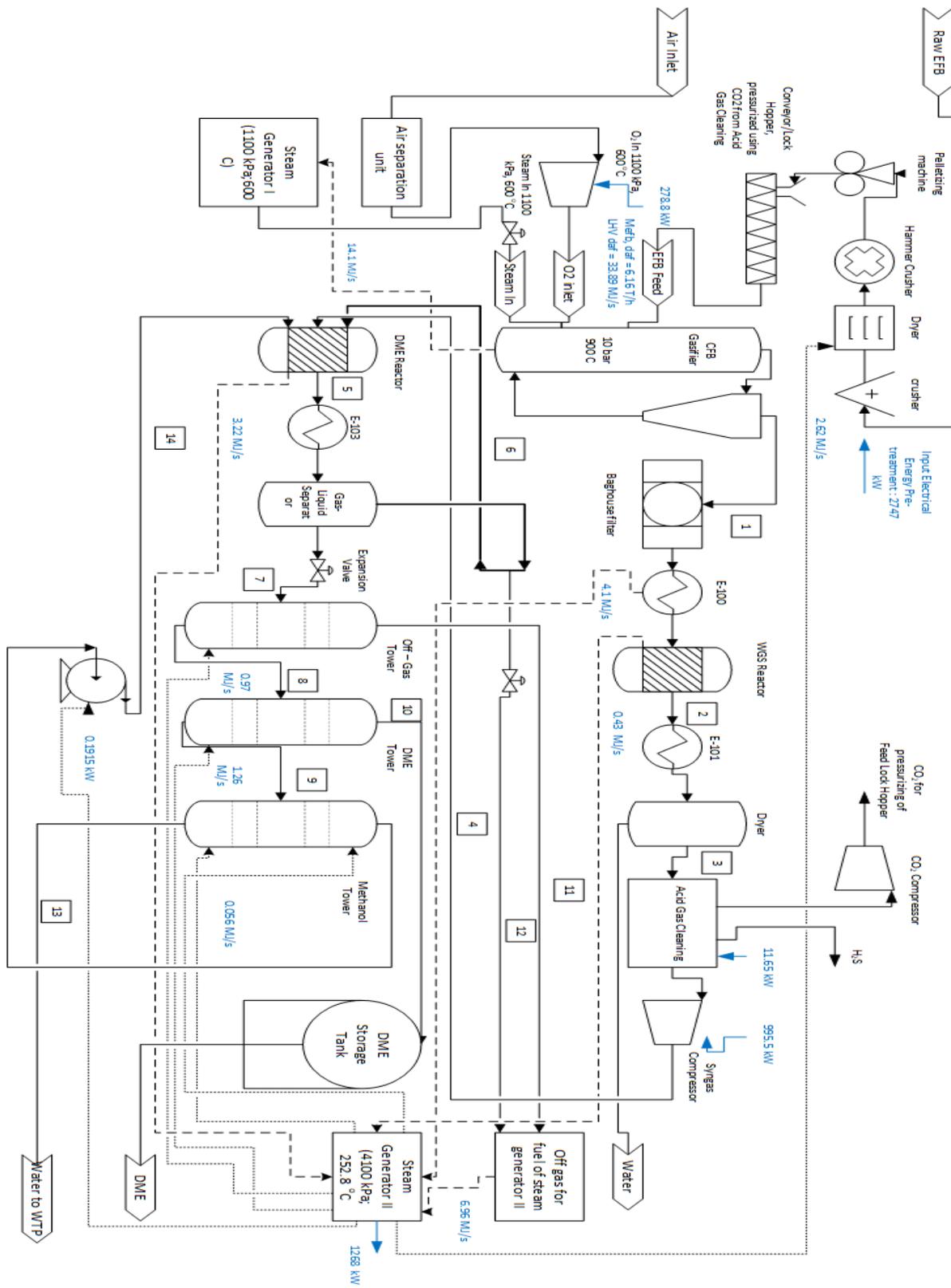
Fig. 1. Process flow diagram DME production based on EFB gasification

DME tower has 10 stages and feed stage is feed number 3 from the top. The bottom product of DME Tower which were methanol and water was further separated in methanol tower. Methanol tower has 12 stages, the top product of the distillation in methanol tower was methanol and the bottom product were water. Methanol was recycled, while water delivered to water treatment facility before discharged or re-utilize.

3.9 Steam and power generation.

Steam generation for the process and power generation was from the steam boiler fueled by waste heat from the plant combined with the utilization of off-gas from plant. There were two steam generators available. First, steam was generated by waste heat from CFB gasifier and was named as steam generator I as shown on Fig.1. Second, combination of off-gas boiler with waste heat boiler from WGS reactor, DME reactor, and E-100, all were combined as steam generator II as shown on Fig.1. Power for DME plant was generated by using one steam turbine at steam generator II system.

3.10 Efficiency Calculation

DME $\eta_{product}$ (product efficiency) was calculated by using (2). Formula was adopted from [23].

$$\eta_{product} = \frac{\dot{m}_{product} \cdot LHV_{product}}{\dot{m}_{biomass} \cdot HHV_{biomass}} \qquad (2)$$

Where $\dot{m}_{product}$ is flow rate of product DME in kg/h, and $\dot{m}_{biomass}$ is flow rate of EFB Biomass in kg/h. LHV$_{product}$ and LHV$_{biomass}$, are the low heating value (in kJ/kg) of the product and biomass respectively.

4. Result and discussion

4.1 Process simulation result

The simulation result on every stream number shown on Fig.1 was tabulated on Table 2. Results showed the total mass and molar flow, operating temperatures, operating pressures, heat flow, and composition of each substance produced. Ratio of H_2 to CO on stream No. 2,3, 4 was equal to 1, and this is required according to JFE technology [15] for direct synthesis of DME (single-stage). Raw DME product was represented by stream No.5. The stream further cooled and separated in gas-liquid separator, where gas product consists mostly CO_2 and unreacted syngas (H_2 and CO), CH_4, and CO_2. The gas product recycled at 95% mol and 5% mol of it delivered and mixed with top product of off-gas tower, further was utilized as fuel of steam boiler for power generation and process consumption.

The liquid product of gas-liquid separator was expanded from 5000 kPa to 1000 kPa, to follow operating condition of DME purification section [12]. Methanol produced at stream No.9 was recycled into DME reactor. Stream No.10 was DME product with purity 99.9 %, since DME has similarity with LPG in term of physical properties, its handling and storage are similar to LPG [26]. Yield of DME over input EFB for the model developed was 50%. Table 3 shows mass of EFB input and DME output, LHV of EFB input and LHVof DME output, and DME product energy efficiency.

Table 2. Material stream and stream composition of DME plant

Stream No.		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Vapour Fraction		0.9932	1	1	1	1	1	0.2532	0	0	0
Temperature	C	900	400	25	25	260	15	-14	49	150	43
Pressure	kPa	1,000	997	997	5000	5000	5000	1000	999	999	950
Molar Flow	$kgmole/h$	602	605	601	528	1,027	819	156	76	9	67
Mass Flow	kg/h	11,400	11,478	11,404	8,200	33,970	25,684	6,672	3,325	239	3,086
Heat Flow	MJ/h	-41,080	-54,627	-60,855	-28,918	-218,000	-176,900	-44,300	-15,620	-2,112	-13,520
Mole Frac (%)											
H_2		35.00	41.51	41.79	47.58	9.68	11.29	0.47	0.00	0.00	0.00
CO		48.47	41.62	41.91	47.71	17.26	20.12	1.70	0.00	0.00	0.00
CO_2		6.66	13.22	13.31	1.52	41.60	41.65	41.19	0.00	0.00	0.00
H_2O		6.46	1.02	0.34	0.39	0.31	0.05	1.80	3.71	31.95	0.05
CH_4		2.20	2.19	2.21	2.51	14.04	15.99	3.20	0.00	0.00	0.00
H_2S		0.19	0.19	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N_2		0.26	0.25	0.26	0.29	2.00	2.32	0.21	0.00	0.00	0.00
CH_3OH		0.00	0.00	0.00	0.00	0.62	0.06	3.78	7.81	68.02	0.01
CH_3OCH_3		0.00	0.00	0.00	0.00	14.48	8.53	47.64	88.48	0.04	99.94

4.2 Power consumption and generation

Total electrical power consumption of main unit/section in DME plant was shown on Table 4. Power generated by steam turbine was 1268 kW. According to Table 4, there was deficit 2717.19 kW on the electricity for the DME plant to run. Steam cycle converts 13519 kW waste heat into 1268 kW electricity. This is corresponding to 9.4% electrical efficiency. To overcome deficit on electricity, generator coupled with internal combustion engine (ICE) should be added for power generation. Fuel used for ICE is DME itself as a product from the DME plant. Type of ICE utilized is diesel engine and the fuel used is DME, since DME can be used as replacement for diesel fuel [26].

DME most prominent characteristic is high cetane number that makes DME can be considered as a replacement of Diesel fuel [26], with modification on fuel tank.

Table 3. Energy eefficiency of DME plant

Parameters	Unit	Value
$\dot{m}_{biomass}$	Kg/h	6160
$LHV_{biomass}$	MJ/kg	19.81
$\dot{m}_{product}$	Kg/h	3080
$LHV_{product}$	MJ/kg	28.8
$\eta_{product}$	%	73

Table 4. Power cconsumption of DME plant

Plant Section/Unit	Power Consumption (kW)
Recycle pump	0.1915
Air Separation Unit	1214
Pre-treatment EFB	2747
Acid Gas Cleaning	11.65
CO2 compressor	12.35
Power Deficit	**-2717.19**

By selecting diesel engine as genset prime mover, high thermal efficiency can be achieved, in this study the thermal efficiency of the ICE was 45 % [27]. Compressors in DME plant needs huge power to run, and this is supplied by ICE as prime mover of compressor. Table 5 shows the power consumption of compressors prime mover. Power required for refrigeration and compression of syngas consumed huge amount of power and supplied by ICE as prime mover. With 45% efficiency, total DME required to be supplied to power generation ICE is 754 kg/h, in order to generate deficit power at 2717.19 kW. While DME required by compressors is 1098 kg/h. From total 3086 kg/h DME produced, almost two-third of it is used as ICE fuel.

Table 5. Power consumption of compressor prime mover

Prime Mover ICE	Power Consumption (kW)
Oxygen compressor prime mover	279
Syngas Compressor prime mover	956
Refrigeration compressor prime mover	2725

Based on the result, conversion of CO on the simulation was 64% at 5000 kPa and 260 $^{\circ}$C. It was tally with the experiment result in [15], where CO conversion was higher than 50% at 5 MPa and 260°C. The efficiency of this model ($\eta_{product}$) is 73% for pre-treated EFB, and this is slightly different with the result given by JFE process at 69.4% when using natural gas as the feed. The efficiency for torrefied biomass as reported by [12] was 67%, while untreated biomass only 60%. This study revealed that $\dot{m}_{product}$ was 50% of $\dot{m}_{biomass}$, and energy efficiency from EFB to DME was 73%. Conversion of torrefied biomass model into DME as studied by [7] was 54%, and it is quite close with the result obtained in this study. To run the plant electricity is required, and it can be fulfilled by the waste heat utilization through steam generation and genset, where genset fuel was using DME as final product.

5. Conclusion

The model of DME plant was designed and simulated by using Aspen Hysys. Simulation of the model was based on EFB gasification, conducted in CFB gasifier. The results of the simulation were in good agreement with reference data, especially for DME yield and CO conversion. The electric power for DME plant based on EFB gasification was provided by itself, where all the power supplied by steam cycle and ICE fueled by DME product. Total electric power required is 4096 kW. Total power required for compressor prime mover is 3960 kW. DME can be used to replace LPG and Diesel fuel, because of its physical properties and high cetane number. $\dot{m}_{product}$ produced at 50% of $\dot{m}_{biomass}$ and $\eta_{product}$ from simulation was 73% for pre-treated EFB. In the future study, DME plant model developed will be used as a basis for techno-economic analysis of bio-DME plant based on gasification of EFB.

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