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STUDY ON DOUBLE-EFFECT DISTILLATION PROCESS FOR SEPARATING METHANOL-WATER USING ASPEN PLUS V10

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ABSTRACT

Methanol (also known as CH_3OH, methyl alcohol, hydroxymethane, wood alcohol, or carbinol) is a widely used primary raw material. It is one of the first organic chemicals to find extensive laboratory and industrial use. Methanol and water are ideal binary systems that can be separated by conventional distillation. This study aims to separate methanol-water using a simulated double-effect distillation process in Aspen Plus. To obtain a higher purity of methanol and consider the high energy consumption of the distillation process, double-effect distillation with a double column was used. Furthermore, the single-column and double-effect distillation processes can be simulated by Aspen Plus software. The software version used in this simulation is Aspen Plus V.10 with NRTL thermodynamics methods as binary interaction parameters. The double effect distillation column was equipped with a heat exchanger, splitter, and pump. Moreover, a design specification is needed to get the purity of methanol as wanted. Compared to each column process, the temperature profile of each column process is directly proportional to the number of stages. By simulation process that has been carried out, the purity of methanol in the single-column process and double-effect distillation process is slightly different with 97.1% and 97.2%, respectively. In the double-effect distillation process, columns C1 and C2 save 0.6% and 0.37% of energy in the single-column process, respectively. It indicates that the double-effect distillation has obvious advantages over single-column distillation in terms of purity of methanol and energy saving.

***Keywords**:* double-effect distillation, economic calculation, methanol, process simulation.

1. INTRODUCTION

Distillation is one of the most important and widespread methods of thermal separation in the modern process industry, distillation has been widely applied in the petrochemical, chemical, metallurgical, food, and textile industries. Representing a large proportion of global energy use, it is estimated that around 43% of thermal energy is used for industrial applications [1]. In particular, refinery alone is responsible for about 40% of heat energy consumption in the chemical process industry [2] which is a driving force for the various energy saving programs that have been launched to improve refinery performance. The concept of heat integration was first introduced nearly 70 years ago to reduce its energy consumption [3]. The basic idea of heat integration is that a hot process stream exchanges heat with a cold process stream [4].

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Furthermore, methanol, also known as CH_3OH, methyl alcohol, hydroxymethane, wood alcohol, or carbinol, is one of the first organic chemicals to be commonly used in laboratory and industry as the basic raw material [5, 6]. In Europe before 1900, methanol was known as a heating fuel and was obtained by distillation of the destructive wood [7]. Along year by year, advances in distillation make it possible to develop the process in a meaningful way. Multi-effect Distillation or MED is one of the most effective processes in distillation.

MED schemes have been developed and applied in the industry due to their energy saving effect. MED for seawater desalination and liquid mixture separation has made tremendous progress, especially with the advantages of easy operation and substantial energy savings. In an MED system, for example, in double-effect column distillation with two columns, the top vapor of the first column generated from the first column reboiler is used to heat the second column reboiler. So, the consumption of heating agents for the reboiler can be reduced, and the corresponding energy consumption can be reduced by about 50%. For multi-effect distillations with three or more columns, the energy consumption can be further reduced. For example, for a three-effect distillation with three columns, the energy consumption can be reduced by about 33%. In the MED system, the total temperature difference between the first column reboiler and the last column reboiler is distributed in each column. This implies that the temperature difference for each column decreases as the number of columns increase. To meet the specified reboiler evaporation rate, its heat transfer area must be increased. Therefore, the cost of the reboiler increases, while the energy consumption decreases as the number of columns increase [8].

The separation of methanol and water via distillation should be easy. The relative volatility between the key compounds is relatively high, around 3.0, and the liquid surface tension and fluid density difference are both high [9]. Most of the separation in methanol-water still uses conventional distillation which consumes a lot of energy.

According to the discussion above, this research uses the double-effect distillation process as an enhanced process from the single-column distillation process. Therefore, the aim of this study is to separate methanol-water using simulated double-effect distillation in Aspen Plus. Methanol and water are an ideal binary system that can be separated by conventional distillation. In order to obtain a higher purity of methanol and consider the distillation process high energy consumption, it can use double-effect distillation with the double column. In addition, energy consumption and total annual costs (TAC) for the two schemes are comprehensively discussed. It is hoped through this research that new techniques for separating mixtures can be developed, then the advantages and disadvantages of methods can be fully explored.

2. METHODOLOGY

2.1. Materials and Methods

A mixture of methanol and water (60:40, w/w) was fed into the column at a rate of 100 kg/hr. Simulation of the process was carried out using Aspen Plus software V.10. The model selected for property calculations in the simulator depended on the operation type. The NRTL model was selected for the thermodynamics property method.

2.2. Distillation Process

The simulation process is basically divided into two processes, i.e. single-column distillation and double-column distillation.

a. Single Column Distillation

The single-column distillation is an original process, and the double column distillation is an enhanced process. The Aspen Plus main flowsheet is shown in Figure 1. The number of theoretical stages, the feed stage, and the reflux ratio required for the column were initially calculated and simulated by Radfrac block in Aspen Plus. To get the optimal setting of the column, use NQ curve analysis.

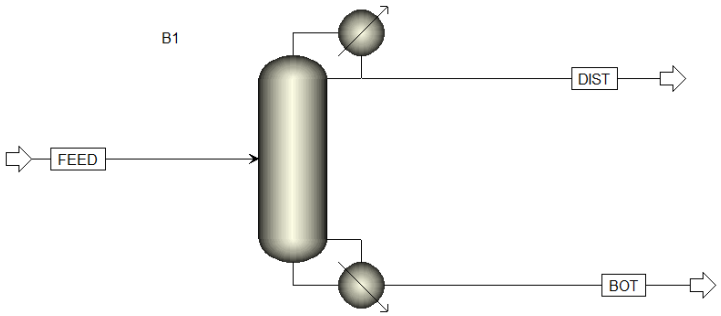

Figure 1. Aspen main flowsheet for single column distillation

The specific steps of the simulation for the single-column distillation process are as follows:

1. Open the Aspen plus V.10 software and add methanol and water as the component list.
2. Choose NRTL as the physical properties method based on the component list.
3. Move to Simulation Bar to make the main flowsheet. Use the radfrac column and set the stream input and output.
4. Click feed stream to input the temperature (20°C), the total pressure (101325 kPa), the flow basis (100 kg/hr), and the mass fraction of methanol and water (0.6 and 0.4, respectively).
5. Click the blocks section to input the parameter of the column. The calculation type is equilibrium then fills in the number of stages, distillate rate, and reflux ratio.
6. Add design specifications to set the purity. Do the design specification two times, then fill the desired mole purity of the product and adjust which would become the bottom and distillate.
7. Go to Vary to create independent variable to see the effects on methanol and water. Do the variation two times, the first variable should be filled as Distillate rate, the lower bound is 20, and the upper bound is 50. Then the other variables must be Reflux ratio, the lower bound is 0.1, and the upper bound is 5.
8. To get the optimum setting of the column, use NQ Curve analysis. Fill the lower limit, upper limit, and step size.
9. Run the simulation.

Single column distillation is an original process of distillation yet has one column that is operated. The Aspen Plus diagram for the single column distillation process is

shown in Figure 1. The design single tower scheme and detailed condition can be seen in Figure 2.

Single column distillation is labeled as B1 and has three streams input and output. The stream input is feed and the stream output source is divided by two streams, there are from condenser and reboiler. The output streams consist of distillate stream and bottom stream. B1 has 20 stages, and the feed stage is 13. The diameter of column B1 is 0.1008 m.

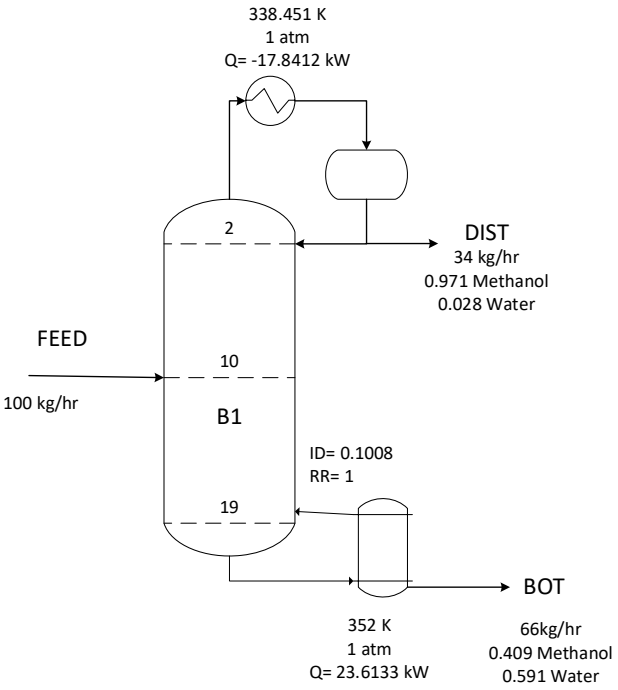

Figure 2. Design for single column distillation

b. Double Column Distillation

Double-effect distillation is one of a process for separating methanol-water, which is an enhanced process from a single column process. Double-effect distillation process simulated after getting the result of two tower process simulations. The double-effect distillation process has two columns equipped with a heat exchanger. The design double-effect distillation process is shown in Figure 3.

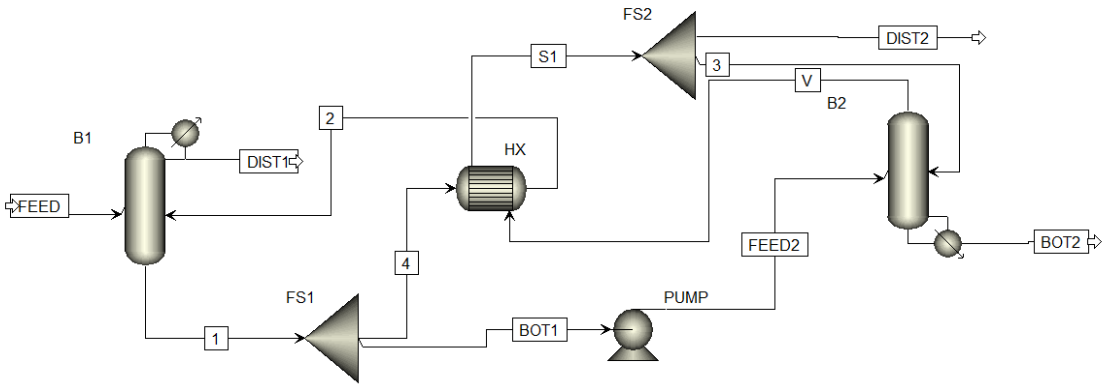

Figure 3. Aspen main flowsheet for double-effect distillation

The specific steps of the simulation for the double column distillation process are as follows:

1. Open the Aspen plus V.10 software and add the components list.
2. Choose NRTL the physical properties method based on the component that will be used.
3. Move to Simulation Bar to make the main flowsheet. Use the radfrac column and set the stream input and output.
4. Click feed stream to input the temperature (20°C), the total pressure (101325 kPa), the flow basis (100 kg/hr), and the mass fraction of methanol and water (0.6 and 0.4, respectively).
5. Click blocks section to input the parameter of the column. The calculation type is equilibrium and fills in the number of stages, distillate rate, and reflux ratio.
6. Add design specifications to set the purity. Do the design specification two times, then fill the desired mole purity of the product and adjust which would become the bottom and distillate products.
7. Go to Vary to create independent variable to see the effects on methanol and water. Do the variation two times, the first variable should be filled as Distillate rate, the lower bound is 20, and the upper bound is 50. Then the other variables must be Reflux ratio, the lower bound is 0.1, and the upper bound is 5.
8. To get the optimum setting of the column, use NQ Curve analysis. Fill the lower limit, upper limit, and step size.
9. Click the pump and fill the discharge pressure.
10. Run the simulation.
11. Click blocks to fill the column and input the parameter. The calculation type is equilibrium and changes the number of stages, distillate rate, and reflux ratio.
12. Add design specifications to set the purity. Do the design specification two times, then change the desired mole purity of the product and adjust which would become the bottom and distillate.
13. Go to Vary to create independent variable to see the effects on methanol and water. Do the variation two times, the first variable should be filled as Distillate rate, the lower bound is 20, and the upper bound is 70. Then the other variables must be Reflux ratio, the lower bound is 0.1, and the upper bound is 5.
14. Click FS1 and fill stream 4.
15. Click FS2 and fill stream 3
16. Click the pump and fill the discharge pressure.
17. Run the simulation.

The double-effect distillation process has two columns labeled C1 and C2. C1 column did not have a reboiler because the output stream to a splitter. C1 has 10 total stages and the feed stage at stage 5. The diameter column C1 is 0.1032 m. From the C1 column distillation process, obtained the purity of methanol is 0.952, which is approximately equal to 95.2%. The bottom output from C1 was streamed to the splitter. Splitter has two outputs, one became an inlet for heat exchanger named stream 4, and

the other one is a bottom stream that is generated by column C1 and flows to the pump. Stream bottom 1 flowed to the pump. From the pump flows to C2 as feed. C2 column did not have a condenser. C2 has 12 total stages and the feed stage at stage 8. Diameter column C2 is 0.069 m. All the processes can be seen in Figure 4.

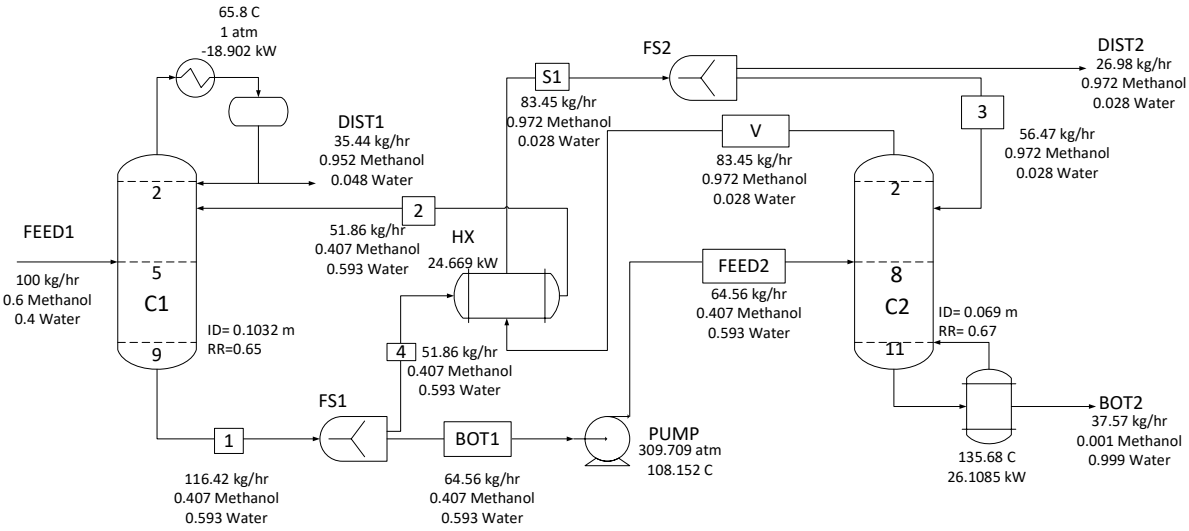

Figure 4. Design for double-effect distillation

2.3. Optimization

Single column and double column were optimized using NQ curve analysis. Figure 5 and Figure 6 are the NQ curve analysis for each scheme. NQ curve analysis could see where the suitable total stage number and feeding position be. In the single-column distillation process, from the graph can be seen that it is very slow to change at stages 19-20. Therefore, it is the suitable total stage number and feeding position. The suitable total feed number is 19 and the feeding position is in stage 14. Meanwhile, the double-column distillation process looks very slow to change at stages 21-22. It means that the suitable total stage is 21 with the suitable feed stage is in stage 13.

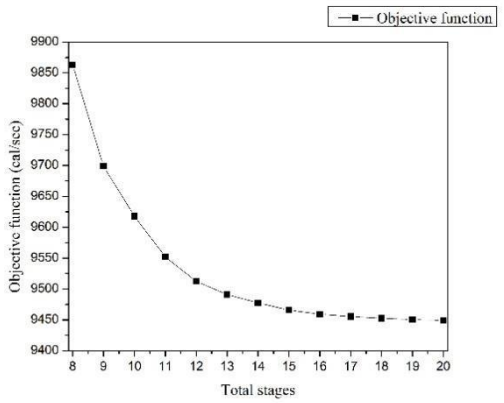

Figure 5. NQ curve single column analysis

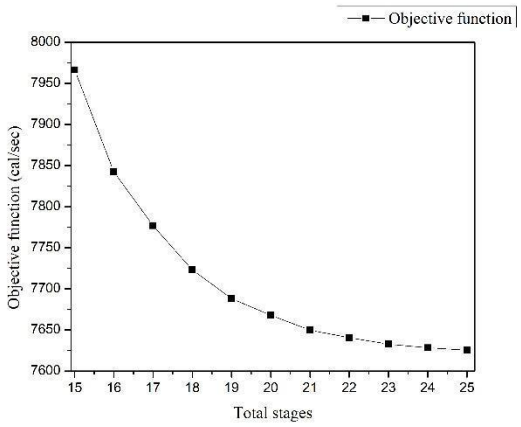

Figure 6. NQ curve double column analysis

Figures 7, 8, and 9 are the result of doing sensitivity analysis in a single column and double column distillation processes. It can be seen that the graph form of both processes is the same. For purity methanol, the greater the value of stage, the greater the purity of the methanol produced. For reboiler duty, the larger the value of the stage, the smaller the energy required. There is a meeting point between methanol purity and reboiler duty in the early stage.

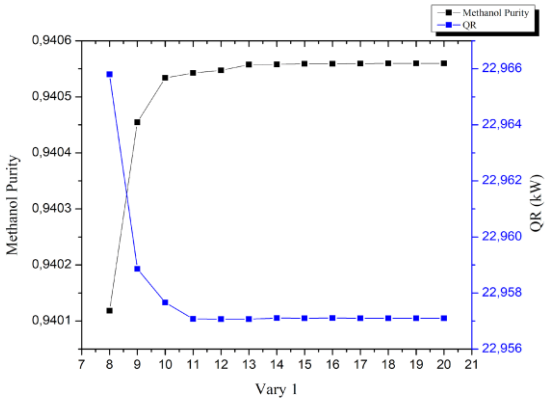

Figure 7. Sensitivity analysis NT single column

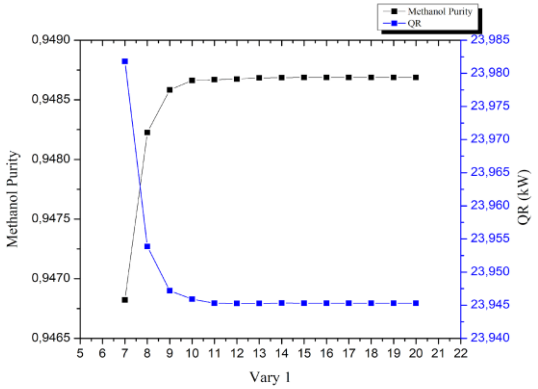

Figure 8. Sensitivity analysis NT double column B1

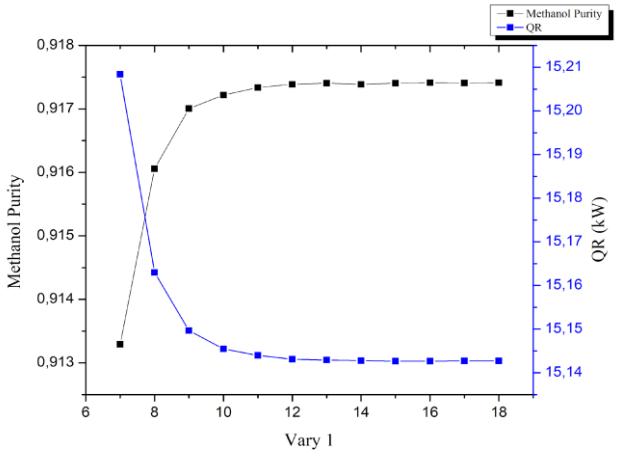

Figure 9. Sensitivity analysis NT double column B2

Figures 10, 11, and 12 are the result of doing sensitivity analysis in a single column and double column distillation process. It can be seen that the graph form of both processes is the same. For purity of methanol, the greater the value of the reflux feed stage, the greater the purity of the methanol produced. For reboiler duty, the larger the value of the feed stage, the smaller the energy required.

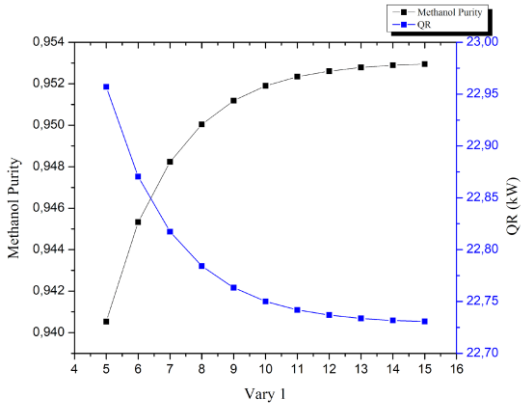

Figure 10. Sensitivity analysis feed position single column

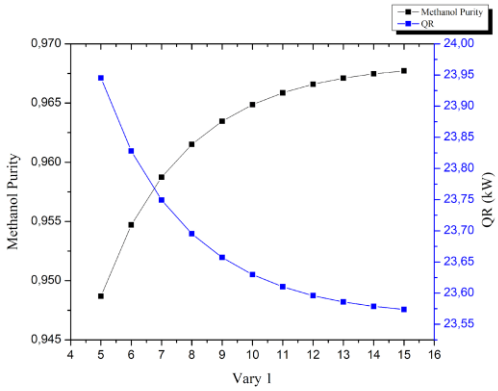

Figure 11. Sensitivity analysis feed position double column B1

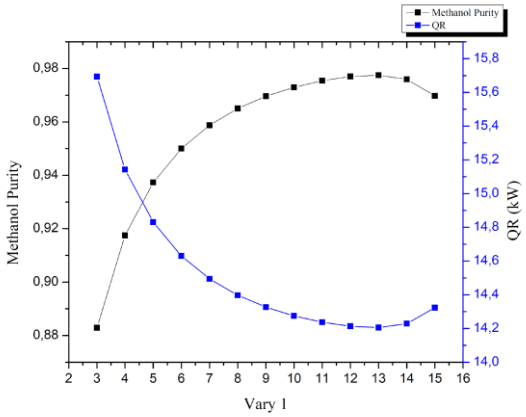

Figure 12. Sensitivity analysis feed position double column B2

The figures below are the result of doing sensitivity analysis in a single column and double column distillation process. It can be seen that the graph form of both processes is the same. For purity of methanol, the greater the value of the reflux ratio, the greater the purity of the methanol produced. In case of reboiler duty, the greater the value of the reflux ratio, the larger the energy required. In all processes, there is constant change in reboiler duty.

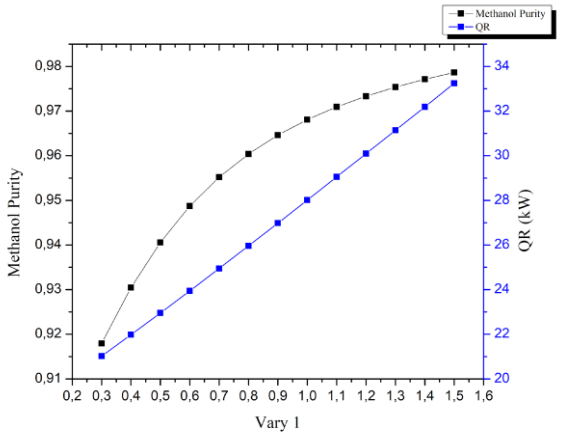

Figure 13. Sensitivity analysis reflux ratio single column

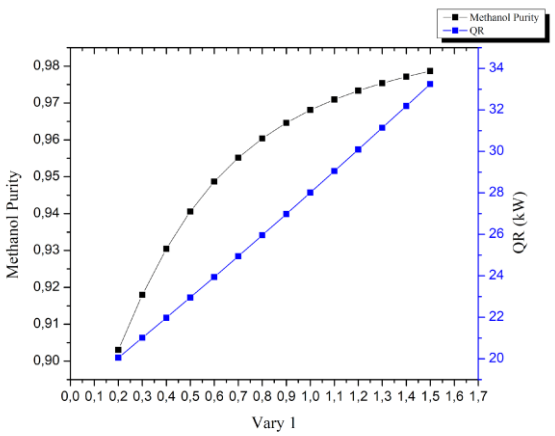

Figure 14. Sensitivity analysis reflux ratio double column B1

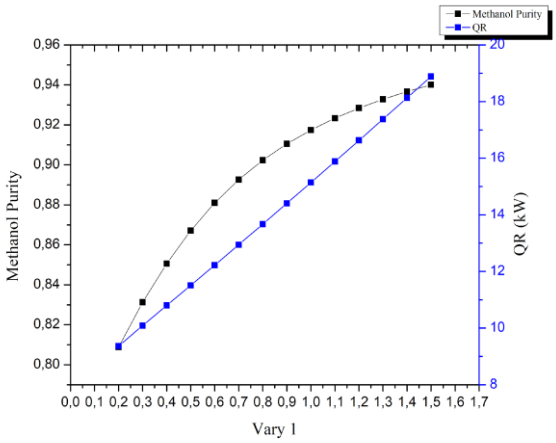

Figure 15. Sensitivity analysis reflux ratio double column B2

3. RESULTS AND DISCUSSION

Based on the simulations that have been carried out, the temperature profile, liquid composition, and vapor composition of each column process are obtained. As seen in Figure 16, the graph indicated that the temperature rises as the number of stages increases. Moreover, to get the high purity of the final product, the number of stages should be increased. However, the pressure will increase as the stage increases. According to Raoult's law, at low pressure, the vapor of the mixture approaches ideal behavior and follows the ideal gas law [10]. Therefore, the temperature will increase as the stage increases.

Additionally, from the single-column distillation process, the purity of methanol is 0.971, which is approximately equal to 97.1%. Whereas the double-effect distillation process obtained the purity of methanol is 0.972, roughly equivalent to 97.2%.

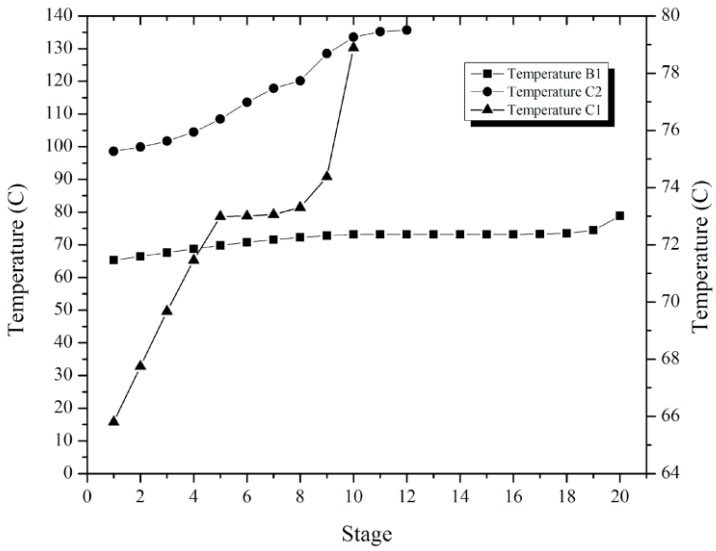

Figure 16. Temperature profile in B1, C1, and C2

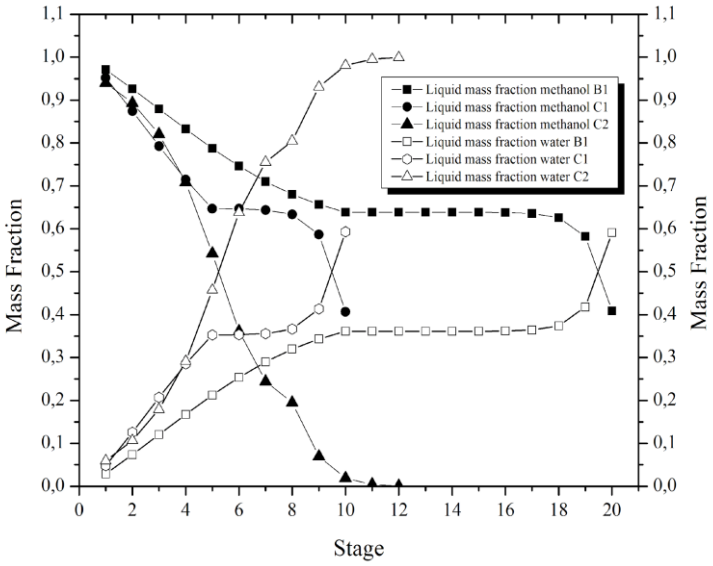

Figure 17. Liquid composition B1, C1, and C2

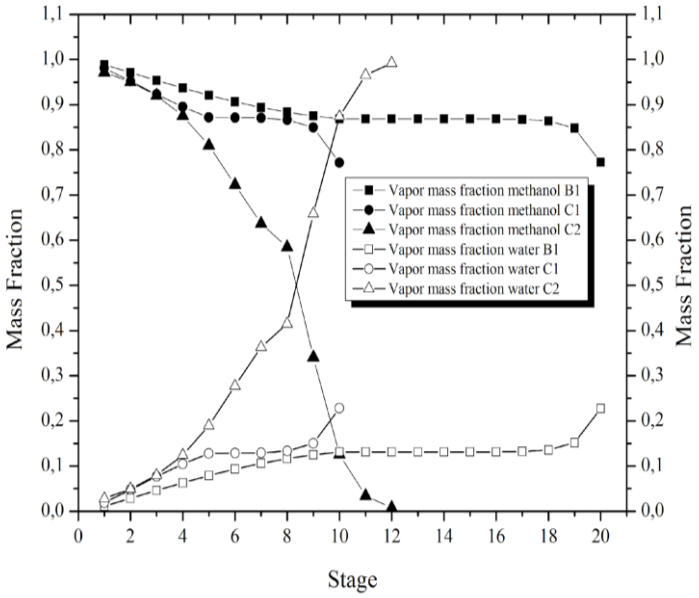

Figure 18. Vapor composition B1, B2, and C2

Figures 17 and 18 show the vapor and liquid composition of each column distillation. From the figures above can be seen that the liquid and vapor mass fraction of methanol decrease as the stage increase, it happens because the temperature given in the stage is too high, so a lot of the mixture is ready to change into vapor phase [11].

The overall result from the simulation will then be optimized based on the analysis TAC (total annual cost economy) to get the best design based on TAC to get the design that best and most efficient. The TAC for single-column distillation and double column distillation was calculated in excel. TAC stands for a total annual cost. Here, TAC includes the annual capital

investment and the annual operating cost, and the payback period is assumed to be 3 years. The expression is as follows the Equation 1.

$$TAC = \frac{capital\ cost}{payback\ period} + annual\ operating\ cost \quad (1)$$

The annual operating costs consist of cooling and heating costs. Whereas, the capital costs comprise the costs of distillation tower, sheet, and heat exchanger.

Table 1. TAC for every column

	C1 single column	C1 double-effect column	C2 double-effect column
NS	10	10	10
NF	10	5	8
NT	20	10	12
ID (m)	0.1008	0.1032	0.069
Q_C (kW)	-17.8412	-18.902	-
Q_R (kW)	23.6133	-	26.1085
Heat transfer area (Δ_C)	-1.5065	-1.5961	-
Heat transfer area (Δ_R)	1.1946	-	1.3208
Total capital cost (10^4\$)	6.465	3.193	3.38
Annual energy cost (10^4\$)	5.432	0.193	5.805
TAC (10^4\$)	2.698	1.084	1.707

Information:
NS: number of entrainer
NF: number of feed
NT: number of stage
ID: diameter
Q_C: condenser duty
Q_R: reboiler duty

Based on the single-column distillation process, the number of the theoretical stage is 20, the column diameter is 0.1008 m, the condenser duty is -17.8412 kW, and the reboiler duty is 23.6133 kW. The TAC value obtained from the calculation is 2.698x10^4\$/y. Double-effect distillation process is needed to calculate TAC in both columns since it has two columns in its process. With this value in C1, the number of the theoretical stage is 10, the column diameter is 0.1032 m, and the condenser duty is -18.902 kW. The TAC value obtained from the calculation is 1.084 x10^4\$/y. Column C1 saves energy 0.6% from energy in single-column distillation. While this value in C2, the number of the theoretical stage is 12, the column diameter is 0.069 m, the reboiler duty is 26.1085 kW. The TAC value obtained from the calculation is 1.707 x10^4\$/y. This column saves energy 0.37% from energy in single-column distillation. The total TAC is sum up from TAC in C1 and TAC in C2. TAC in the double-effect distillation process is 2.791 x10^4\$/y.

According to the simulation that has been done, although the two processes only has $\pm$0.1% of purity differences and $\pm$930\$/y of TAC differences, the recommendation scheme is a double-effect distillation process with a separating condenser and reboiler assist in the

operation of the process. Since each column has its own condenser and reboiler, operation is simpler than in the original internally heat integrated distillation column [12].

4. CONCLUSION AND SUGGESTION

This simulation study is to determine the most suitable operating conditions for the separation of the methanol-water using double-effect distillation. To obtain the best conditions and configuration, NQ curve analysis and sensitivity analysis was done. The temperature and composition profiles were obtained for the double-effect distillation column.

Design simulation of the single-column process and double-effect distillation process has been created and simulated by Aspen Plus V.10. The purity of methanol obtained is around 0.971, which is approximately equal to 97.1%. Meanwhile, the double-effect distillation process has two columns that are operated which are C1 and C2. The purity of methanol obtained is 0.972, approximately equal to 97.2%. Column C1 and C2 saving energy is 0.6% and 0.37%, from energy in the single-column process, respectively. TAC of each process was also calculated. The payback period is assumed to be 3 years. The total capital cost from the single-column process is 6.465 x10^4\$. Meanwhile, the total capital cost is C1 and C2 is 3.193 x10^4\$ and 3.38 x10^4\$, respectively. TAC in the single-column process is 2,698x10^4\$/y, and the TAC in the double-effect process is 2,791 x10^4\$/y. Therefore, according to the simulation that has been done, the more favorable scheme distillation process in order to get a higher purity of the product and more saving energy, the double-effect distillation process scheme is.

For further research conducted in the future, another simulation process should be implemented to get a higher purity of methanol, lower energy consumption and TAC.

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