

HASIL CEK_Process Design Study of Methyl Tertiary-Butyl Ether Production Using Reactive Distillation

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Process Design Study of Methyl Tertiary-Butyl Ether Production Using Reactive Distillation

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Abstract—The increasing of gasoline demand cause, the need for octane number booster additives such as methyl tertiary-butyl ether, ethyl tertiary-butyl ether, triacetin and other additives is increasing. Methyl tertiary-butyl ether is one of the non-metallic substances that can be used as an octane number booster additive in gasoline up to 93.7 octane numbers and is not harmful to the environment because it does not form peroxide compounds. Methyl tertiary-butyl ether can be made by reacting methanol and isobutylene using the Amberlyst-15 catalyst on reactive distillation at a temperature of 70-90°C and 11 bar pressure. In this study, the effects of mole ratio of isobutylene and methanol and changes in reactive distillation design to methyl tertiary-butyl ether concentrations was examined. The best ratio of moles of isobutylene and methanol is 1:1.25. The design of reactive distillation for optimal methyl tertiary-butyl ether results is methanol feed on stage 9 with the number of stage 17, reactive zone in stage 2-11 with rectification zone in stage 1 and stripping zone in stage 12-17, reflux ratio 6. In the simulation process with a capacity of 100,000 tons per year using Aspen Plus, the conversion of methanol is 99% with the concentration of methyl tertiary-butyl ether is 97.48%.

Keywords—methyl tertiary-butyl ether, additives, reactive distillation

I. INTRODUCTION

A. Additives

Based on data from the National Energy Council, world oil production is projected to increase 11 million barrels per day in 2012 to 98 million barrels per day by 2035 [1]. This has resulted in the need for octane booster additives for gasoline fuels such as Methyl tertiary-butyl ether (MTBE), Triacetin [2] and other Bio-additive ingredients increase.

MTBE is a volatile compound made as a by-product of petroleum processing by reacting methanol and isobutylene [3]. Currently, methyl tertiary-butyl ether is being actively used to increase octane numbers from gasoline.

TABLE I. EFFECT OF MTBE CONCENTRATION ON OCTANE NUMBER OF GASOLINE

MTBE Concentration	Octane Number
0%	85.29
5%	87.30
10%	88.70
15%	89.80
20%	92.20
25%	93.70

Table 1 shows that the greater concentration of MTBE added to gasoline without other additives of octane booster, then higher octane number of the compound [4].

Ethyl tertiary-butyl ether is recognized as a suitable mixture for ethanol in gasoline. Ethyl tertiary-butyl ether is mixed into gasoline around 10-20%, usually around 9-12% where fuel consists of 70-84% gasoline and 5-20% ethanol. Ethyl tertiary-butyl ether dissolves alcohol in gasoline thereby significantly increasing octane numbers [5].

Triacetin has been used for pharmaceutical and cosmetics industry. On the other hand, triacetin is a promising alternative chemical to be transformed into fuel additive [6]. Adding 10% of triacetin to biodiesel can give better performance as compared to the pure biodiesel [7].

B. Materials and Reactive Distillation

The material used in this study was Methanol with 99% purity, Isobutylene with 32% purity and Amberlyst-15 as a catalyst.

Reactive Distillation (RD), combination of reaction and separation, is an alternative to the reactor which is followed by traditional distillation, especially when the mixture resulting from the reaction coming out of the reactor forms one or more azeotrope which is difficult to separate. The combination of reaction and separation in a single operating device not only reduces production costs but also provides other benefits such as uniform reaction heat, eliminating azeotrope, increasing conversion and higher selectivity [8].

The process that uses reactive distillation can increase the reactant conversion to close to 100% and combine the reactor with a separator so as to minimize operating costs. Besides methyl tertiary-butyl ether, reactive distillation is used to produce triacetin from glycerol [9].

C. Research Objective

The objective of this study was to determine the effect of mole ratio of materials and the effect of reactive distillation design changes on methyl tertiary-butyl ether concentration produced.

II. RESEARCH METHODOLOGY

A. Effect of Mole Ratio methanol and Isobutylene

The MTBE etherification reaction can be carried out in reactive distillation at 70 - 90°C and 11 bar pressure. The catalyst used is Amberlyst-15. The kinetics model in the reaction between isobutylene and methanol is (1), (3) and (4).

$$r = k \frac{\alpha_{IB}}{\alpha_{MeOH}} - \frac{1}{K_s} \frac{\alpha_{MTBE}}{\alpha_{MeOH}^2} \quad (1)$$

The temperature depends on the reaction rate constant k given by the Arrhenius equation (2).

$$k = k^* T^* \exp \left(-\frac{E}{R} \frac{1}{T T^*} \right) \quad (2)$$

$$r_{forward} = 3.67 \times 10^{12} \times \exp \left(\frac{-92440}{RT} \right) \frac{X_{IB}}{X_{MeOH}} \quad (3)$$

$$r_{backward} = 2.67 \times 10^{17} \times \exp \left(\frac{-134454}{RT} \right) \frac{X_{IB}}{X_{MeOH}^2} \quad (4)$$

Because the reaction is in the form of first order, there is an excess raw material for more optimal results [10].

B. Process Design of Methyl Tertiary-Butyl Ether

In this study, the methyl tertiary-butyl ether plant with a capacity of 100,000 tons/year using reactive distillation was designed using Aspen plus simulation software. Then the results will be analyzed the effect of design changes from reactive distillation with variations in the effect of the location of the methanol feed, the effect of the number of stages used, the effect reaction zone location, and the effect of reflux ratio on methyl tertiary-butyl ether concentrations produced.

III. RESULTS AND DISCUSSION

A. Effect of Mole Ratio Methanol and Isobutylene

The methyl tertiary-butyl ether formation reaction of methanol and isobutylene is a one-order reaction with a mole ratio of raw material 1:1. Addition of moles comparison of raw materials can affect the methyl tertiary-butyl ether concentration produced. The effect of the mole ratio of methanol and isobutylene is shown in figure 1.

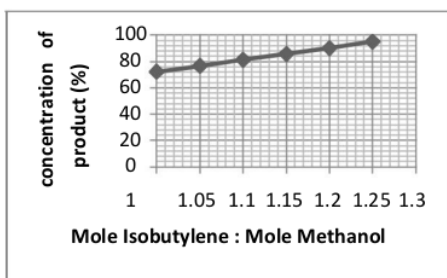


Fig. 1. Effect of mole ratio of methanol and isobutylene

Figure 1 shows that the higher the ratio of moles of isobutylene to moles of methanol, the higher the concentration of methyl tertiary-butyl ether produced. At a ratio of 1:1 the concentration of methyl tertiary-butyl ether produced was 72.23% while the ratio of 1:1.25, methyl tertiary-butyl ether concentration reached 94.88%.

B. Effect of Feed Methanol Location

From the results, the location of the methanol feed in the reaction zone affected the methyl tertiary-butyl ether concentration produced. The effect of methanol feed location can be seen in Figure 2. Reactive distillation was designed with 16 stages consisting of rectification zones at stage 1-3, reactive distillation zone on stage 4-10 and stripping zone on stage 11-16. The effect of feed methanol location shown in figure 2.

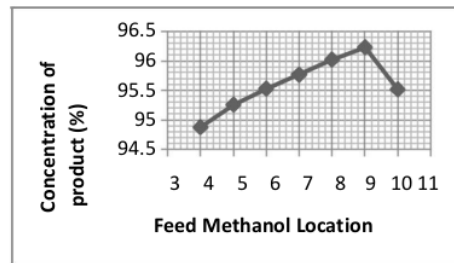


Fig. 2. Effect of feed methanol location

Figure 2 Shows that the greatest concentration of MTBE is obtained if the methanol feed is entered through the stage which is in the lower area of the reaction zone because of the increasing contact between methanol and isobutylene, resulting in more MTBE concentrations. Methanol entering stage 9, will be "pushed" upwards by MTBE, whose fraction is lighter so that contact with isobutylene is greater in the reaction zone and produces higher purity products.

The concentration of MTBE decreases if methanol is entered through stage 10, this is because the isobutylene stage feed which is a light phase is above the methanol feed stage so that the contact reactants in the reaction zone are reduced because isobutylene goes up the reaction zone while methanol down the reaction zone so that the product is produced a little.

C. Effect of the Number of Stage Effect of Reaction Zone Location

The number of stages on RD affects the amount of methyl tertiary-butyl ether concentration produced, the effect can be seen in Figure 3.

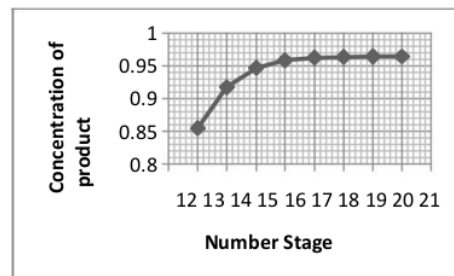


Fig. 3. Effect of the number of stage

Figure 3 shows the MTBE concentration produced increases with increasing number of stages but at stage 17 to a higher number of stages, a small increase in MTBE

concentration. This is because the addition of the number of stages will affect the location of the feed from methanol and the number of separating zones added.

D. Effect of Reaction Zone Location

The number of reaction zones can show how much contact the raw material requires and how many separations are needed to obtain maximum methyl tertiary-butyl ether results. The effect of the location of the reaction zone on the methyl tertiary-butyl ether concentration produced can be seen in Table 2.

TABLE II. EFFECT OF REACTION ZONE LOCATION

Reaction Zone	MTBE Concentration (%)
2 – 11	97.74
3 – 11	97.10
4 – 11	96.23
5 – 11	95.51

Table 2 shows the greatest MTBE concentration obtained in the stage 2-11 reaction zone of 97.74%, this shows that with the reaction zone on stage 4-11, the rectification zone at stage 1-3 and the stripping zone on stage 12-18 contact occurs. the best between raw materials and separation occurs well.

E. Effect of Reflux Ratio

The addition of reflux will increase the performance of separating and recycling raw materials that do not react to the reaction zone, thereby increasing conversion. Another effect of the addition of reflux is the reduced concentration of the raw material in the distillate and the temperature in the reaction zone will decrease.

MTBE purity will initially increase with increasing reflux ratio, reaching maximum concentration, then it will decrease if the reflux ratio increases. The effect of reflux ratio on the concentration of MTBE products is shown in figure 4.

The purity of MTBE products will always increase as the reflux ratio increases as long as the tower operates normally. When the reflux ratio is too small, the separation does not work properly so the product purity is low. When the reflux ratio is too high, the residence time in the reaction zone is too short to produce a product with a high concentration so that the product's purity will decrease.

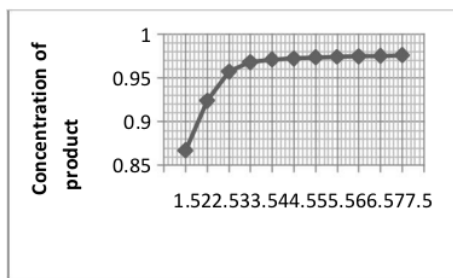


Fig. 4. Effect of reflux ratio

Figure 4 shows that the MTBE concentration had a large increase until the reflux 3.5 ratio was close to constant, this was due to the reduced reactants that had to be refluxed because most of them had become products. The best reflux ratio to produce the methyl tertiary-butyl ether product with the highest concentration is with a reflux ratio of 7, which is 97.59%, but the increase is not too far from the results of MTBE in reflux ratio 6 which is 97.48%. If the reflux ratio is increased by more than 7, the product purity will decrease.

IV. CONCLUSIONS

From the results of the study, it can be concluded that the optimal operating conditions to produce methyl tertiary-butyl ether are at temperatures of 70-90°C 11 bar pressure and reflux ratio 6, with reactive distillation in the form of reactive zone in stage 2-11, rectification zone at stage 1 and stripping zone on stage 12-17.

Methanol feed is flowed in stage 9 because methanol is the heaviest substance among the other components so it will tend to flow down the reaction zone then "pushed" upwards and will react with isobutylene fed on stage 3. With reflux ratio 6 so that the material residence time the standard in the reaction zone is not too short, resulting in high concentration of methyl tertiary-butyl ether.

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