Energy Transition with Dimethyl Ether(An Alternative Fuel to Diesel) to minimise the Environmental Impact

Introduction

Energy is vital to the advancement of modern society. Two energy sources exist renewable (such as geothermal, solar, hydropower and wind) and non-renewable energy (such as fossil fuels: coal, oil, and natural gas). Fossil fuels, particularly oil-based liquid fuels, which are non-renewable, almost satisfy the existing energy demand. Fossil resources are the primary source for meeting current energy needs through their diversity: diesel, petrol (for transportation), liquefied petroleum gas (for heating and cooking) and many other industrial building blocks such as propylene, butylene and ethylene (obtained through steam cracking). The demand for fuels and value-adding chemicals keeps rising. It must be tackled because there is a dramatic decrease in oil production and significant environmental issues, such as large carbon dioxide emissions, which causes global warming. Hence, the need to find an alternative to oil-based fuels. Much research is being undertaken to meet the growing demand for energy by creating new and more efficient technologies using available raw materials such as natural gas, coal and biomass instead of petroleum. These potential energy sources help generate synthesis gas, a versatile intermediate for chemical production and fuels. It is also considered a realistic way of using vast available sources because directly converting the sources mentioned above into fuels and valuable chemicals is practically not feasible.

Dimethyl ether is known for its environmental friendliness as a fuel. As shown in Table 1 It can be liquefied at a pressure of approximately 6 atm (at room temperature) or temperature of about -25^{o}C (in atmospheric pressure); therefore, it can be distributed or stored like Liquefied petroleum gas (LPG). It is a suitable replacement for diesel fuel due to its high cetane number (55-60) range which is greater than diesel fuel. DME has gained significant attention as an environmentally friendly alternative fuel because of its good burning characteristics, low SOx, NOx emissions and high cetane number.

Another main concern that needs to be addressed when considering alternative fuel is using existing infrastructure, including transport, handling, storage and distribution. This is necessary to reach economic viability. Dimethyl ether can be regarded as one of the potential fuels to achieve such. Dimethyl ether (DME) has continued to attract research interest as a possible replacement for liquefied petroleum gas and diesel due to the reduced emission of environmentally hazardous compounds. There are two processes for producing DME: a direct and indirect synthesis. The direct process has gained more research focus than the indirect due to its favourable thermodynamics and economics.

Table 1 *Physical properties of DME and other alternative fuels (Mondal and Yadav, 2019)*

Properties	DME	LPG	Diesel
Formula	CH_3OCH_3	C_2-C_5	-
Molecular weight, g/mol	46	44.09	-
Vapour pressure at 20^{o}C	5.1	8.4	-
Liquid density, g/cm^3	0.67	0.49	0.86
Cetane number	55-60	5	40-55
Boiling point, ^{o}C	-24.9	-42	125-400
Low Heating Value - LHV (kJg^{-1})	28.62	46.35	41.66
Sulfur content, ppm (parts per million)	0	-	~250

The reactions that occur in the direct process are as follows (Mondal and Yadav, 2019):

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H^{o}_{298} = -90.63 \text{ kJ/mol} \qquad \text{(Eq. 1)}$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H^{o}_{298} = -49.50 \text{ kJ/mol} \qquad \text{(Eq. 2)}$$

$$2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O \qquad \Delta H^{o}_{298} = -23.56 \text{ kJ/mol} \qquad \text{(Eq. 3)}$$

$$CO+H_2O \leftrightarrow H_2+CO_2 \qquad \Delta H^o_{298} = -41.13 \text{ kJ/mol} \qquad \text{(Eq. 4)}$$

The overall reaction is:

$$3CO + 3H_2 \leftrightarrow CH_3OCH_3 + CO_2 \qquad \Delta H^o_{298} = -245.95 \text{ kJ/mol} \qquad \text{(Eq. 5)}$$

A product in each step is a reactant in the next step, which increases the process's synergistic effect, leading to a higher conversion of syngas in a single step. This is beneficial for thermodynamics (Fleisch et al. 2012).

Fluidised bed reactors have high mass and heat transfer efficiencies and have been suggested by researchers as ideal for the direct process (Mondal and Yadav, 2019). The synthesis of DME from syngas is highly exothermic. Therefore, an efficient reactor is required industrially to produce a suitable yield of DME. Abashar et al. (2017) proposed using a multiphase fluidised bed reactor for the process with the potential of maximising yield.

A modified dual-phase fluidised bed reactor model provided by Jafari et al. (2004) for simulation in UniSim will be adopted. The modified dual-phase model comprises a bubble phase in plug flow and an emulsion or dense phase in continuous flow. In contrast, Lu et al. (2004) adopted a model composed of a bubble phase in plug flow and an emulsion or dense phase in plug flow. This study aimed to simulate and evaluate the direct synthesis of DME using a dual-phase fluidised bed reactor. A comparison was carried out between the fluidised bed model adopted by Lu et al. (2004) and the modified model proposed by Jafari et al. (2004). The fluidised bed reactors have high mass and heat transfer efficiencies, which are more appropriate as the production process from syngas is naturally exothermic (Mondal and Yadav, 2019).

Method

The process of producing DME was modelled and simulated using the UniSim simulator, which assists in carrying out automated calculations for the procedure. UNIversal QUAsi Chemical (UNIQUAC) activity model was selected for the process. The significant operations in the simulation include the production of syngas from natural gas, Synthesis of DME from syngas and Purification of DME. (Figure 1)

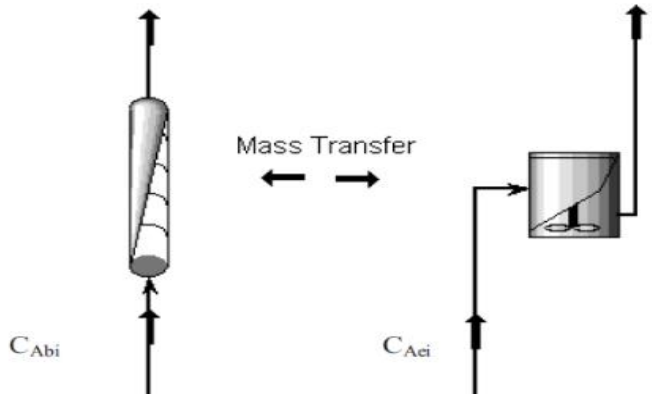

Figure 1 *Model of dual-phase fluidised bed reactor (Jafari et al. 2004)*

The simulation of the direct synthesis of DME was carried out. Despite its extensive use in chemical industries, a fluidised bed reactor module is not provided in process simulation programs. The UniSim process simulation program consists of only ideal reactors like Plug flow reactor (PFR) and Continuous stirred tank reactor (CSTR). A fluidised bed reactor is a non-ideal reactor and cannot be classified as only a PFR or a CSTR because the bubble and emulsion phase must coexist in the reactor (gas-solid fluidisation) (Jafari et al. 2004). Therefore, a combination of two ideal reactors in which the PFR represents the gas flow through bubbles and the CSTR represents the gas flow through the emulsion was used to model the dual-phase fluidised bed reactor.

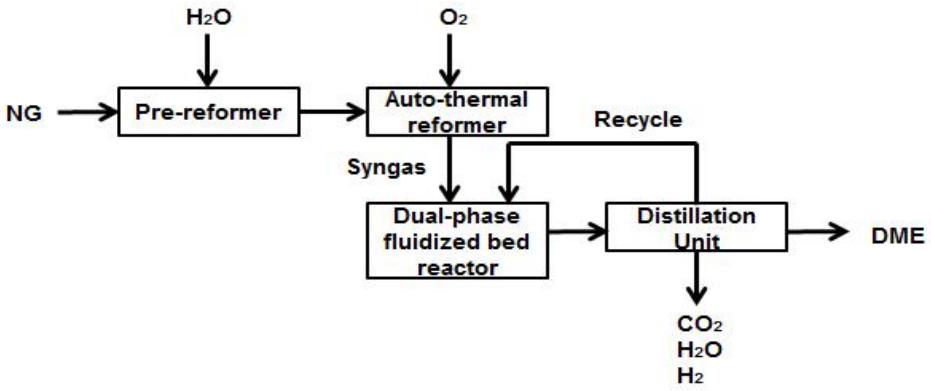

Figure 2 *Block flow diagram for the synthesis process from natural gas*

Lu et al. (2004) studied the performance of DME synthesis in a fluidised bed reactor through experiments. It was concluded that the efficiency of fluidised bed technology was greater than that of the slurry reactor and fixed bed technology for DME synthesis. The results for CO conversion and DME selectivity under the same conditions were 17% and 70% for the slurry reactor, 10.7% and 91.9% for fixed bed reactor and 48.5% and 97% for the fixed fluidised bed reactor. Compared with the fixed bed and slurry reactor, the fluidised bed reactor had negligible gas-solid mass transfer resistance and excellent temperature control due to the vigorous mixing of catalyst particles (Figure 2).

Fluidised bed reactors are generally modelled as multiphase systems comprising two or separate phases. Toomey and Johnstone (1952) originally proposed the two-phase theory of fluidisation. This theory explains that the gas-fluidised bed includes two phases; a bubble phase consisting of voids primarily free from particles and an emulsion phase composed of solid particles & interstitial gas.

In the simulation study by Lu et al. (2004) fluidised bed reactor used the P-P model (i.e. bubble phase and dense/emulsion phase were assumed to be in plug flow). But, according to Jafari et al. (2004), modelling the bubble phase in plug flow and emulsion phase in continuous flow for the fluidised bed is closer to real-life performance. This discovery led to this present study.

Results

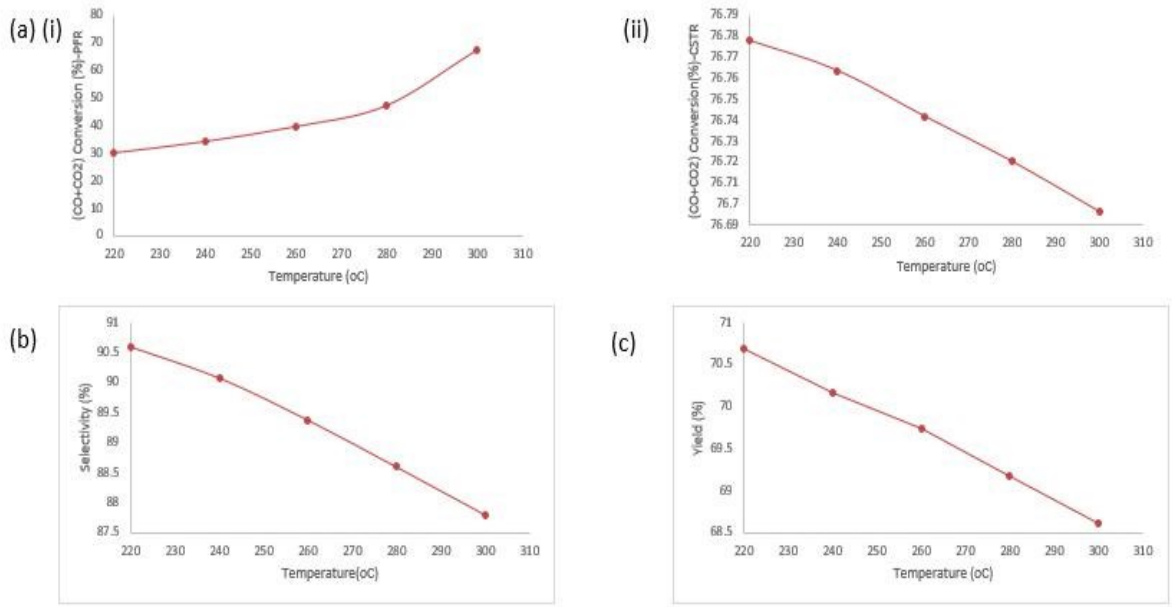

Figure 3 *Effect of temperature on (a) (CO +CO_2) Conversion in (i) PFR (ii) CSTR (b) DME Selectivity (c) DME Yield*

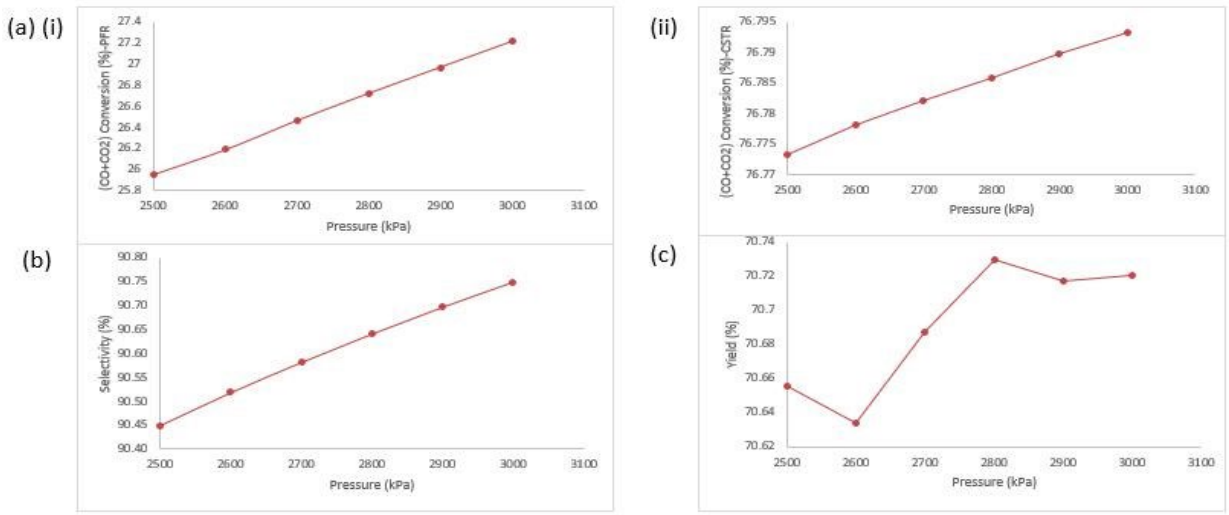

Figure 4 *Effect of pressure on (a) (CO +CO_2) Conversion in (i) PFR (ii) CSTR (b) DME Selectivity (c) DME Yield*

The simulation was conducted to investigate the influence of operating parameters such as temperature and pressure on CO, (CO+CO_2) conversion, selectivity and yield of DME. The temperature and pressure range used for this study were (220^{o}C – 300^{o}C) and (2500 kPa – 3000 kPa) respectively.

The results obtained at 260^{o}C and 2700 kPa were 89.4% DME selectivity, 69.7% DME yield, 99.994% CO conversion and 76.74% (CO+CO_2) conversion (Figure 3 & 4).

Conclusion

As shown in Figures 3 & 4 . the results indicated that the dual-phase configuration of a fluidised bed was efficient for DME production. The modified model of the dual-phase fluidised bed reactor as proposed by Jafari et al. (2004) used in this study (bubble phase in plug flow and emulsion phase in continuous flow) generally gave improved results (99.994% CO Conversion, 76.74% (CO + CO_2) Conversion, 89.4% selectivity and 69.7% DME yield) compared to that of Lu et al. (2004) (bubble and emulsion/dense phase both in plug flow) with CO conversion and DME selectivity as 48.5% and 97% respectively at 260^{o}C.

This study also proved that the second bed is susceptible to the composition of the catalyst bed, which was mainly observed in the CSTR at temperature increase. From the cost analysis, the return on investment is positive. Thus, producing DME using a dual-phase fluidised bed reactor is profitable.

Finally, future research should compare the efficiency of reactive dividing-wall columns (RDWC) with fluidised bed reactors in directly synthesising DME for industrial and commercial applications.

References

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