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Sensitivity Analysis of Bioethanol Simulation from Microalgae with Pressure Swing Distillation Process

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ABSTRACT

Energy is an important parameter in the social and economic development of a country. Thus, it is necessary to seek renewable energy to supply energy needs in Indonesia. The production of bioethanol from microalgae as a biofuel is one way to reduce the use of fossil fuels. Microalgae has an advantage over other types of biomass sources due to its high biomass productivity and do not compete with agricultural crops for land and water resources. In the bioethanol production process, the ethanol and water form an azeotrope mixture of 95.6% of ethanol at 1 atm and 78.15°C. The objective of this research was to analyse and determine the operating conditions and the optimum distillation column configuration which results in high ethanol purity according to fuel specifications (fuel grade ethanol). The method of pressure-swing distillation was applied to separate the azeotrope of ethanol-water and obtain high purity ethanol. A simulation model of bioethanol production with pressure-swing distillation system was conducted by using Aspen Plus V10. In this research, the influence of process parameters such as distillation column pressure, reflux ratio, feed stage location, and the number of theoretical stages was analysed by using model analysis tools. The results showed that the obtained bioethanol purity of 99.9% with the condenser and reboiler duty of the LP column -79.931 kW and 667.651 kW, respectively; while the HP column is -47.627 kW and 57.698 kW.

1. Introduction

The development of renewable energy is currently needed to meet the global demand of fuel oil. Energy plays an important role in the social and economic development of a country where its primary sources are from non-renewable resources. The massive use of fossil fuels led to the problems such as depletion of its reserves, negative environmental impacts, worsening climate change and increasing greenhouse gasses emission [1]. Thus, it is a critical concern to develop an

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alternative energy resource to minimize the utilization of fossil fuel and maintain the environmental sustainability.

Biofuels such as bioethanol emerged as a promising solution to reduce the use of fossil fuels supply. Bioethanol is an ethanol derived from biomass, especially biomass containing glucose and cellulose [2]. Bioethanol can be used as a fuel both in its pure form and as a premium mixture [3]. As a premium mixture, bioethanol has a role, among others, as an additive that can increase the octane number which results in an increase of the fuel quality, furthermore high oxygen content in bioethanol can increase the combustion process in the engine [4].

A wide variety of potential feedstock from all around the world can be utilized for bioethanol production [5]. One of the feedstock that can be used for bioethanol production is microalgae. Microalgae have become an alternative raw material for bioethanol production after the commodity sap, or cassava [6]. Microalgae are ideal feedstock because they produce high biomass and do not compete with agricultural crops for land and water resources. Microalgae can be found and grow in seawater, salt water, and even municipal waste [7].

Microalgae have already caught the attention of biofuel researchers from all over the world and considered as photosynthetic microorganisms capable of producing large amounts of biomass containing lipids, proteins, or carbohydrates [8, 9]. Most of the microalgae can store highly concentrated lipid which can exceed 70% by weight of dry biomass [10, 11]. The carbohydrate content was also found to be relatively high which is up to 50% of dry weight for some species such as *Scenedesmus*, *Chlorella*, and *Chlamydomonas* [12, 13].

From these considerations, the microalgae *Chlamydomonas reinhardtii* is used since it has a high starch content, as well as a parameter in determining the composition of the microalgae to be used as a component of the feed into the simulation. Several studies have been carried out using microalgae such as *Chlorella vulgaris* was reported to obtain 0.890 g/g of bioethanol [14]. Harun and Danquah [15] obtained 0.520 g/g of bioethanol even though the acid hydrolysis was only considered as pre-treatment on microalgal biomass. Choi *et al.,* [16] had performed enzymatic pretreatment of algal biomass *Chlamydomonas reinhardtii* UTEX 90, the study reported 235 mg ethanol/g algae was produced.

In the production process, most of the bioethanol industry uses the fermentation process to produce ethanol with a concentration of 8-12%. Bioethanol can be produced through simple biomass fermentation and distillation processes. In the ethanol-water distillation process, there is an azeotropic point that is difficult to achieve into pure ethanol (99.5%) through a simple distillation process [17]. Several ethanol purification processes are used to exceed its azeotropic point, such as extractive distillation [18], membrane technology [19], adsorptive distillation [20], and Pressure Swing Distillation (PSD) [21].

PSD is a method of ethanol-water separation using different pressures under distillation conditions. Different pressures are intended to purify a mixture by degrees past its azeotropic point. In this distillation system, the distillation is carried out in stages using two distillation columns operating at different pressures [21]. The weakness of this method is knowing the pressure difference between the two columns [22].

Recently, Kiran and Jana [22] proposed a hybrid heat integration scheme for bioethanol separation through the PSD route by integrating an internal heat integrated distillation column with fewer internal heat exchangers and a vapor recompression column. Loy *et al.*, [23] reported fuel-grade ethanol production via pressure swing adsorption is better than extractive distillation using ethylene glycol with 15% lower separation cost and ethanol recovery rate 99.7%. Zhang *et al.*, [24] studied a heat-integrated PSD process for separating the minimum-boiling azeotrope ethyl acetate and ethanol for a 33.33 % saving on energy, reduce CO_2 emissions by 31.33 % and save 26.64 % of

the TAC compared to the conventional process. There are also other energy-saving methods that are applied to PSD processes.

Therefore, this study will purify bioethanol from microalgae using the PSD method using Aspen Plus V10 software through a sensitivity analysis to determine the operating conditions and the optimum distillation column configuration which results in high ethanol purity according to fuel specifications (fuel grade ethanol).

2. Methodology

This research is in the form of a simulation using process design-based software, Aspen Plus V10. This design scheme has a basic idea where bioethanol produced without a purification process still has 3 main components, namely CO_2, water, and ethanol. Meanwhile, in the process of using it, only bioethanol with a moisture content of less than 0.2 vol% is used to prevent corrosion of the engine interior [23]. The NRTL properties model was chosen to predict the VLE (Vapor-Liquid Equilibrium) of the ethanol/water system. The process specification experimental data used was based on the research of Battisti *et al.*, [25] for the initial investigation stage with the condition that the number of theoretical stages of the Low-Pressure (LP) column was 39, reflux ratio was 2.126, fresh feed stage was 23, recycle was 13, atmospheric pressure; The High-Pressure (HP) column with the number of theoretical stages was 42, the reflux ratio was 1.669, the feed stage was 13, the pressure was 10 atm. The main parameters that affect the distillation process included pressure, reflux ratio, location of the feed stage, and the number of theoretical stages. Therefore, these four parameters will be analysed for their effect on the process of purifying bioethanol from microalgae. The limits of the variable optimization range are determined as follows: column pressure LP (0,1 atm ≤ P1 ≤ 1 atm) and HP (10 atm ≤ P2 ≤ 14 atm), reflux ratio of LP column and HP (0,1 ≤ RR ≤ 3), LP column stage (12 ≤ NT1 ≤ 39) and HP (12 ≤ NT2 ≤ 42), LP column fresh feed stage (13 ≤ NF1 ≤ 28), recycle feed LP column (5 ≤ NR ≤ 28), HP column stage feed (2 ≤ NF2 ≤ 41).

The simulation was conducted using two column consists of LP column and HP column. The main flowsheet of this simulation was presented in Figure 1.

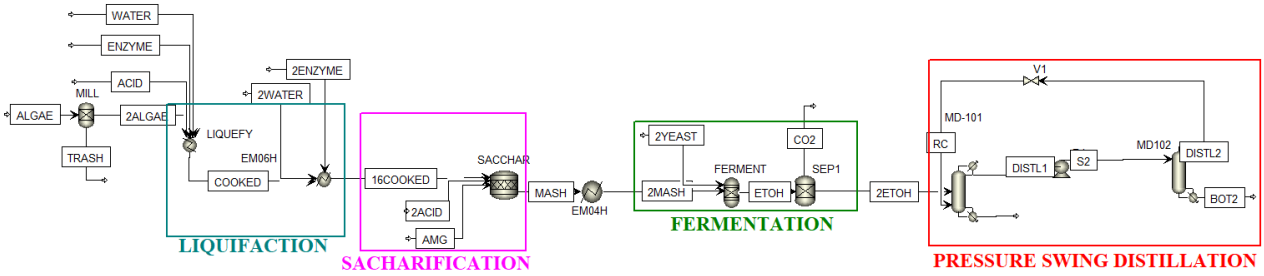

Fig. 1. The pressure swing distillation process flow diagram

3. Results

3.1 Preliminary Simulation

3.1.1 Reactor

The concentration of ethanol as a feed-in is taken from research that has considered the sugar fermentation process. Moncada *et al.*, [26] showed that beer from sugarcane biorefinery contains 7 to 10% by weight of ethanol, while Huang *et al.,* [27] suggested that the concentration of ethanol in

the broth from the fermenter lies between 5 and 12% by weight. In this study, the fermenter outflow that will be used as feed still consists of various components consisting of 4 wt% ethanol, 92 wt% water, and other components in small amounts (≤1 wt%). The process is designed to produce >99.8 wt%.

3.1.2 Pressure Swing Distillation

The main parameters that affect the distillation process are pressure, reflux ratio, location of the feed stage, and the number of theoretical stages. Therefore, these four parameters will be analyzed for their effect on the process of purifying bioethanol from microalgae. At the initial investigation stage, the specification data used were based on research by Battisti *et al.*, [25] with the condition that the number of theoretical stages of the LP column was 39, reflux ratio was 2.126, fresh feed stage was 23, recycle was 13, atmospheric pressure; HP column with theoretical stage number is 42, reflux ratio was 1.669, feed stage was 13, pressure was 10 atm. Table 1 shows a the results comparison between the literature and in this study.

Table 1
Comparison of Simulation Results of Initial Investigation Process

Items	Literature Result [25]	Research Result
LP Column		
• Top Product Composition (ethanol/water)	0.851/0.149	0.864/0.136
• Bottom Product Composition (ethanol/water)	0.005/0.995	0.044/0.920
• Condenser duty (kW)	3,456.1	-80.388
• Reboiler duty (kW)	2,785.1	669.794
HP Column		
• Top Product Composition (ethanol/water)	0.815/0.185	0.850/0.150
• Bottom Product Composition (ethanol/ water)	0.996/0.004	0.995/0.005
• Condenser duty (kW)	1,949.6	-50.783
• Reboiler duty (kW)	2,236.0	59.018

3.2 Sensitivity Analysis of Low-Pressure Column
3.2.1 Effect of pressure on ethanol purity, condenser duty, and reboiler duty

Figure 2 and 3 show that column pressure affects the purity of ethanol, condenser duty, and reboiler duty. In the LP column, the pressure was varied from vacuum pressure to atmospheric pressure and it can be seen that the purity was started to decrease at the pressure of 0.3 atm, this is in line with the study by Huang *et al.*, [28] which stated that the pressure should be less than 0.4 bar. While the effect of pressure on the condenser duty has decreased and the reboiler duty has increased along with the increase in pressure.

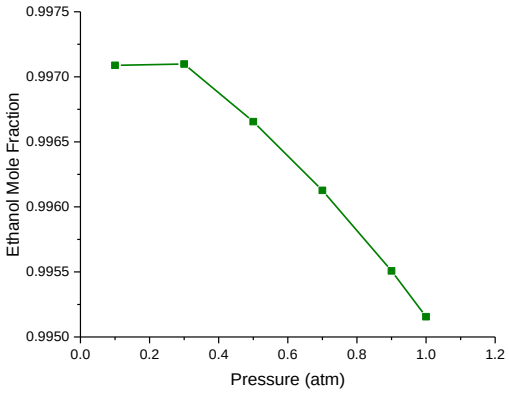

Fig. 2. Effect of Pressure on Ethanol Purity of LP Column

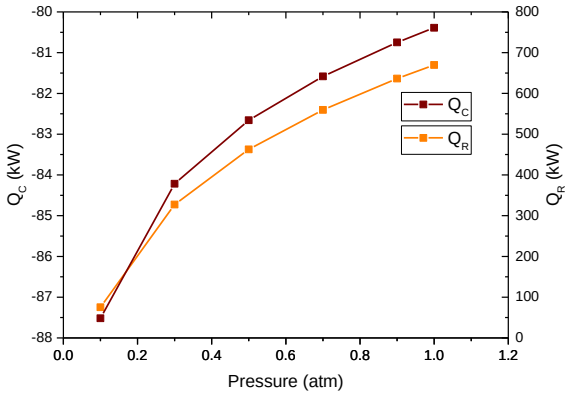

Fig. 3. Effect of Pressure on Condenser and Reboiler duty of LP Column

3.2.2 Effect of reflux ratio on ethanol purity, condenser duty, and reboiler duty

Changes in the value of the reflux ratio in the LP column affect the purity, the higher the ratio the higher the purity as shown in Figure 4. Meanwhile, for the condenser duty and reboiler duty, the variation of reflux ratio causes an increase in the condenser duty and reboiler duty which is shown in Figure 5. This is in accordance with research conducted by Huang *et al.*, [28] which showed an increase in ethanol purity, condenser duty, and reboiler duty with the increasing value of reflux ratio. In this study, the reflux ratio used in the LP column was 2.126. It is due to the insignificant change of ethanol mole fraction at the higher reflux ratio while, the load on the condenser and reboiler increases with increasing reflux ratio, which has an impact on increasing the total annual operating costs [25].

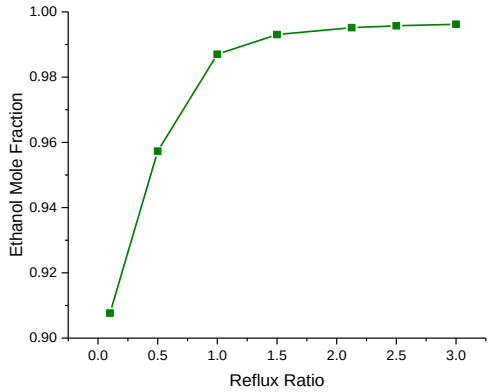

Fig. 4. Effect of Reflux Ratio on Ethanol Purity of LP Column

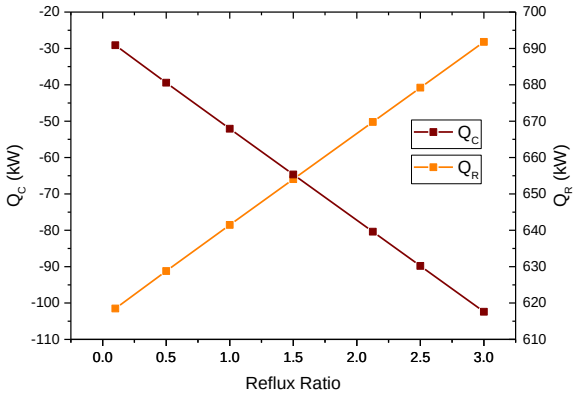

Fig. 5. Effect of Reflux Ratio on Condenser and Reboiler duty of LP Column

3.2.3 Effect of number of stages on ethanol purity, condenser duty, and reboiler duty

Figure 6 and 7 show the effect of the number of stages on the purity of ethanol, condenser duty, and reboiler duty. It can be seen that those variables were highly affected at the number stages up to 23 number of stages. The number of stages has a significant effect to the energy requirements of the condenser and reboiler [29]. Battisti *et al.*, [25] stated that the optimized PSD showed an increase in the number of stages compared to the unoptimized which would compensate for the heat duty in

the reboiler to obtain the same purity as required. Therefore, in this study, the optimum number of stages was 29 (including condenser and reboiler) which showed no change in ethanol purity, condenser duty, and reboiler duty.

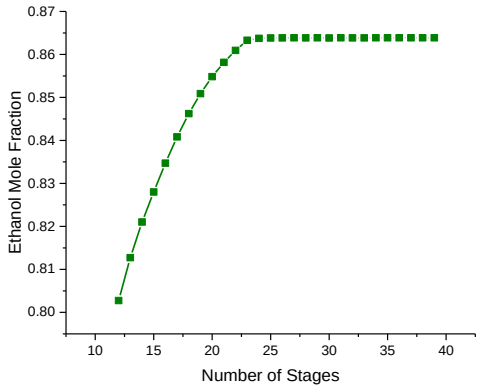

Fig. 6. Effect of Number of Stages on Ethanol Purity of LP Column

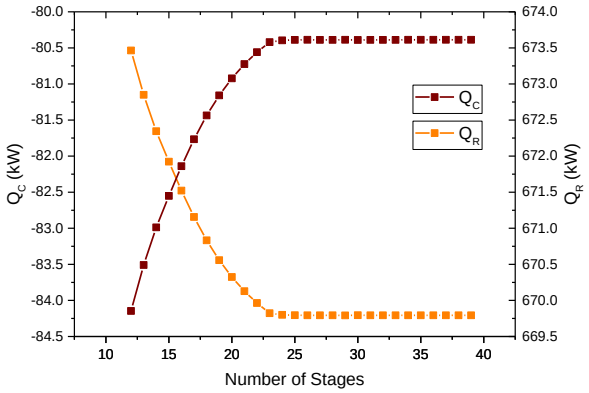

Fig. 7. Effect of Number of Stages Condenser and Reboiler duty of LP Column

3.2.4 Effect of feed stage on ethanol purity, condenser duty, and reboiler duty

Figure 8 and 9 show the significant effect of fresh feed stages on ethanol purity, condenser duty, and reboiler duty on the LP column. While the effect of recycle feed stage on those variables were shown in Figures 10 and 11. In this study, the sensitivity study was conducted separately. During the sensitivity study of fresh feed stage, the recycle feed stage remained the same. The optimum frees feed stage obtained was 28. Optimum recycle feed stage was conducted by using the optimized fresh feed stage. The optimum recycle feed stage was 9 with an ethanol purity of 99.6%, condenser duty of -79.896 kW, and reboiler duty of 669.303 kW. High feed position of distillation column will lead to an increase in the energy consumption of the distillation tower and the purity of the resulting product [28, 30].

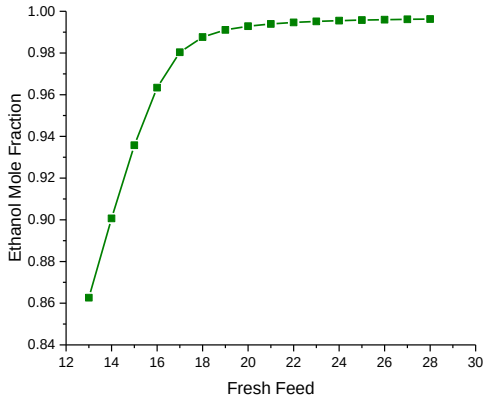

Fig. 8. Effect of Feed Stage on Ethanol Purity on Fresh Feed LP Column

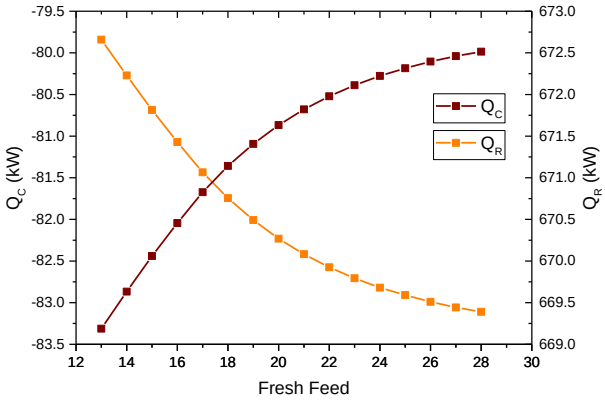

Fig. 9. Effect of Feed Stage on Condenser and Reboiler duty of LP Column on Fresh Feed LP Column

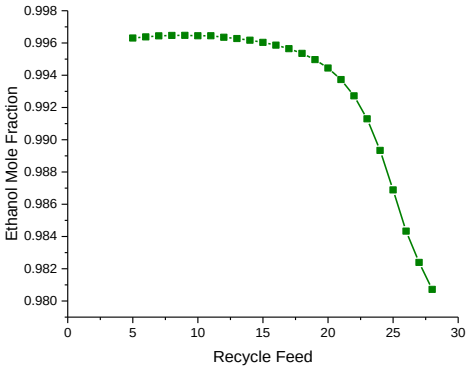

Fig. 10. Effect of Feed Stage on Ethanol Purity in LP Column Recycle

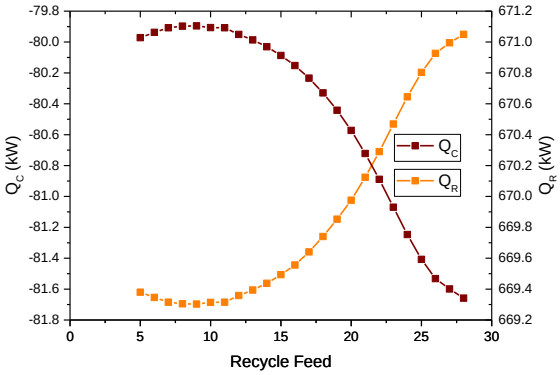

Fig. 11. Effect of Feed Stage on Condenser and Reboiler duty on LP Column Recycle

3.3 Sensitivity Analysis of High-Pressure Column

3.3.1 Effect of pressure on ethanol purity, condenser duty, and reboiler duty

Figures 12 and 13 show the effect of pressure in HP Column to the ethanol purity, condenser duty, and reboiler duty. The increasing pressure in HP column from 10-14 atm, also increase the purity of ethanol and condenser duty, however it decreases the reboiler duty. This is in line with the study conducted by Luyben [31], where the greater the pressure difference, lead to the greater force the shift in the azeotropic composition.

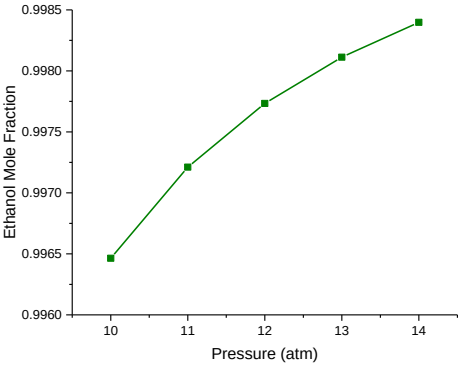

Fig. 12. Effect of Pressure on HP Column Ethanol Purity

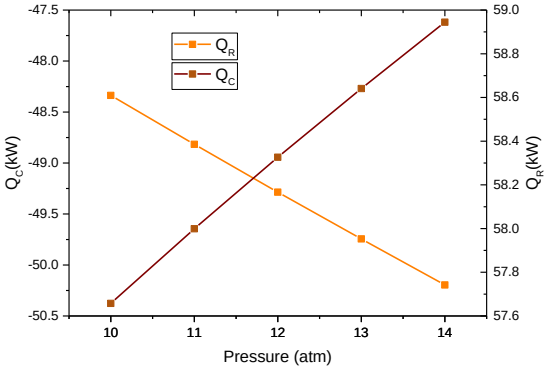

Fig. 13. Effect of Pressure on Condenser and Reboiler duty HP Column

3.3.2 Effect of reflux ratio on ethanol purity, condenser duty, and reboiler duty

The effect of the reflux ratio value on the HP column affects the purity which is shown in Figure 14. Increases in the reflux ratio value also increase ethanol purity. Meanwhile, for the condenser duty and reboiler duty are shown in Figure 15, the variation of reflux ratio causes a decrease in the condenser duty and increase in reboiler duty. This is following research conducted by Huang et al. [28]. In this study, the reflux ratio value of the HP column used is 1.669 because the reflux ratio value above shows a significant change in the condenser duty and the reboiler duty.

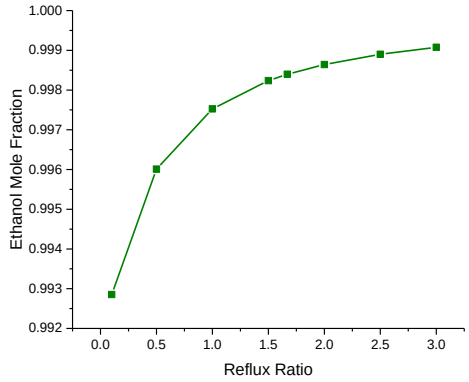

Fig. 14. Effect of Reflux Ratio on Ethanol Purity of HP Column

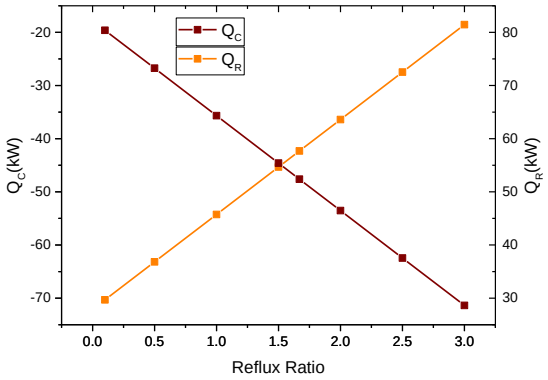

Fig. 15. Effect of Reflux Ratio on Condenser and Reboiler duty of HP Column

3.3.3 Effect of number of stages on ethanol purity, condenser duty, and reboiler duty

Based on Figure 16 and 17, variations in the number of stages on ethanol purity, condenser duty, and reboiler duty showed a significant effect up to the number of stages 42, this is following research conducted by Battisti *et al.,* [25] and Loy *et al.*, [29]. The optimum configuration for the number of HP column stages is 42 (including condenser and reboiler).

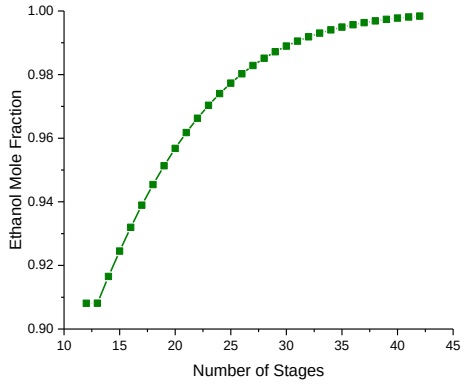

Fig. 16. Effect of Stage Number on HP Column Ethanol Purity

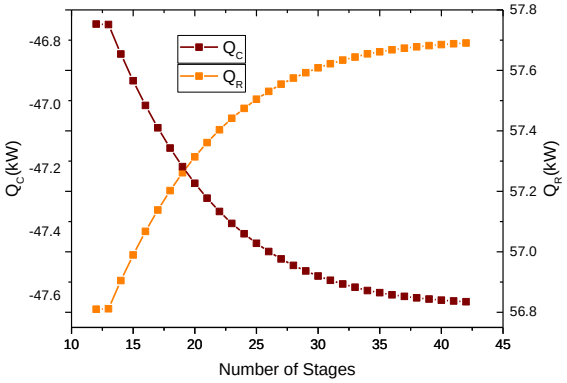

Fig. 17. Effect of Number of Stages on Condenser and Reboiler duty for HP Columns

3.3.4 Effect of feed stage on ethanol purity, condenser duty, and reboiler duty

Figure 18 and 19 show the effect of feed stage to the ethanol purity, condenser duty, and reboiler duty on the HP column. At this sensitivity study, the number of stages was fixed at 42. The feed stage variation shows a significant effect on the ethanol purity, condenser duty, and reboiler duty, this is following the research conducted by Huang *et al.*, [28] and Yang *et al.*, [30]. The best feed position for the HP column was found at stage 7 with an ethanol purity of 99.9%, condenser duty of -47.627 kW, and reboiler duty of 57.698 kW.

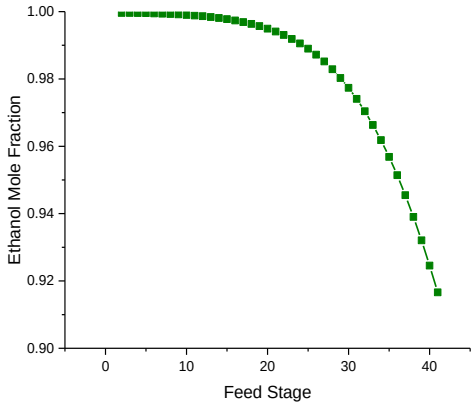

Fig. 18. Effect of Feed Stage on HP Column Ethanol Purity

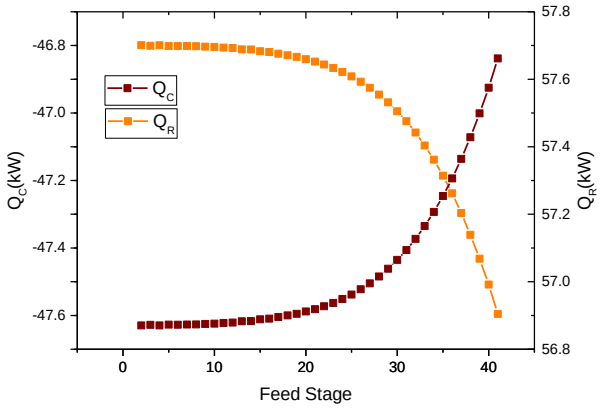

Fig. 19. Effect of Feed Stage on Condenser Duty and HP Column Reboiler Duty

3.4 Optimum Condition Pressure Swing Distillation System Parameters

Based on the results of the sensitivity analysis of the PSD system, the optimum operating parameters can be seen in Table 2. Based on these parameters, the data profile of the ethanol-water composition in the LP and HP columns is obtained, and temperature data profiles in the LP and HP columns.

Table 2
Optimum Conditions PSD System Parameters

Column	Number of Stages	Feed Stage	Reflux Ratio	Pressure
LP	29	28[1] dan 9[2]	2.126	1 atm
HP	42	7	1.669	14 atm

[1]Fresh feed stage dan [2]Recycle feed stage

Figure 20 and 21 show the profile of the ethanol-water composition at each stage of the LP and HP columns. Meanwhile, Figure 22 and 23 show the temperature profile of each stage of the LP and HP columns. The large temperature changes especially from stage 26 to 29 at LP column indicates a region where the composition (water or ethanol) changes significantly [32]. There is an increase in temperature that occurs near the bottom of the LP column as the water is concentrated near 100°C. In the HP column, the minimum azeotropic boiling point is drawn at the top of the column, because the purified anhydrous ethanol has a higher temperature than the azeotropic mixture and exits at the bottom of the column.

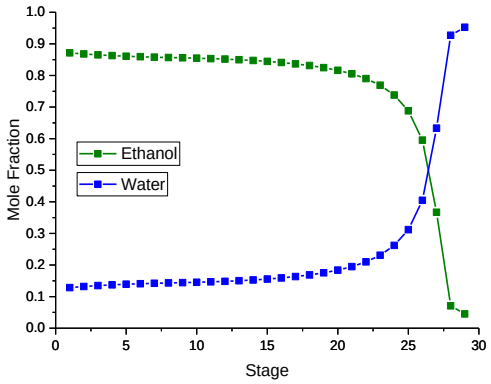

Fig. 20. LP Column Ethanol-Water Composition Profile

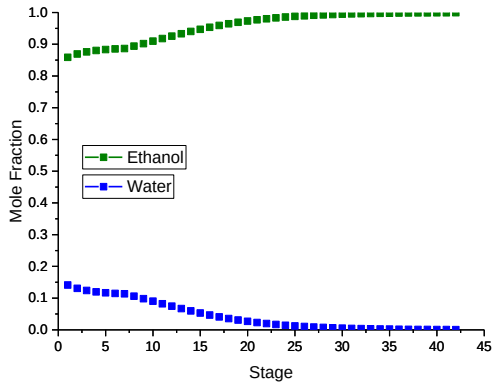

Fig. 21. HP Column Ethanol-Water Composition Profile

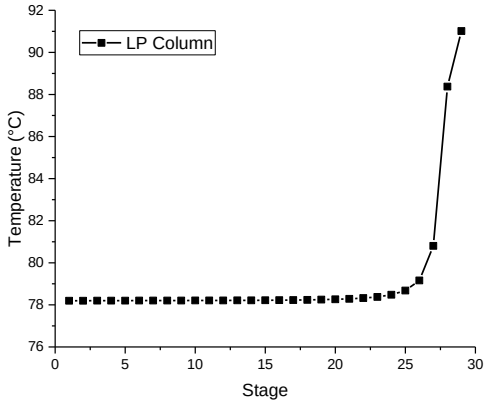

Fig. 22. LP Column Temperature Profile

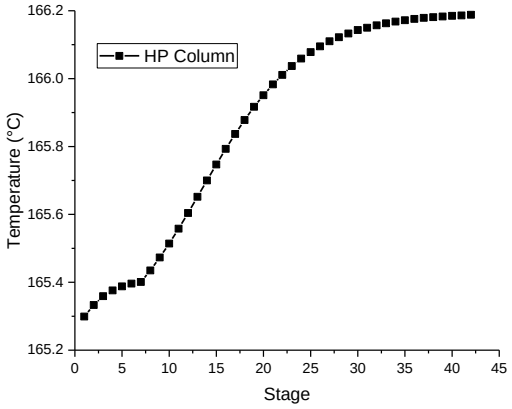

Fig. 23. HP Column Temperature Profile

4. Conclusions

The Pressure Swing Distillation method for bioethanol purification from microalgae was simulated using Aspen Plus. The results showed that the bioethanol with purity of 99.9% was obtained with an energy consumption at the condenser duty and the reboiler duty of the LP column was -79.931 kW and 667.651 kW respectively. While the condenser duty and reboiler duty of HP column was -47,627 kW and 57,698 kW, respectively. The effect of the pressure has a significant effect on the purity of ethanol, condenser duty and reboiler duty. The optimum operating conditions obtained for the LP column and HP column were 1 and 14 atm respectively. The effect of the reflux ratio in PSD column (LP and HP) shows that the higher reflux ratio will increase the ethanol purity, condenser and reboiler duty. The optimum reflux ratio for LP and HP column was 2.126 and 1.669 subsequently. The effect of the number of stages and feed stage (feed location) also show a significant effect on the purity of ethanol, condenser duty, and reboiler duty. The optimum column configuration for LP column was 29 number of stages with fresh feed at stage 28 and recycle feed at stage 9. While, the HP column configuration was using 7 number of stages 42, with a feed stage of 7.

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