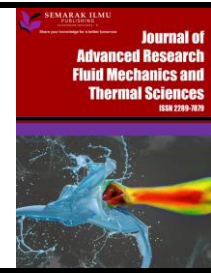




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Cost And Product Optimization of Upgrading Light Naphtha Using Pressure Swing Adsorption Method by Aspen Adsorption Simulation

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ABSTRACT

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Light naphtha is an organic compound produced from the distillation process that is often sold at a low price because of its poor performance, especially in the value of Research Octane Number (RON). The goal of this study was to improve the quality of naphtha to become a useful fuel with qualifying performance that is High Optimum Mogas Component (HOMC) by using the Pressure Swing Adsorption (PSA) method with the help of Aspen Adsorption simulations to find the most optimal combination of zeolite adsorbents (Beta and 5A) to use in the process. The principle of this quality improvement is to separate the compounds contained in naphtha that have low RON values from those that have high RON values so that the performance of naphtha that has gone through the adsorption process can be maximized. For this study, the RON target from HOMC is 95, while the value of RON for feed light naphtha ranges from 61-65. There are three compounds simulated in this PSA process, n-pentane and n-hexane as compounds that want to be separated because they have low RON values from isopentane which has a high RON value. Furthermore, after acquiring the combination of adsorbents that resulted in the products that have the highest RON, the economic potential of all variables was evaluated to get the most optimal process to use. The economic potential is also analyzed to find the profit of the PSA process. The most optimal results are obtained when the adsorbent configuration produces the product with the highest RON and produces high economic potential. The results showed that the most optimal adsorbent combination is to use 30% Zeolite Beta; 70% Zeolite 5A with product results having the highest RON of 84 and economic potential of US\$ 114,410,163.92.

1. Introduction

Over time, the urgency of the world to the energy crisis is very high and many countries are making efforts to maintain their energy security [1]. Indonesia, as the country with the fourth most populous population in the world, has an impact on the high energy needs in Indonesia. In meeting domestic energy needs, Indonesia has so far still made fossil fuels a primary energy source such as fuel oil. In 2019, Indonesia's energy consumption fuel type became the main choice of the community

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touching 42% of energy consumption or 415.8 million oil barrels equivalent. This consumption is projected to be increased with an average growth rate of 2.8% per year. The impact of the energy crisis and high energy needs then encourage development to improve the efficiency of the use of fuel oil in terms of performance [2]. In order to improve the quality of fuel required by the community, a mixed material is required to improve the fuel performance, such as High Octane Mogas Component (HOMC). High Octane Mogas Component (HOMC) is a high-octane hydrocarbon compounds which consist of aromatic hydrocarbons and olefins and used as a mixed material to obtain better fuel performance [3]. One method to increase the aromatic hydrocarbons and olefins in light naphtha is pressure swing adsorption (PSA).

Several studies and studies relevant to PSA on upgrading chemical commodities including naphtha have been carried out several times. Chang et al. studied the influence of adsorber models and studies related to the influence of operating specifications on adsorption performance [4]. Dobladez et al. studied an external influence in the form of the influence of the type of adsorbent used on adsorption performance [5]. Chen et al. studied the pressure-swing adsorption process to upgrade biogas quality [6]. Pruksathorn et al. studied the modelling from adsorption in the liquid or solution phase to obtain pure ethanol [7]. Barcia et al. studied the octane upgrading of naphtha which containing pentane/hexane with pressure swing adsorption method [8]. Pratiwi et al. do a simulation about hydrogen purification by Pressure Swing Adsorption [9]. Anugraha et al. studied that the light naphtha can be used as raw materials to become commercial fuels using blending method [10].

However, the operations that have been implemented until now can be said to still not implement process efficiency that meets the needs of two aspects, namely the economic aspect and the quality aspect of the products produced later. In addition, from several existing studies, slices were obtained to support this research by developing an analysis of equipment specifications that are suitable for use by reviewing the costs and profits generated, because there has been no study that leads there. Therefore, in this study, a study and simulation of process swing adsorption processes to upgrade light naphtha which considering economic aspects and product quality aspects were carried out. The light naphtha used in this study refers to light naphtha product from mini oil rig in our previous study [11].

2. Methodology

To simulate the upgrading of light naphtha to HOMC via PSA methods, a reduced light naphtha composition system comprising three compound groups based on their size was chosen. Thermodynamic properties are calculated via the Peng-Robinson Equation of State (PR-EOS). The simulation environments were employed on Adsim (Aspen Technology, Inc.) to dynamically simulate PSA phases: adsorption and bed regeneration. In addition, Microsoft Excel (Microsoft Corporation) was used for estimating isotherm parameters by fitting adsorption isotherms onto adsorption equilibrium data from the literature for pure n-pentane, n-hexane, and iso-pentane with 5Å Zeolite and zeolite beta respectively.

2.1 Data Collection

Data collection about how light naphtha is described as the molecule composition. One used method that is dependent on pressure variables is Pressure Swing Adsorption (PSA). PSA is one of the adsorption methods with high pressure operated and when a fluid flow through it, some component will be adsorbed because of high pressure [4]. For the liquid light naphtha used in this study, the properties are itemized in Table 1. The concept of the separation of PSA is by the molecular

size of the component in the fluid so if we want to use this method as upgrading of light naphtha, it needs to specify the molecular size of the component in light naphtha as Table 1 [11,12].

Table 1
 Composition and Molecular Size of Light Naphtha

Components	Composition (mol%)	Molecule Width, l (Å)	Molecule Length, p (Å)
Butane	0.11	2.17	8.334
N-Pentane	13.3	4.154	9.87
N-Hexane	30.72	4.154	10.617
Heptanes	2.6	4.150	11.5
2-Methyl-Pentane (2 MP)	10.4	5.50	9.316
3-Methyl-Pentane (3 MP)	9.37	5.467	11.782
2,3-Di-Methyl-Butane (2,3 DMB)	1.66	5.72	8.045
iso-Pentane	11.69	5.90	8.334
Cyclohexane (CH)	5.84	0.69	6.0
Methyl-Cyclo-Pentane (MCP)	8.69	6	-
Benzene	3.18	6.7	7.4
2,2-Di-Methyl-Butane (2,2 DMB)	0.49	6.744	8.031
Cyclo-Pentane (CP)	1.95	6.79	-
Feed fraction that will be used in simulation:			
N-Pentane	0.1333		
N-Hexane	0.3272		
iso-pentane	0.533		

PSA needs some properties to be characterized such as isotherm parameters that represent the reaction between components used with the adsorbent about how many components will be adsorbed into the adsorbent in some of operating conditions [14].

The adsorbent also needs to be specified, to be used in upgrading light naphtha. Zeolite is the most suitable adsorbent to be used, but zeolite has so many types, such as 4A, 5A, BETA, 10X, 13X, and so on with each of its characteristics. Zeolite 5A and BETA is most likely to be used as adsorbent of hydrocarbons because of light naphtha's molecular size, so this paper will use a combination of two adsorbents in PSA and analyze which one has the best performance and highest economic potential and can be used as commercial.

ASPEN Adsorption is the software that has features to simulate Pressure Swing Adsorption. It can specify the adsorber beds specification, feed and product stream, cycle and valve scheduler for PSA, and the others that supported from the experimental data of Pressure Swing Adsorption. It is used in this experiment to simulate the case described before. The result hopefully can be a recommendation about the PSA and adsorbent configuration for PSA installation in the real plant.

2.2 Process Modelling

To simulate the upgrading of light naphtha to HOMC via PSA methods, a reduced light naphtha composition system comprising three groups based on their size was chosen. Thermodynamic properties are calculated via the Peng-Robinson Equation of State (PR-EOS). The simulation environments were employed on Adsim (Aspen Technology, Inc.) to dynamically simulate PSA phases: adsorption and bed regeneration. In addition, Microsoft Excel Solver (Microsoft Corporation) was used for estimating Langmuir isotherm parameters by fitting adsorption isotherms equilibrium data from the literature for pure n-pentane, n-hexane, and iso-pentane with 5Å Zeolite and zeolite beta respectively.

2.2.1 Adsorption isotherms

The type of isotherm used in this study is Langmuir type 3, so it requires four isotherm parameters obtained from the results of previous experiments. Type isotherm Langmuir 3 uses maximum loading by paying attention to temperature and partial pressure variables with 4 independent parameters which can be more accurate compared to Langmuir 1 or Langmuir 2. The Langmuir isotherm describes an increasing surface of occupancy as a function of pressure up until the entire surface area is coated with the molecules. The type of 1, 2, and 3 describes of how much the parameters is applied in the equations [15].

Based on Santos et al., the type of base parameter used in determining isotherm parameters there are two types of database data, namely concentration or partial pressure [16]. Because in this study the temperature applied in the naphtha light feed of 473 K and a pressure of 8 bars, the form of light naphtha in these conditions is gas, so the database data used is partial pressure. The equation used as a data fitting later is Langmuir 3 as written on Eq. (1).

$$W_i = \frac{(IP_1 + IP_2 \cdot T) \cdot IP_3 \cdot \exp\left(\frac{IP_4}{T}\right) \cdot P_i}{1 + IP_3 \cdot \exp\left(\frac{IP_4}{T}\right) \cdot P_i} \quad (1)$$

where W_i (kmol/kg) is the loading of species i ; T and P_i stands for temperature (K) and partial pressure of species i (bar), respectively; and IP_1 (kmol/kg), IP_2 (kmol/kg/K), IP_3 (bar^{-1}) and IP_4 (K) are the Langmuir III parameters.

Figure 1 show the adsorption equilibrium isotherm experimental data for n-pentane, isopentane and n-hexane in Zeolite Beta and Zeolite 5A from Barcia et al. and Silva et al [17,18]. The calculation of parameters will later use the above equation to get *loading* in calculations and obtain calculation results that will later be adjusted to the *error* method with experimental data so that four isotherm parameters are expected with *solver* calculations on *the spreadsheet* by minimizing errors and summarize in Table 2.

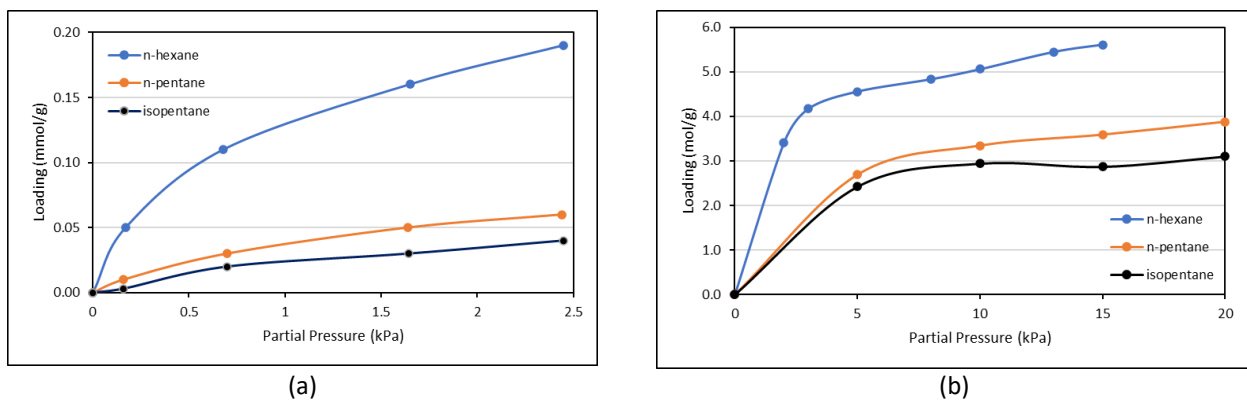


Fig. 1. The adsorption equilibrium isotherm for n-pentane, isopentane and n-hexane: (a) Zeolite Beta; (b) Zeolite 5A [17,18]

Table 2

Langmuir III Parameters for Adsorption on Zeolite Beta and Zeolite 5A

Adsorbent	Zeolite Beta				Zeolite 5A			
Component	IP1 (mol/g)	IP2 (mol/gK)	IP3 (1/bar)	IP4 (K)	IP1 (mol/g)	IP2 (mol/gK)	IP3 (1/bar)	IP4 (K)
<i>n-pentane</i>	0.0013	-2.69E-06	0.013	4000.00	0.00081	0.0000003	0.28	2100
<i>n-hexane</i>	1.00	-0.002	-0.003	5002.48	0.00079	2E-09	0.59	2360
<i>i-pentane</i>	0.0013	-2.75E-06	0.0136	3976.64	-	-	-	-

2.2.2 Adsorbent selection

The selection of adsorbent methods for adsorption is due to the separation process using zeolite has a high selectivity value and uniform pore size on a high surface area. Where one of the zeolites that has a good performance in increasing the octane value of the hydrocarbon mixture is Zeolite 5A which has a pore diameter of 5A with a Linde type A lattice structure with Ca cation, where the diameter value is between the diameter or size of the linear and branched alkane. Thus, resulting in a high selectivity value for hydrocarbon separation.

The derived properties for the adsorbent are presented in Table 3. The selection of these two bed layers is an attempt to increase the octane value again where zeolite beta has been shown to be used as a layer that separates the C6 single chain from the total mixed compounds thus increasing the average value of THE RON obtained [18].

Table 3
 Properties of Zeolite 5A and Zeolite Beta [8]

Properties	BETA	5A
Inter Voidage (ϵ_i)	0.49	0.314
Intra Voidage (ϵ_p)	0.4	0.35
Pore Diameter (A)	6.7	5
Bulk solid density of adsorbent (ρ_p) (kg/ m ³)	1.180	1.130
Adsorbent particle radius (R_p) (m)	7.95×10^{-4}	7.95×10^{-4}
Shape Factor (Sfac)	0.8	1.0
Mass Transfer Coefficient of iso-pentane (1/s)	0.5003	0
Mass Transfer Coefficient of n-hexane (1/s)	0.0513	0.0577
Mass Transfer Coefficient of n-pentane (1/s)	0.2844	0.4017
Adsorbent Specific Heat Capacity (Cps) (MJ/KgK)	0.865	0.865
Constant for heat of adsorption of Isopentane (MJ/kmol)	-58.7	0
Constant for heat of adsorption of n-hexane (MJ/kmol)	-84.5	-59.41
Constant for heat of adsorption of n-pentane (MJ/kmol)	-63.8	-55.23
Specific Area of Adsorbents (a_p) (1/m)	1924.52	2588.6

2.2.3 Process variables

Based on Figure 1, the two beds are installed with these specifications and assumptions on simulation. The specifications and assumptions used for both beds on simulations are tabulated in Table 4. The specification of the operating condition as controlled variables are listed on Table 5 below. Two Beds are applied and connected with some valves and pressures set to control the flow when PSA is operated and simulated. The full flowsheet is displayed in Figure 2. The basic explanation of the overall process is when adsorption is applied to Bed 1, Bed 2 will depressurization and vice versa. There are some operation units used, they are

- i. B1 & B9: Bed Adsorber (Used to specify the isotherm and adsorption parameter)
- ii. B2: Product Block (used to display the result of PSA main product)
- iii. B4: Feed block adsorption (used to specify the component list and operating condition of the feed)
- iv. B23: Waste Block (used to display the result of PSA undesired product)
- v. T1, T2: Gas Void in Bed (used to specify the initial condition of pressure and as the pressure setter on and under beds)

- vi. TP, TF, TW: Gas Void Between Bed (used to specify the initial condition of pressure and as the pressure setter between beds)
- vii. VF, VF1, VF: Valve Feed (used to specify the adsorption flow in a cycle, either on or off)
- viii. VP, VP1, VP2: Valve Product (used to specify the main product flow in a cycle, either on or off)
- ix. VW, VW1, VW2: Valve Waste (used to specify the undesired product flow in a cycle, either on or off)

Table 4

Vessel Specification

Parameter	Description
<i>Component List</i>	Using n-pentane, n-hexane, dan i-pentane as representative from unstability component in <i>light naphtha</i>
<i>Fluid Packages</i>	Peng Robinson
Layers	Double Layer (Zeolite Beta and Zeolite 5A)
Layer Type	Vertical 1-D
Heat Exchanger Type	None
<i>Discretization Method</i>	QDS 1
<i>Material / Momentum Balance Assumption</i>	<i>Convection Only / Ergun Equation</i>
<i>Kinetic Models</i>	<i>Solid with Lumped Resistance</i>
<i>Isotherm</i>	<i>Langmuir 3 with Partial Pressure variable</i>
<i>Energy Balance Assumption</i>	<i>Non-Isothermal with No Conduction with specifying heat transfer coefficient dan heat of adsorption</i>
<i>Reaction</i>	None

Table 5

Operating Conditions

Specification	Value
Feed Flowrate (m ³ /h)	70.7
Feed Pressure (bar)	10
Product Pressure (bar)	8
Operating Temperature (K)	473

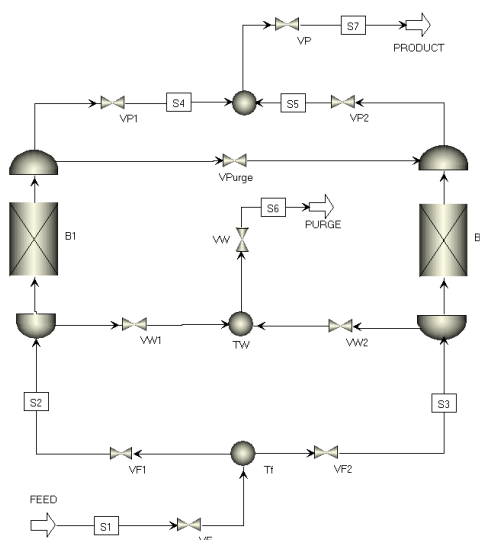


Fig. 2. Full Flowsheet of PSA

With two beds applicated, it needs to specify the step of PSA with cycle organizer. A cycle contains of 4 steps with a schedule as listed below in Table 6. The time is set as 90 hours with 5 cycles, so every cycle has 18 hours. The cycle time applied is because of adsorption and desorption process is ideally operated in 8 hours and each of blowdown process in 1 hour as Step 1 with 8 hours, step 2 with 1 hour, step 3 with 8 hours, and the rest with 1 hour [19]. Code of 0 represents that valve is closed, 1 is totally open, and 2 is open with specified Valve Characteristic value (Cv).

Table 6
 Scheduling of Valve in Pressure Swing Adsorption Process

Step	Process	VF	VF1	VF2	VP	VP1	VP2	VW	VW1	VW2	V Purge	Time (hours)
1	Adsorption Bed 1, Purge Bed 2	1	1	0	1	1	0	1	0	1	2	8
2	Blowdown Bed 1, Pressurize Bed 2	1	0	1	1	0	1	1	1	0	0	1
3	Adsorption Bed 2, Purge Bed 1	1	0	1	1	0	1	1	1	0	2	8
4	Blowdown Bed 2, Pressurize Bed 1	1	1	0	0	1	0	1	0	1	0	1

2.3 Variable and Performance Analysis

2.3.1 Variable analysis

The main goal of this experiment is to optimize the cost and product of upgrading light naphtha using Pressure Swing Adsorption (PSA), so it uses the variable in adsorbent ratio customizing with range 10% in every variables. The two variables used as explained before are 5A Zeolite and BETA Zeolite, with these specifications listed in Table 7.

Table 7
 Variables of Experiment

Variables	1	2	3	4	5	6	7	8	9	10	11
5A Zeo	100%	90%	80%	70%	60%	50%	40%	30%	20%	10%	0%
BETA Zeo	0%	10%	20%	30%	40%	50%	60%	70%	80%	90%	100%

2.3.2 Performance analysis

With the product of the desired adsorption process is High Octane Mogas Component HOMC. In determining the octane value of HOMC determined will be based on one of the HOMC mass production that has been carried out by PT. Pertamina Refinery Unit (RU) IV Cilacap which has research octane number (RON) value of more than 93. So that a calculation of RON from the results of simulation products based on the composition of isomerization obtained with Eq. (2).

$$RON = \sum_{i=1}^N v_i (RON)_i \tag{2}$$

where v_i is volume fraction of species i , RON_i is the research octane value of species i and N is the total species in the mixture.

The RON product will be calculated based on multiplication between the volume fractions of each composition with the RON value of each composition that has been set. The RON database are obtain from literature [20,21]. The end result of the adsorption process generally has a higher RON value

than crude naphtha, but the value is still much lower than 95. Therefore, to achieve the expected RON value, the product of PSA process is blended with a certain amount ethanol to reach the RON value of 95. The ethanol addition amount is calculated using the following Eq. (3)

$$V_{ethanol} = \frac{V_{HC}(95-RON_{HC})}{(RON_{ethanol}-95)} \quad (3)$$

where $V_{ethanol}$ is the additional ethanol volume, V_{HC} is the volume of hydrocarbon product from PSA process, $RON_{ethanol}$ is RON value of ethanol and RON_{HC} is RON value of hydrocarbon product from PSA process.

2.4 Economical Analysis

The economic analysis in this study is focused on the Total Annual Cost (TAC) and Economic Potential (EP). The formula for calculating the Total Annual Cost (TAC) is taken from Robin Smith, 2005 which are obtained from Total Operating Cost (\$/ year) and Annualized Capital Cost (\$/year) [22]. The calculation of economic potential (EP) of upgrading light naphtha is obtained from the difference between income per year with the total annual cost and income tax that must be incurred [23].

$$TAC = \text{Annualized Capital Cost} + \text{Operating Cost} \quad (4)$$

$$EP = \text{Income Sales} - TAC \quad (5)$$

The basis economy used here is the cost of adsorbent and it will make a great difference between each of the economic potential variables. The cost of the adsorbent is listed in Table 8 below.

Table 8
 Adsorbent Prices on 2021

Adsorbent	Prices Range (Year 2021)
Zeolite 5A	US\$1,5-US\$3/kg
Zeolite Beta	US\$100-US\$300/kg

Beside it, there are some basis price that used in calculating the economical aspect, such as energy costs that also will make difference between variables, listed on Table 9.

Table 9
 Basis Economy and Energy Cost

Utility	Prices Range (Year 2021)
Steam	\$12 c/t
Cooling Water	\$1 c/t
Electricity	\$1.5 c/MJ

3. Result and Discussion

3.1 The result of PSA Simulation and Product Analysis

Simulation of PSA supply the result of the purity of iso-pentane as the highest quality of component and RON calculation. The one variable with the highest RON number is the best performance variable. The result is supplied in Table 10.

The Table 10 presents that the best performance of the adsorbent combination is when we use 90% Zeolite BETA and 10% Zeolite 5A. This represents that Zeolite BETA is more effective to use when adsorbing light naphtha because of its pore diameter is >6,7 A so it is possible that all of the components is adsorbed inside them. This is because 6,7 A is larger than all of the molecular width in light naphtha when the molecule is flowing in a radial direction. Zeolite 5A has 5 A diameters which are only can adsorb components with molecule size below it, like n-butane, n-pentane, n-hexane, and heptanes. The 90% BETA : 10% 5A variable has the highest purity of iso-pentane, but it has slightly differences with some variables like 80%:20% ; 70%:30% ; 60%:40% ; 30%:70%. If the RON number is counted, it also presents a little difference from other variables. So, it can't be said that 90% BETA: 10% 5A is the most optimum adsorbent combination. It needs to be reviewed from economic aspect. The RON calculation is provided in the Figure 3.

Table 10
 The purity of iso-pentane based on simulation

Variable (Beta:5A)	% Iso-Pentane	% n-Pentane	% n-Hexane
100% Beta	0.883	3.63E-21	0.11604
90% : 10%	0.975919	3.03E-23	0.0240813
80% : 20%	0.975884	1.30E-22	0.0241158
70% : 30%	0.975595	3.01E-29	0.024405
60% : 40%	0.974765	8.13E-27	0.0252347
50% : 50%	0.973951	0	0.0260486
40% : 60%	0.972782	1.02E-23	0.0272178
30% : 70%	0.975308	1.72E-23	0.0246918
20% : 80%	0.945438	4.93E-24	0.0545621
10% : 90%	0.901064	1.01E-19	0.0989362
100% 5A	0.892799	1.51E-21	0.107201

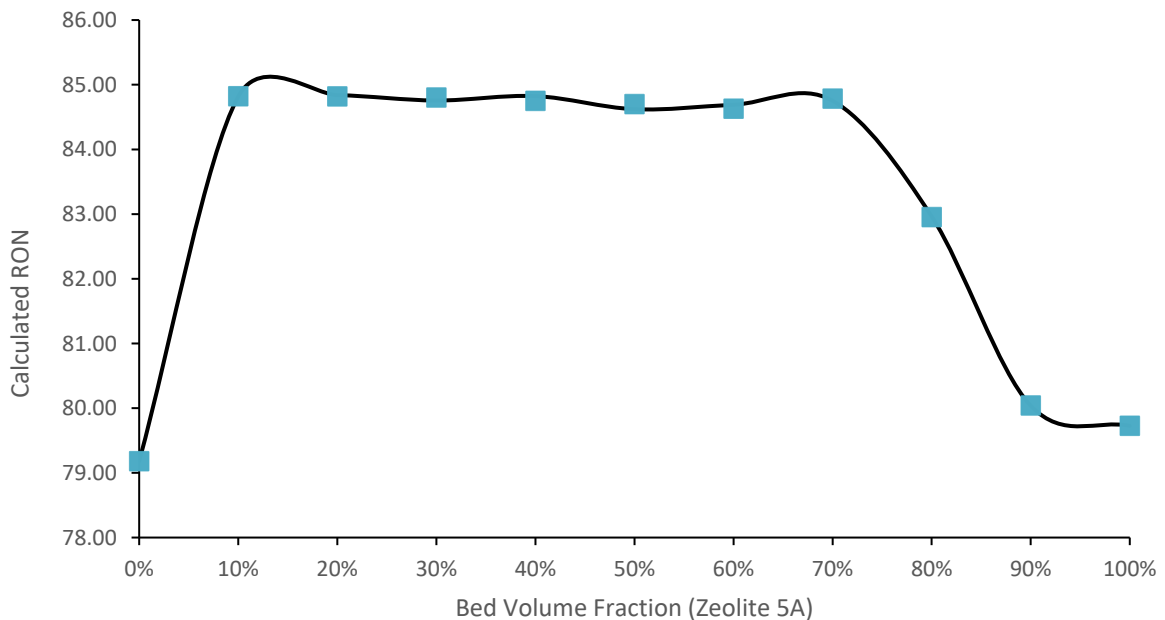


Fig. 3. Effect of Adsorbent Composition to RON

The concept of RON calculation is fraction of component multiplied with RON of individual component. From the RON calculation, it can be said that some of variables has the same number of RON. It supports the statement before that it needs to be reviewed from economical aspect. The

highest RON of all variables is 84.8 which is far from the HOMC RON target, so that it is needed to be blend with ethanol with RON 120. The target RON is 95, so the higher RON from the PSA output will need fewer amount of ethanol that also reduce the capital and operation cost invested. Figure 4 shows the ethanol needs of every variable.

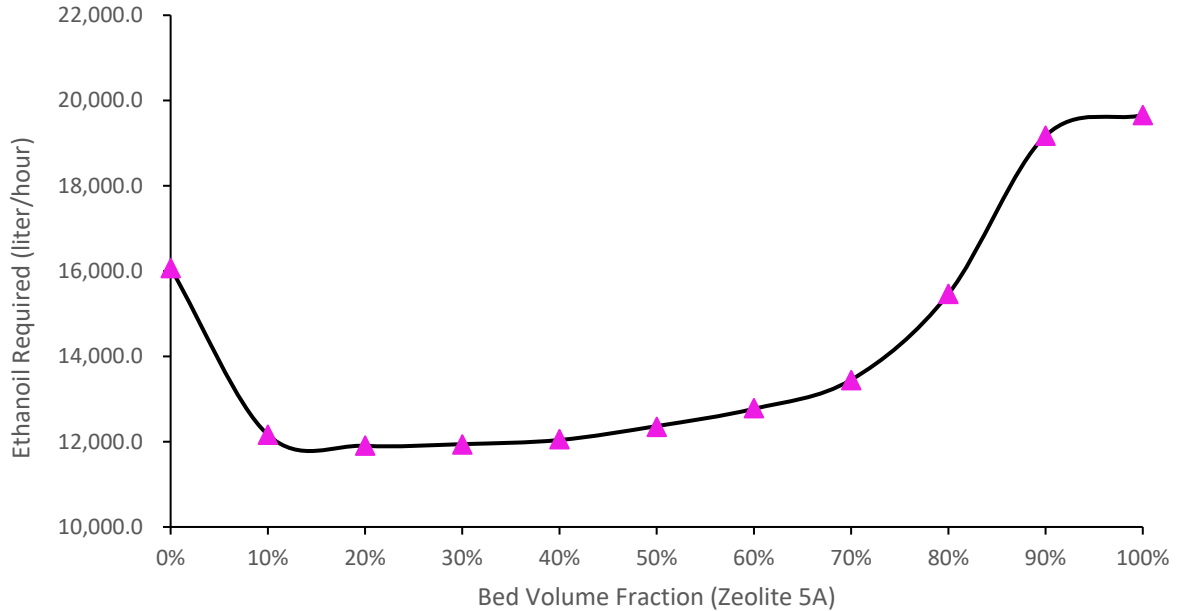


Fig. 4. Amount of Ethanol Requirement in Various Adsorbent Composition

3.2 Economic Aspect

The method of economic aspect calculation is the Total Annual Cost (TAC) method which is combination of Total Operating Cost and Annualized Capital Cost. Annualized Capital Cost is the annualized value total of capital cost invested in operation unit used, such as adsorber beds, compressor, heater, and cooler, operating cost invested to steam, electricity and cooling water, and fixed charge that invested to annual cost beside two points before, such as: tax, assurance, and others. The Total Operating Cost is the cost incurred of the process operation such as raw materials cost and energy cost. The TAC invested in every variable is shown in Figure 5. Maximum Point of total annual cost happen if the adsorber use ratio of 100% Zeolite 5A and the minimum point happen if the adsorber use ratio of 80% Zeolite 5A : 20% Zeolite BETA.

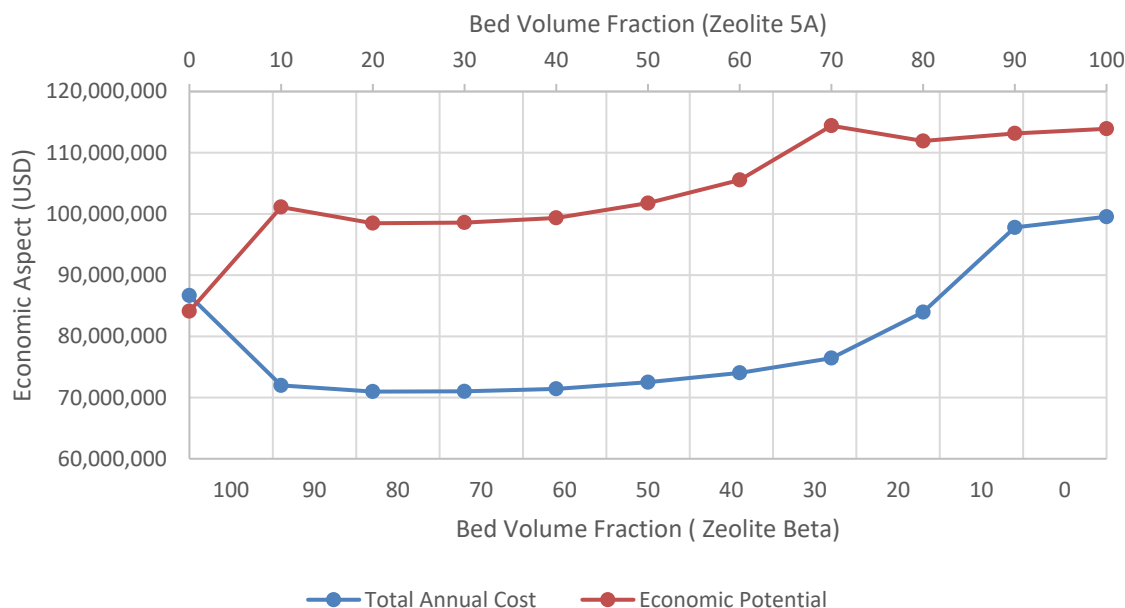


Fig. 5. Economic Potential and Total Annual Cost Invested in Various Adsorbent Composition

From the graph, it can be said that the fewest annual cost is in variable 70% BETA and 30% 5A with US \$ 76,447,067.17 every year. This is because the 5A zeolite is cheaper than zeolite BETA.

The Economic Potential is obtained from the difference between income sales per year with the total annual cost. If the gasoline price is stable in every condition, then the fewest TAC invested will provide the highest economic potential, that shown in Figure 5. The maximum point of economic potential happens if we apply ratio of 70% Zeolite 5A and 30% Zeolite BETA and the minimum point happens if we apply ratio of 100% Zeolite BETA.

To produce the maximum RON product using PSA with zeolite beta and 5A arranged in two layers because it is more optimal. This is shown in Figure 5, where the economic potential is higher than the total annual cost for the variation in volume of zeolite used in PSA. However, different results are shown when using 100% beta zeolite, where the economic potential is higher than the total annual cost. One reason for this to occur is because the capital costs and operating costs for preparing beta zeolite as an adsorbent are higher than 5A zeolite so that the total annual cost for the 100% beta zeolite variation is higher than the economic potential

4. Conclusion

The results from this work demonstrate the feasibility of using the PSA cycle method to achieve high-octane gasoline from light naphtha. Simulations were performed to evaluate the performance of the PSA cycle with a dual layer of adsorbent. The bed consists of a zeolite 5A layer to retain linear paraffin and a zeolite beta layer to separate monobranched C6 from the enriched fraction. The effects of different percentages of the zeolite 5A to zeolite beta ratio were evaluated. The dynamic simulations demonstrate that the judicious choice of these variables can improve the octane quality of the enriched fraction compared to the conventional processes for the separation of n-paraffins. Based on research conducted, it can be concluded that to get the greatest economic potential value is obtained when the adsorbent configuration conditions in the PSA process on a 30% BETA: 70% 5A ratio, with 95 as the final RON value of the product and economic potential of US\$114,410,163.

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