# Parametric Study for Production of Di Methyl Ether (DME) as a Fuel from Palm Wastes

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Dissertation submitted in partial fulfilment of the requirement for the Bachelor of Engineering (Hons) (Chemical)

MAY 2014

Universiti Teknologi PETRONAS Bandar Seri Iskandar 31750 Tronoh Perak Darul Ridzuan

## **CERTIFICATION OF APPROVAL**

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A project dissertation submitted to the Chemical Engineering Programme Universiti Teknologi PETRONAS (UTP) in a partial fulfilment of the requirement for the BACHELOR OF ENGINEERING (Hons) (CHEMICAL)

Approved by;

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MAY 2014

## **CERTIFICATION OF ORIGINALITY**

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

(MUHAMAD NORILLYAS BIN HUSSIN)

## ABSTRACT

Dimethyl Ether (DME) as one of the second generation of Biofuels can be produce traditionally from the petroleum based feed which involve two steps of production (methanol synthesis from the syngas and DME synthesis from methanol). Recent study shows that DME production process is now possible to be done with biomass as the raw material and single step for DME production process has been developed. In this paper, single step process of DME production was used and simulated using the HYSYS Simulation Software V8.0. Empty Fruit Bunch from palm wastes is the main feed for the process which having four main parts: gasification, water gas shift, CO<sub>2</sub> removal and DME Synthesis. In addition, a parametric study was conducted on the DME production process. The results shown that Oxygen to Biomass ratio (O/B) of 0.37 and Steam to Biomass Ratio (S/B) of 0.23 will give a H<sub>2</sub>/CO feed ratio of 1. Pressure and temperature effect towards the production of DME process was tabulated and 1000kpa, 140°C respectively were found to be the optimum condition for DME production at H<sub>2</sub>/CO feed ratio of 1.

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## **CHAPTER 1: INTRODUCTION**

#### **1.0 OVERVIEW**

Chapter 1 was discussing mainly the background of the project. The purposes and the objectives of the project were identified with respect to the problem statement issued. Furthermore the scope of works for this project also were presented in this chapter.

## **1.1 BACKGROUND**

Projected by The International Energy Outlook 2013 (IEO, 2013), world energy consumption now is about 56 percent between 2010 and 2040. Total world energy use rises from 524 quadrillion British thermal units (Btu) in 2010 to 630 quadrillion Btu in 2020 and to 820 quadrillion Btu in 2040. World energy consumption based on Key World Energy Statistics 2013, International Energy Agency (IEA, 2013) is now currently at more than 8 000 Metric Ton of Oil equivalent (MTOE) for year 2011.

Figure 1 shows the distribution of the source of world energy that has been used. About 80 % of all primary energy in the world consumed is comes from fossil fuels. Unfortunately, we have to realize that fossil fuel is non-renewable energy which someday it will be depleted. In addition the burning of fossil fuel and natural gas is causing the emission of greenhouse gases (GHG).

With regards to energy shortage and global warming crisis, the possibility of producing fuel from biomass and wastes has been even more promising as it involves the renewable sources. Thus for now, the development and research on Biofuels production becomes more serious. The 1<sup>st</sup> generation of Biofuels liquid production such bioethanol (produced primarily form food corps) is well established. Classification of Biofuels generation is based on the production source. First





FIGURE 1: World Total Final Energy Consumption from 1971 to 2011

In fact, there are already exists a commercial first generation of biofuels supported by the government in many countries. For example Corn Ethanol in United State of America, sugarcane ethanol in Brazil and for biodiesel derived from vegetable oil is in Germany, Austria and France. These biofuels are derived from food crops and from the viewpoint of economics, environment, land use, water and chemical fertiliser, there is a strong preference for the use of woody, grassy materials as well as agricultural residue and wastes as the feed stock. Thus second generation of Biofuels such bio-methanol, bioethanol, dimethyl ether (DME), FT (Fisher-Tropsch) fuel, synthetic natural gas and hydrogen via gasification and synthesis is more promising.

#### **1.2 PROBLEM STATEMENT**

Dimethyl ether (DME) as one of biofuels can be produced from biomass such agricultural wastes. The DME production is traditionally involving two steps of process, first methanol production from the gasification process of biomass and next the dehydration of methanol to produce DME.

Two steps of DME production process seems not economical and has the equilibrium limitation poses by methanol synthesis (Marchionna et. al., 2008). Thus most recent study started to analysed the opportunity of the single step of DME production process by using biomass as the feed. Ju et. al. (2009), and Zhu et. al. (2010) are the study which performed the simulation of the DME production from biomass to analyse the process parameters. Both works is using dried woody and diatomic gases respectively as the feed for the single step DME production process.

In addition, the reaction conditions for DME production process are really important and giving a significant effect towards the product produced.  $H_2/CO$  feed ratio, temperature and pressure are the main factor that gives effect to the process.

Fortunately for Malaysia, abundant agricultural waste is available especially EFB. Thus this study will be focusing on optimizing EFB as the feed for DME production process.

### **1.3 OBJECTIVE**

There are two main objectives for this study, which are.

- i. To perform the simulation of Dimethyl Ether (DME) production process by using Empty Fruit Bunch (EFB) as a feed.
- ii. To perform the parametric study towards the Dimethyl Ether (DME) production process.

The study is conducted by using HYSYS simulation software

## **1.4 SCOPE OF STUDY**

The study will involve in performing the simulation of Dimethyl Ether (DME) production process from Empty Fruit Bunch (EFB). The effect of the parameters towards the process also will be analysed. The DME production process will involve four major parts namely; gasification of the biomass, Water gas Shift reaction, CO<sub>2</sub> Removal and DME synthesis reaction. Single step DME production process is used and the process parameters will be varied to get the best and optimum production process. The process parameters involved for the study will be;

- 1. Operating Temperature of DME synthesis reaction
- 2. Operating Pressure of DME synthesis reaction
- 3. Composition of feed (H<sub>2</sub>/CO ratio)
- 4. Oxygen to Biomass ratio (O/B)

## **CHAPTER 2: LITERATURE REVIEW AND THEORY**

#### **2.0 OVERVIEW**

Chapter 2 is discussing the literature on the past researches that has been done for DME production process. It started with giving the view of the biomass potential in becoming the alternative energy source. Followed by the characteristic of DME and the reaction for DME production process.

## 2.1 ALTERNATIVE ENERGY FROM BIOMASS

Biomass as per 'Biomass regulation 2001/77/EG' is defined as the biological degradable fraction of products, wastes and residues from agriculture, forestry and the biological degradable fraction industrial and household wastes. Biomass is considered as renewable energy and CO<sub>2</sub> neutral in its lifecycle. Plants absorb CO2 from the air and convert it into complex biochemical compound like lignin and cellulose through photosynthesis. At next stage, the same amount of CO<sub>2</sub> is released by burning the biomass.



FIGURE 2: Life cycle of Biomass

The European Parliament has approved the EU guideline to increase the share of biofuels in all transport fuels (diesel and petrol) up to 5.75 % in 2010, 10 % in 2020 although only 1.4 % of bio-automotive fuels is, at present, produced from biomass (Zhang W., 2009). This is one of the examples of government initiative to enhance and support the usage of biofuels. Other support that came is from the nongovernmental organization such Volvo. Well known company in automotive industry which already implement the usage of renewable fuel in their trucks. Volvo Trucks is the first truck manufactured to carry out comprehensive customer-based field tests involving Bio-DME fuel.

Dimethyl ether produced form biomass is known as Bio-DME. It offer a higher energy efficiency and low level of greenhouse gases emission. Research by Volvo DME (2012), Bio-DME has 95 % lower carbon emission than diesel and no soot particulate emission. In addition it has five times better land usage than biodiesel and high energy efficiency in relation to other biofuels.

Bar graph below show the performance of DME compared with the other renewable energy and also fossil fuel.



DME has the highest well-to-wheel energy efficiency, 25% better than synthetic diesel fuel, and the lowest greenhouse gas emissions of any biomass-based fuel.

Well-to-wheel analysis for energy efficiency and greenhouse gases (Courtesy – A. Roj, Volvo Technology Corporation). These estimates include production, transport, and end use GHG emissions. KEY: DME dimethyl ether; MeOH methanol; CNG compressed natural gas. RME rapeseed methyl ester; GHG greenhouse gas.

#### FIGURE 3: Comparison of Performance between DME as a fuel with other

sources

#### **2.2 DIMETHYL ETHER (DME)**

Dimethyl ether (typically abbreviated as DME), also known as methoxymethane, wood ether, Dimethyl oxide or methyl ether, is the simplest ether with a chemical formula of CH<sub>3</sub>OCH<sub>3</sub>. It is a colourless, slightly narcotic, non-toxic, highly flammable gas at ambient conditions, but can be handled as a liquid when lightly pressurized. The properties of DME are similar to those of Liquefied Petroleum Gas (LPG). DME burns with a visible blue flame and is non peroxide forming in the pure state or in aerosol formulation (Troy et. al., 2005). DME is the organic compound which is degradable in the atmosphere and not a greenhouse gas.

#### **FIGURE 4: DME structure**

C<sub>2</sub>H<sub>6</sub>O / CH<sub>3</sub>OCH<sub>3</sub> H<sub>3</sub>C CH<sub>3</sub>

DME has historically been used as a propellant in consumer products. DME can be used in a wide variety of consumer applications, namely personal care (e.g., hairspray, shaving creams, foams, and antiperspirants), household products, automotive, paints and finishes, food products, insect control, animal products, and other related applications.

Based on International DME Association, DME has a remarkable potential for increased use as an automotive fuel, for electric power generation, and in domestic applications such as heating and cooking. Recent attraction on DME application is as a fuel. Promising fuel applications include:

- LPG Blending and Substitute
- Diesel Blending and Substitute
- Power Generation
- Acetylene Substitute

Recently, China has been blending DME with LPG in significant volumes. The Chinese government has been promoting DME blends. Egypt is also developing a DME project to reduce dependence on LPG imports. The properties of DME suggest that it could be a substitute for diesel as a transportation fuel, with the attraction of enhanced environmental performance. Several bodies are actively researching the use of DME as a substitute for diesel vehicle fuel. The IEA (International Energy Agency) is co-coordinating research as part of the Implementing Agreement on Alternative Motor Fuels (IEA/AMF). Among the many organizations involved are automotive manufacturers such as Volvo, Renault and Peugeot. Volvo has developed a DME fuelled engine for buses. In Japan, a number of demonstration vehicles and small scale filling stations have already been built. Early tests by a number of companies have shown promising fuel efficiency results compared with traditional diesel vehicles. Programs on cars are also being promoted in North America and Western Europe.

Property	DME	Diesel
Density at 20 °C [kg/l]	0.67	0.83
Lower heating value [MJ/kg]	28.4	43.1
Cetane number	<mark>60</mark>	50
Fuel equivalence	0.59	1
GHG [gCO <sup>2</sup> eq/MJ]	Waste wood DME: 5	
	Farmed wood DME : 7	

 TABLE 1: Comparison between DME and Diesel

DME is one of those fuels: vastly superior cold starting, literally smokeless, quieter combustion, no fuel waxing in cold climates to clog fuel lines, low  $NO_x$  emissions, lower well-to-wheel greenhouse gas emissions than diesel fuel, and potentially a  $CO_2$  absorber in its production.

## 2.3. DME PRODUCTION & REACTION

DME is conventionally produced by converting natural gas (mainly methane) to syngas to produce methanol followed by methanol dehydration to dimethyl ether (Troy et. al., 2005). Methanol synthesis process from syngas (derived from Syngas) is highly exothermic reaction whereas methanol dehydration is endothermic reaction. In total the heat of reaction for whole process is about 258.6kLmol<sup>-1</sup>. Below is listed the overall chemical equation of DME production form natural gas.

Methanol synthesis



## FIGURE 5: Block Diagram of DME Synthesis from Biomass

Natural gas is not the only raw material to produce syngas. Organic waste or biomass can also produce syngas through gasification process which will be then used for methanol synthesis and methanol dehydration as illustrated in Figure 5 above. This study will be using palm wastes as the raw material, specifically the empty fruit bunch (EFB) and the chemical compound will be  $C_{3.4}$  H<sub>4.1</sub>O<sub>3.3</sub> (Laohalindanond et. al., 2006).

Figure below illustrated the path of syngas  $(CO + H_2)$  to DME.



**FIGURE 6: Syngas to DME Route** 

#### 2.4 SINGLE STEP OF DME PRODUCTION

Recently the production of DME has been improved by using only single step of DME synthesis. Previously, the DME synthesis process will go through methanol synthesis and methanol dehydration separately, but in single step both reactions are combined in one reactor (Ju et. al., 2009), equation (1) to (5). Single step of DME synthesis is more economical and has overcome the equilibrium limitation poses by methanol synthesis (Marchionna et. al., 2008). Single step DME synthesis highly depends on the bi-functional catalyst or so called the hybrid catalyst. The catalyst will have two active sites corresponding to methanol synthesis and methanol dehydration, respectively which will be stacked in Fixed-bed reactor.

$$CO + 2H_2 \longrightarrow CH_3OH$$
 (1)

$$2CH_{3}OH \longrightarrow CH_{3}OCH_{3} + H_{2}O \qquad (2)$$

$$CO + H_2O \longrightarrow H_2 + CO_2$$
 (3)

Overall reaction

$$3CO + 3H_2 \longrightarrow CH_3OCH_3 + CO_2$$
 (4)

If reaction (3) does not participate, the total DME synthesis reaction can be expressed as;

$$2CO + 4H_2 \longrightarrow CH_3OCH_3 + H_2O$$
(5)

There are two main typical technologies of single step DME Synthesis, Hardlor Topsoe and JFE. The Hardlor process adopts at feed composition of  $H_2/CO$  ratio of 2 which is favourable for reaction (4) while JFE technology using  $H_2/CO$  ratio of 1 and favor reaction (5). For this study the composition of the feed will be vary to find the best condition.

## **CHAPTER 3: METHODOLOGY**

#### **3.0 OVERVIEW**

Chapter 3 is focusing on the method and technique to be used in conducting the study. The main tool for the research is discussed and the parameter involved is further describe. In order to have a better and structural work attitude, timeline of the project also is produced. Some assumption is also mentioned which is involved with the study.

### **3.1 PROJECT FLOW CHART**

Presented below is the flow chart of this study. It start with the literature review of the related past paper on the DME production process followed by the developing the block diagram and conducting the simulation work. The works continues by doing the data gathering and analysis and finished with discussion and conclusion.

## 1.Literature Review

- Gathering information from previous research regarding the relevant reaction involved (Gasification reaction, Water gas Shift, DME Synthesis)
- Additional literature regarding the physical properties of Palm Waste (Empty Fruit Bunch, EFB) to be used in simulation.

## 2.Simulation

- Developed the block diagram of the DME Production process from EFB.
- Simulation of DME Production process using HYSYS simulation software.
- Validation of the simulation work

- Simulation data is extracted and analysed.
- Parametric study (temperature, pressure, O/B ratio and H<sub>2</sub>/CO ratio) are performed and compared with past work.

## 3. Discussion and Conclusion

• Conclusions are made based on simulation data and trend of the process data based on the parametric changes.

## **3.2 GANTT CHART AND KEY MILESTONE**

Table 2 shows the timeline and gantt chart of the project. This timeline is adapted from the FYP 2 Guidelines.

Process

Milestone O

 TABLE 2: FYP 2 Gantt Chart

No	Detail Work	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Project work continues														
2	Submission of Progress Report							0							
3	Project work continues														
4	Pre-SEDEX										0				
5	Submission of Draft Final Report											0			
5	Submission of Dissertation (soft														
6	bound)												$\cup$		
7	Submission of Technical Paper												$\circ$		
8	Viva													$\circ$	
9	Submission of Project Dissertation (hard bound)														0

### **3.3EXPERIMENT METHODOLOGY**

#### **3.3.1 Research Tools and Equipment**

This study is using Aspen Hysys V8.0 Simulation software to simulate the DME Production process. Hysys Simulation software is a software developed for design, steady state simulation and optimization of a chemical process. Parametric study on DME production process were conducted once the DME production process simulation is develop.

#### 3.3.2 Research procedure

Parametric study of DME production process will be focus on the single step DME Synthesis process. Ju et.al. (2009), Zhu et. al. (2010) and Lu et.al. (2004) are the main source of the guidance for this research. The research procedures for this study are;

- 1. Understand the background for chemical reaction of single step DME synthesis.
- 2. Develop the block diagram of DME production process.
- 3. Identification of the variables (operating parameters) for the process.
- 4. Develop the simulation model for DME production process using HYSYS Simulation Software.
- 5. Variation on the variable and data gathering.
- 6. Tabulate and analyse the findings from the parametric study.

#### 3.3.3 Parametric Study

There are many factor that could affect the performance of a process such temperature, pressure, composition, flow etc. Table 4 below listed the selected parameter for the parametric study of DME production process as a fuel from palm wates. Selection of the parameters are based on the previous research Ju et.al. (2009), Zhu et. al. (2010) and Lu et.al. (2004) which give the biggest significant effect towards

the process. Each parameters are varied on different condition and value to investigate and explore the effect on the DME production process.

Parameter
Hydrogen to Carbon Monoxide (H <sub>2</sub> /CO) ratio
Reaction Temperature
- DME synthesis
- Syngas Synthesis( Gasification)
Reaction Pressure
Oxygen to Biomass ratio (O/B)

## **TABLE 3: Research Parameter**

## **3.3.4 Process Assumption**

In parametric study of DME production process, there are a few assumption considered in the process development and modelling.

- a) Ideal reaction condition
- b) The reaction occur isothermally and at constant volume.
- c) Tar formation in the process are negligible in the calculation.
- d) Perfect mixing and uniform temperature and pressure distribution in the gasifier.

## **CHAPTER 4: RESULT AND DISCUSSION**

#### **4.0 OVERVIEW**

In this chapter, the outcome from the experimental work were tabulated and analysed based on the respective criteria selected. Starting with the discussing the feedstock for the process which is Empty Fruit Bunch of Palm Wastes which is identified as the potential feed stock due to its availability and properties. Next, block diagram for the whole process was develop followed by simulation model in Hysys. The study continued by investigating the effect of selected operational parameter towards the DME production process.

## 4.1 EMPTY FRUIT BUNCH AS BIOMASS FEEDSTOCK

Feedstock for this process is empty fruit bunch (EFB) due to its availability and its potential for the gasification process. The proximate chemical component and analysis of EFB are given in the Table 3, Laohalidanond K et. al. (2006). The molecular formula for EFB is  $C_{3.4}H_{4.1}O_{3.3}$  (basis of 1kg biomass) with molecular weight of 97.77kg/kg mol.



FIGURE 7: Empty Fruit Bunch form palm wastes:

Component	Proportion
Proximate analysis (%)	
Cellulose	59.7
Hemicellulose	22.1
Lignin	18.1
Ultimate analysis	
С	48.79
Н	7.33
Ν	0
0	36.3

#### TABLE 4: Elemental analysis of Empty Fruit Bunch (EFB)

## 4.2 DME PRODUCTION PROCESS BLOCK DIAGRAM

The overall process route for DME production from palm wastes involved series of reaction namely Gasification, Water Gas Shift, CO<sub>2</sub> Removal and single step DME Synthesis as illustrated in Figure 7. During gasification stage, EFB is gasified together with an oxygen and steam (10MPa, 540°C) line. There are five (5) major reaction involve in gasification process as listed in Table 5 (Partial Oxidation, Gasification, Boudouard, Methanation, and Methane Reforming). The C, H and O component of the EFB will be reacted and transform to produces H<sub>2</sub>, CO, CO<sub>2</sub> and CH<sub>4</sub>. Later the gas produced is transported into Water Gas Shift (WGS) reactor to modulate the H<sub>2</sub>/Co ratio to the desired value. Water stream (215°C, 4MPa) is added in WGS stage to control the temperature of the WGS reactor. The modulated gas the being transferred to DME Synthesis reactor. DME synthesis involved 2 main reaction; Methanol synthesis and Methanol Dehydration.



FIGURE 8: DME production process block diagram

## 4.3 PROCESS SIMULATION MODEL IN HYSYS

The developed simulation model, as shown in figure 8 below, derived from the equation listed in Table 5. The configuration consist of four major section, Gasification (Partial Oxidation, Gasification, Boudouard, Methanation, and Methane Reform), Water Gas Shift, CO<sub>2</sub> Removal and DME Synthesis. Peng- Robinson property package was used as thermodynamic property package. Rstoic Module was introduced to simulated the Partial Oxidation reaction, Co<sub>2</sub> Removal and DME synthesis, while RGibbs module which based on the gibbs free energy minimization approach was used to simulated the Gasification, Methanation and Methane Reforming reaction (Ju et.al. 2009).

100 kg/h of Pre-treated are fed together with the Oxygen and Steam (514°C, 10MPa). Into Conversion Reactor which partial oxidation reaction occurred to transform EFB into CO<sub>2</sub> gas and H<sub>2</sub>O. Next, the product and unreacted EFB continues the journey into Gasification Reactor which three simultaneous reaction are happening (Gasification, Methanation and Methane Reforming). The gas product from

Gasification Reactor which mainly  $H_2$  and CO gas later were send into the Water Gas Shift (WGS) Reactor to modulate the  $H_2$ /CO molar ratio to the required value. This work adapted the JFE technology which adopt a  $H_2$ /CO ratio of 1 (Ju et.al. 2009).

WGS reaction was used and 70% of CO conversion was set. The product stream next entering the purifications section which  $CO_2$  Removal reaction take place.  $CO_2$  Removal Reaction was simulated using Rstoic Module in the conversion reactor. The top product of the reactor which  $CO_2$  free stream next transported into DME Synthesis Reactor which modulate by conversion reactor. 90% conversion on H<sub>2</sub> basis was set for the reaction to occurs. DME Synthesis Reactor was modulated by Rstoic Module.



**FIGURE 9: DME Production Process Simulation Model** 

# TABLE 5: DME production process reaction scheme

Re	Reaction Reaction scheme			
Gasification	Partial Oxidation	$C_{3.4}H_{4.1}O_{3.3} + 2.775O_2 \rightarrow 3.4CO_2 + 2.05H_2O$	Conversion: 97%	
	Gasification	$C_{3.4}H_{4.1}O_{3.3} + 0.1H_2O \leftrightarrow 2.15H_2 + 3.4CO$	3.139 x 10 <sup>12</sup>	
Boudouard		$C_{3.4}H_{4.1}O_{3.3} + CO_2 \leftrightarrow 4.4CO + 0.9H_2O + 1.15H_2$	1,238 x 10 <sup>10</sup>	
	Methanation	$C_{3.4}H_{4.1}O_{3.3} + 8.05H_2 \leftrightarrow 3.4CH_4 + 3.3H_2O$	1.435x 10 <sup>11</sup>	
	Methane Reforming	$CH_4 + H_2 0 \leftrightarrow CO + 3H_2$		
Water gas shift		$CO + H_2O \leftrightarrow H_2 + CO_2$	70%	
CO <sub>2</sub> Removal		$CaO + CO_2 \leftrightarrow CaCO_3$	99%	
DME synthesis		synthesis $3CO + 3H_2 \leftrightarrow CH_3OCH_3 + CO_2$		

\* K<sub>e</sub>= Equilibrium coefficient

## 4.4 EFFECT OF H<sub>2</sub>/CO RATIO

 $H_2/CO$  ratio on feed gas is an important factor in DME production processes. It can be varied by either changing the molar flow of Steam or Oxygen stream into the process. As this work is adopted the JFE Technology in developing the DME synthesis reaction equation, a  $H_2/CO$  ratio of 1 is needed. Based on the simulated work the desired ratio was achieved when having a 370 kg/hr of Oxygen stream with 23 kg/hr of Steam stream in a basis of 1000 kg/hr of EFB as a feed.

Comparison	Feed	Oxygen to Biomass ratio ( O/B)	Steam to Biomass ratio (S/B)	H2/CO Ratio
This work (EFB)	This work (EFB) 100 kg/hr		0.23	1
Ju F. 2009 (Dried Woody) 75.6 tan/hr		0.370	0.143	1

TABLE 6: S/B and O/B Ratio when H<sub>2</sub>/CO is 1

The outcome of the finding was compared with previous work. Some deviation were identified in order to obtain  $H_2/CO$  ratio of 1 especially for steam to biomass ratio. For this study, the required steam to biomass ratio was 0.23 whereas Ju F. (2009) reported a 0.143 of steam to biomass ratio. While for the oxygen to biomass ratio there was not much different.

This deviation in getting a  $H_2/CO$  ratio of 1 can be explain by the different in the feed used. Ju F. (2009) was using dried woody biomass as the feedstock while this work is using EFB as the feed. Different in the properties of the feed might give different result as dried woody is having a higher content of oxygen compared to EFB. Dried woody contains 41.90 per cent of Oxygen while EFB having only 36.3 percent

of oxygen. Other than that, Ju F. (2009) have included a heat recovery steam generation system to produce steam in the WGS stage and DME Synthesis stage which could give effect on the hydrogen amount in the process.

Shown below in graph 1 is the effect of  $H_2/CO$  mole ratio in feed gas of DME Synthesis Reactor towards the production of DME. The variation of  $H_2/CO$  ratio was done from 0.5 till 3.5. It can be clearly seen that the trend of production of DME is increasing in the early ratio up till 0.2126 mol fraction of DME before goes down when the ratio keep increasing. The most optimum value of the ratio was proven to be 1 as suggested by JFE technology.



FIGURE 10: Effect of H<sub>2</sub>/CO ratio on DME production

Compared with the experimental done by Zhu Y. (2008), the DME yield was increasing when the H<sub>2</sub>/CO ratio is 2 before being decreasing. This different might occurs as Zhu Y. (2008) was using a combination of pure gas as the feed to symbolized as biomass.

#### 4.5 EFFECT OF OXYGEN TO BIOMASS RATIO (O/B)

Oxygen to biomass ratio (O/B) also giving a significant effect towards DME production. Oxygen is need in the gasification section which will react with the EFB in partial oxidation reaction to produced  $CO_2$  and  $H_2O$ . The oxygen is supplied at 170kpa and 25°C which was in the same condition with the supplied feed, EFB. The effect of O/B on  $H_2$  produced and DME produced was tabulated in the graph 2 below. The increase in O/B ratio makes the production for  $H_2$  gas and DME reducing.



FIGURE 11: Effect of Oxygen to Biomass (O/B) ratio on DME production

process

#### **4.5 EFFECT STEAM TO BIOMASS RATIO (S/B)**

Effect of steam flow into the DME production process also affecting the production. The optimum S/B ratio for the process is below 2 as the DME produced will be decreased when the S/B is more than 2. In contrast the Hydrogen produced after WGS reactor is keep increasing when S/B increasing.



Although hydrogen is highly used in DME synthesis reaction, but limiting reactant now changed to CO as the hydrogen is supply in excess. That explain why the DME produced in not linearly with the hydrogen produced. Both Hydrogen and Carbon Dioxide is needed in producing DME.

#### **4.6 EFFECT OF PRESSURE**

The effect of pressure towards the process also being studied by correlating it with the amount of DME produce. Different set of pressure were used to show the significant effect of it as shown in graph 3.



FIGURE 12: Effect of pressure towards DME production

Starting with the lowest possible pressure for reaction to occur which is at 170kpa, the pressure of the feed is increase gradually until 3000kpa. In order to have a better result, pressure of the steam and oxygen feed is keep maintain at 10 Mpa. Operating temperature of the DME Synthesis section also was maintain at 140°C which found to be the optimum temperature for DME production. From the run, we could see a trend of the DME production responding towards the various operating pressure.

The DME production started to increase while we increase the pressure. This trend is maintain up till pressure 100kpa where it started to show a decreasing trend.

The DME produced keep decreasing when the pressure increased. The optimum production happen at 100kpa.

## **4.7 EFFECT OF TEMPERATURE**

Temperature also is giving a significant effect towards DME production. Studied had been done to investigate the behaviour and trend of DME production in different temperature. The result of the simulation study for effect of temperature were tabulated in figure 14.



FIGURE 13: Effect of temperature towards DME production

From graph above, the trend of DME produced is in a decreasing trend as the temperature increase. When arrive at 300°C, the production is at the minimum and approaching zero limit. This situation might happening as the reaction of DME synthesis is highly exothermic which mostly favoured low temperature condition.

## **CHAPTER 5: CONCLUSION AND RECOMMENDATION**

As a conclusion, both objectives of the project is achieved. Single step of DME production process is simulated by using HYSIS simulation software and parametric study was performed on it to identify the optimum condition. In getting  $H_2$ /CO feed ratio of 1 for DME production, om37 of O/B and 0.27 S/B is needed

Operating parameter is giving a significant effect towards the DME production process especially  $H_2$ /CO ratio as the DME synthesis reaction is highly dependent on the Hydrogen and Carbon Monoxide as the reactant. Pressure and temperature are also giving direct effect towards the process.

Hopefully the research will benefit human in long term as we now facing the issue of depletion of fossil fuels and the emission of Green House Gases. Thus DME which is the 2<sup>nd</sup> generation of Bio-fuels seems as the best alternatives option after the 1<sup>st</sup> generation. By utilizing the wastes from agriculture activities like palm wastes to produce DME; we will make a better world tomorrow.

As a recommendation, a future work might do the double step of DME production process as to see if there is significant different between the single step. Furthermore, it also can be done in future by analysing the production process by using other type of biomass such food wastes.

## REFERENCES

Biomass Registration (2001) Biomass Registration 2001/77/EG

- Ju, F., Chen, H., Ding, X., Yang, H., Wang, X., Zhang, S., & Dai, Z. (2009). Process simulation of single-step dimethyl ether production via biomass gasification. *Biotechnol Adv*, 27(5), 599-605. doi: 10.1016/j.biotechadv.2009.04.015
- Laihong S., Yan G. & Jun X., (2007) Simulation of hydrogen production from biomass gasification in interconnected fluidized beds.
- Lanohalidanond K., Heil J., & Wirtgen C., (2006) THe PRoduction of Synthetic Diesel from Biomass.
- Lu, W.-Z., Teng, L.-H., & Xiao, W.-D. (2004). Simulation and experiment study of dimethyl ether synthesis from syngas in a fluidized-bed reactor. *Chemical Engineering Science*, 59(22-23), 5455-5464. doi: 10.1016/j.ces.2004.07.031
- Murni M., Khairuddin M. Y., & Abrar I. (2010) Simulation of Gasification with INsitu Carbon Dioxide Adsorption of Empty Fruit Bunch into Hydrogen
- Semelsberger, T. A., Borup, R. L., & Greene, H. L. (2006). Dimethyl ether (DME) as an alternative fuel. *Journal of Power Sources*, 156(2), 497-511. doi: 10.1016/j.jpowsour.2005.05.082
- Smith, Robin. (2005). *Chemical Process Design and Integration* (Vol. 1). England: John Wiley & Sons, Ltd.
- The International Energy Outlook 2013 (2013), International Energy Agency. Volvo Bio-DME Facts Sheet. (2012) Volvo Corp.

Volvo Bio-DME Facts Sheet. (2012) Volvo Corp.

- Wen W. L., Li H. T., & Wen. D. X., (2004) Simulation and experiment study of dimethyl ether synthesis from syngas in a fluidized -bed reactor
- Zhang, W. (2010). Automotive fuels from biomass via gasification. *Fuel Processing Technology*, 91(8), 866-876. doi: 10.1016/j.fuproc.2009.07.010
- Zhu, Y., Wang, S., Ge, X., Liu, Q., Luo, Z., & Cen, K. (2010). Experimental study of improved two step synthesis for DME production. *Fuel Processing Technology*, 91(4), 424-429. doi: 10.1016/j.fuproc.2009.05.001