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Simulation of the Effect of Flow Ratio on Methyl Caproate Composition in Fractionated Methyl Ester Based on Palm Kernel Oil

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ABSTRACT

This research consists of five steps. The first is a literature review and *Aspen Plus* simulator review. This review step will not only provide initial data and assumptions, but also determine which thermodynamic data are suitable to be used in *Aspen Plus* for this research. The second step is the data collection step. The data are collected from actual recorded data, such as temperature, pressure, and flow rate, from one of the oleochemicals plants during the June 2023 period, complete with the analysis results. The data and analysis results are collected from several days in the month and are selected based on the normal running conditions of the plant, without any interruptions. The third step is process modeling with the *Aspen Plus* simulator, using the data collected from the literature review and actual plant data. The fourth step is validation of the process model using actual plant data with different modes. The last step is simulation of the process using the valid model to predict the product composition based on predetermined process parameter variations. Based on the actual plant data, a valid model was obtained using the *RadFrac* Unit Operation, with a reflux ratio of 150, stage count at 32 stages, and feed stage at stage 23. The process parameter variations used in the simulation are reflux ratio and side product flow ratio, each with a +/- 10% range. Based on the simulation results, reflux ratio affects *methyl caproate* product composition more than side product flow ratio in the first *methyl ester* fractionation column. This model has the potential to be implemented in the plant to predict the *methyl caproate* composition in case of feed composition changes or deviations in the product composition itself.

Keywords: simulation; fractionation; distillation; methyl ester; methyl caproate; biodegradeble surfactants

INTRODUCTION

The growth of the human population in the world continues to increase every year; in 2023, the human population has reached 7.91 billion people (Cheng et al., 2025). Along with this increase in the human population, the need for consumer goods also rises. The higher the human population in a country, the higher the demand for consumer goods (United Nations, 2022; Haub & Gribble, 2023). Consumer goods are products that can be consumed directly by consumers without undergoing an advanced process to obtain the benefits of the product. Consumer goods are divided into several categories, two of which are personal hygiene products—such as shampoo, soap, and toothpaste—and household products, such as detergents and floor cleaners (Grabner-Kräuter, 2018; Kotler & Keller, 2021). In the production of personal hygiene and household products, active ingredients in the form of surfactants are needed, which function to lower the water surface tension so that impurities are easier to remove (Sarmah et al., 2022; Turovsky et al., 2020; Bi et al., 2023). The most common raw material for making surfactants is fatty alcohol, which is usually produced from petroleum and vegetable oils.

Along with the emergence of environmental concerns, traditional petroleum-based surfactants are increasingly being replaced with more sustainable alternatives, such as those derived from vegetable oils like palm oil, palm kernel oil, and coconut oil (Cholakova & Tcholakova, 2025; Oikonomou et al., 2018). These bio-based surfactants, including alkyl polyglucosides and sucrose esters, are biodegradable, non-toxic, and demonstrate comparable performance in cleaning and emulsification processes (Cholakova & Tcholakova, 2025; Oikonomou et al., 2018; Sarmah et al., 2022). Beyond environmental benefits, substituting petroleum with vegetable oil feedstocks addresses sustainability challenges related to non-renewable resources and reduces the ecological footprint of surfactant production (Sarmah et al., 2022; Turovsky et al., 2020). Life cycle assessment studies have shown that palm kernel oil–based surfactants can lower greenhouse gas emissions, although the environmental impacts may vary with crop cultivation practices (Djolov et al., 2021; Extended surfactants review, 2017). Moreover, innovations such as coconut oil–derived esterquat surfactants exhibit high biodegradability and are effective in fabric softeners, lubricants, and cleaning formulations (Oikonomou et al., 2018; Sarmah et al., 2022). As industries shift toward green chemistry principles, the adoption of vegetable oil–based surfactants continues to grow, representing a crucial step toward sustainable production in personal care and household products (Cholakova & Tcholakova, 2025; Sarmah et al., 2022).

Fatty alcohol is an oleochemical product resulting from a hydrogenation reaction between *methyl esters* and hydrogen. *Methyl esters* themselves are obtained from the reaction of triglycerides in vegetable oils with methanol, assisted by acid and alkaline catalysts to accelerate the reaction. The *methyl ester* that is formed will be fractionated based on the carbon chain, which will later be hydrogenated into *fatty alcohol* with a specific carbon chain. *Fatty alcohol* with carbon chains C12–C14 is the main raw material in the manufacture of *surfactants*. One of the sources of vegetable oils with a primary carbon chain content of C12–C14 that is most often used in the oleochemicals industry is *palm kernel oil*, commonly abbreviated as *PKO* (Chemanalyst, 2023).

Oleochemicals companies in Indonesia usually use *palm kernel oil* as the main raw material in their production process because of its abundant supply and more competitive price compared to other vegetable oils. In the production process, the carbon chain in *fatty alcohol* relies heavily on the *methyl ester* fractionation process to separate the short carbon chains (C6–C10) from the middle and long carbon chains (C12–C20). The fractionation of *methyl esters* is greatly influenced by the temperature and pressure of the fractionation column, as well as the flow rate of the product from the fractionation column. Changes in these operating conditions have a direct effect on the composition and purity of the fractionated *methyl ester*. If the operating conditions are not optimal, the specifications of the *methyl ester* products produced become off-spec and may require more energy to re-process the off-spec products, resulting in the loss of production volume and making the final product less competitive in price.

On an industrial scale, obtaining optimal operating conditions such as temperature, pressure, and product flow rate in the *methyl ester* fractionation column can be done by experimenting with the trial-and-error method. However, this method is time-consuming due to the large volume and carries the risk of off-spec product composition and a high propensity for error if done in a short time. Therefore, to obtain the right and optimal operating conditions for temperature and pressure, as well as to maximize *fatty alcohol* yield, it is necessary to model the *methyl ester* fractionation column process.

In this study, the *methyl ester* fractionation column to be modeled is the first fractionation column of a series of three-stage fractionation and one-stage distillation columns. The real data taken from the plant comes from recorded data in 2023. The data collected include temperature and column pressure, product flow rate, and product composition analysis results. The product composition specifications required by the company will also be used as the basis for simulating process conditions using the obtained model. After that, the model can be studied and used as a basis for predicting the operating conditions of the *methyl ester* fractionation column, thereby reducing the risk of re-processing off-spec products, minimizing production volume loss, and increasing operating cost efficiency so that the price of *fatty alcohol* products remains competitive.

In modeling fractionation columns, some of the commonly used software includes *Aspen Hysys*, *Aspen Plus*, *Chemcad*, and *Simulink*. In addition, other methods such as *Machine Learning* and *Deep Learning* can be used, utilizing actual data as the basis for process modeling. In this study, the software used is *Aspen Plus*, which will then be validated with real data to obtain valid and accurate modeling. The resulting model will be used to predict the operating conditions of the *methyl ester* fractionation column to achieve a composition that meets the plant's requirements.

The production of *fatty alcohols* involves a series of processes, beginning with transesterification of triglycerides into *methyl esters*, followed by fractionation and hydrogenation. The fractionation stage is critical in determining the quality and specification of the final product. However, fluctuations in process parameters such as temperature, pressure, and flow rates can lead to off-spec products, increased energy usage, and reduced profitability. While traditional trial-and-error methods are time-consuming and costly, process modeling and simulation using *Aspen Plus* software offer a more efficient and safer alternative for optimizing operating conditions.

Several previous studies have focused on biodiesel production optimization (Nguyen, 2012; Anene & Giwa, 2016) and the design of distillation systems using simulation tools (Kick et al., 2013; Othman, 2020). However, most of these studies are centered on biodiesel processes or generic distillation columns, with limited focus on the fractionation of *methyl esters* specifically derived from *palm kernel oil* under industrial conditions. This forms the research gap, as few studies provide a detailed and validated model using real plant data to predict the impact of flow and reflux ratio on *methyl caproate* composition.

The novelty of this study lies in its application of real industrial data from a 2023 oleochemical plant in Indonesia to validate and simulate *methyl ester* fractionation using *Aspen Plus*. By focusing on the first column of a multi-stage fractionation system, the study develops a specific and practical model to simulate variations in flow rate and reflux ratio and predict their effect on *methyl caproate* yield.

The objective of this research is to develop and validate a simulation model using *Aspen Plus* for the first *methyl ester* fractionation column, and to evaluate the influence of process parameters—specifically the flow ratio and reflux ratio—on product composition. The benefits of this research include providing a reliable simulation model that can be used by plant operators to optimize operating conditions, reduce production inefficiencies, and serve as a predictive tool for adjusting feed or product targets in response to market or operational changes.

METHOD

The *methyl ester* fractionation column modeling and optimization research was carried out through five main stages: literature review and the use of the *Aspen Plus* simulator, data collection, model creation, model validation, and process simulation. The initial stage involved reviewing the relevant literature to obtain a theoretical basis and assumptions of initial operating conditions, which were then used in modeling. *Aspen Plus* was chosen as a simulation tool because of its comprehensive ability to process physical and chemical *methyl ester* data. The data used for model validation were obtained from actual instrumentation records at one of the oleochemical plants during the period 1–30 June 2023, covering parameters such as temperature, pressure, flow rate, and product composition. This input-output data was assumed to be valid and representative of actual process conditions.

The fractionation column model was developed based on literature, patents, and actual factory data, and then validated by comparing the simulation results against field data. If parameters such as temperature and pressure showed compatibility with the actual data, the model was considered valid and could be used for advanced simulations. This simulation aimed to predict optimal product composition and understand the effect of variations in operating conditions, especially variations in side product flow ratio and reflux ratio, on fractionation results. These two parameters were chosen because they were often adjusted in factory operational practices to achieve the desired product specifications. The process studied in this research focused on the first column of the four-column configuration, namely three fractionation columns and one *methyl ester* distillation column.

This research was conducted at the Computing Laboratory of the Chemical Engineering Study Program, Parahyangan Catholic University located in Bandung, West Java, Indonesia. Data collection was carried out in one of the *sections* at one of the oleochemical companies in Indonesia, namely the Section 7 *Methyl Ester Fractionation Section*. The research work schedule is planned to start in October 2023 – May 2025.

The data used for model validation were gathered from actual plant instrumentation records (1–30 June 2023) at an Indonesian oleochemical facility, covering parameters such as temperature, pressure, flow rate, and product composition. The model was constructed using a combination of DSTWU (shortcut) and RadFrac (rigorous) units, which were configured based on actual operating data and patent references. Model validation was conducted by comparing simulated product compositions against real factory data at a different time point (June 28, 2023). The validation criteria were based on a maximum acceptable deviation of ±5% between simulated and actual product composition, ensuring the model's reliability in replicating industrial performance.

For simulation, two key process parameters—side product flow rate and reflux ratio—were varied by ±10% from baseline values. This range was selected based on operational tolerance commonly applied in industrial settings, where small deviations in flow or heat duty often occur due to process fluctuations or control system adjustments. The goal of this simulation was to assess the sensitivity of methyl caproate composition to these variations, identify optimal conditions, and provide predictive capability to reduce the risk of off-spec production.

RESULT AND DISCUSSION

Research Data

This research uses actual data taken from the first fractionation column of Section 7 Methylester Fractionation Section of one of the Oleochemical factories in Indonesia on June 21 and 28, 2023 at 07.00 complete with operating conditions such as temperature, pressure, and column flow rate as well as the results of product composition analysis. In the first fractionation column in *section 7, there* is a separation of 3 products, namely *methyl esters* C6-C8, C8-C10, and C10-C20.

These products have certain specifications that have been adjusted to the needs of the company. This specification will then also be used in the process validation process, while the operating conditions and product composition analysis results will be used in the initial model making.

The variations in the process carried out are variations in flow rate and bottom temperature of column/*reboiler duty*. The flow rate to be varied is the *side product flow rate* (C8-C10) with a range of +/- 10%. *The reflux ratio* will also be varied in the range of +/- 10%.

Parameter	21 June 2023				28 June 2023			
	Feed	Top	Middle	Bottom	Feed	Top	Middle	Bottom
Flow (kg/h)	30148.6	93.1	2033.9	28021.6	30149.4	112.0	2025.0	28012.4
Pressure (mbar)	8000.0	122.5	144.4	188.3	8000.0	119.8	145.2	196.3
Temperature (°C)	205.6	99.5	148.4	215.7	204.8	97.4	149.3	218.6

Figure 2. Actual Factory Operating Condition Data as of June 21 & 28, 2023

Source: by Researcher

Parameter	21 June 2023			28 June 2023		
	Feed	Top	Middle	Feed	Top	Middle
%C6	0.21	63.52	0.13	0.23	69.67	0.15
%C8	3.36	36.35	57.6	3.82	30.24	55.8
%C10	3.52	0.12	42.12	3.06	0.08	43.66
%C12	50.2	0	0.16	47.78	0	0.39
%C14	15.94	0	0	16.29	0	0
%C16	8.11	0	0	8.52	0	0
%C18:0	1.89	0	0	2.41	0	0
%C18:1	14.42	0	0	15.39	0	0
%C18:2	2.26	0	0	2.40	0	0
%C20	0.09	0	0	0.10	0	0

Figure 3. Feed Composition and Actual Factory Product Data as of June 21 & 28, 2023

Source: by Researcher

Research Model Creation

At the modeling stage, the Operating Units used in modeling the *fractionation column of methyl esters* are DSTWU and RadFrac units. The DSTWU operating unit is used to model the fractional column of *methyl ester* by *the shortcut* method so that data in the form of *reflux ratio* and *minimum theoretical stage will be obtained.* The data obtained from DSTWU will then be used as input for rigorous *models,* in which case the RadFrac operating unit will be used.

In modeling the *methyl ester* fractionation column, the DSTWU operating unit requires 2 DSTWU columns with an *indirect sequence configuration,* where the *feed* will go into the first column and the top product will be separated again in the second column. So that the DSTWU column will have 4 inputs, namely 1 *feed* and 3 *products* whose value will be determined based on actual factory data.

The output from DSTWU and the actual operating conditions will be used as inputs from the RadFrac Operating Unit, resulting in an initial model that will need to be further validated to obtain *a valid* methyl ester fractionation column model.

The operating conditions and composition that will be used at the stage of making the initial model of the *methyl ester* fractionation column are actual factory data on June 21, 2023 with parameters and configurations that can be seen in **Figure 4.** and **Table 5.**

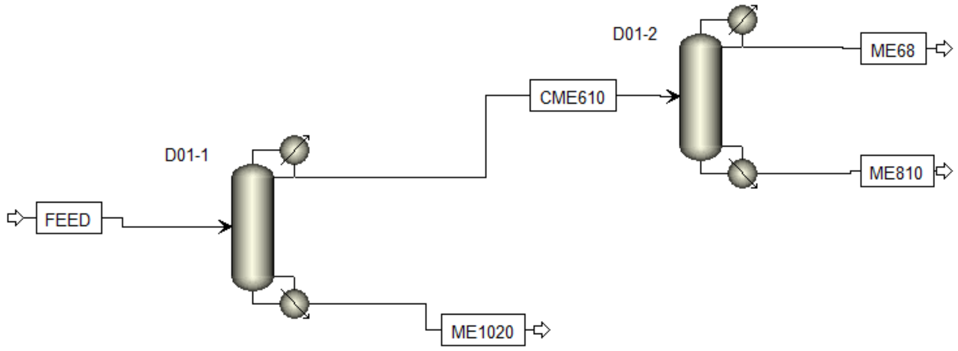


Figure 4. DSTWU Modeling Configuration

Source: by Researcher

Parameter	DSTWU		
	FEED	ME68	ME810
Flow (kg/h)	30148.6	93.0811	2033.91
Pressure (mbar)	8000	122.46	144.42
Temperature (°C)	205.62	99.5	148.4
%C6	0.21	67.34	0.03
%C8	3.36	32.65	48.32
%C10	3.52	0.01	51.65
%C12	50.2	0	0
%C14	15.94	0	0
%C16	8.11	0	0
%C18:0	1.89	0	0
%C18:1	14.42	0	0
%C18:2	2.26	0	0
%C20	0.09	0	0

Figure 5. DSTWU Modeling Parameters

Source : by Researcher

Based on the modeling results above, the output of DSTWU that will be the input from RadFrac can be seen in **Table 6**.

Results	DSTWU		RadFrac	Data Source
	D01-1	D01-2	D01	
Minimum reflux ratio	78.8	4.0	150	Actual
Actual reflux ratio	150.0	7.0		
Minimum number of stage	17.8	5.9	32	DSTWU
Actual number of stage	23.1	8.7		
Feed stage	17.8	4.8	23	

Table 6. DSTWU Modeling Output & RadFrac Input
Source: by Researcher

The configuration and process parameters of the RadFrac operating unit used can be seen in **Figure 2** and **Table 5.**

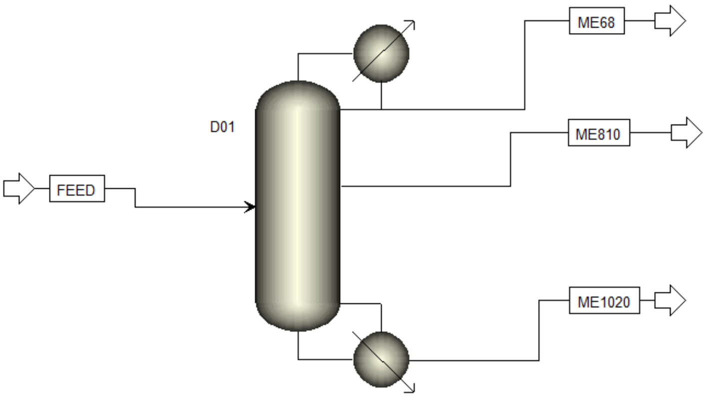
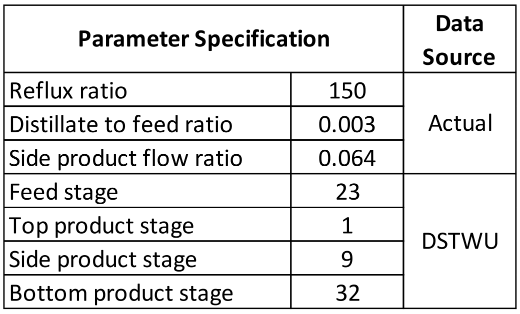


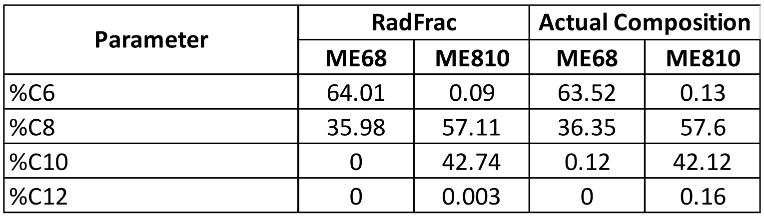
Figure 7. RadFrac Modeling Configuration
Source: by Researcher



Parameter Specification		Data Source
Reflux ratio	150	Actual
Distillate to feed ratio	0.003	
Side product flow ratio	0.064	
Feed stage	23	DSTWU
Top product stage	1	
Side product stage	9	
Bottom product stage	32	

Figure 8. Parameter Pemodelan RadFrac
Source: by Researcher

Based on the above inputs and specifications of RadFrac parameters, with the *same feed composition* and operating conditions, product composition results were obtained from RadFrac modeling which was close to the actual product composition of the factory on June 21, 2023. A comparison of the composition of the RadFrac modeling and the actual composition can be seen in **Figure 9.** below.

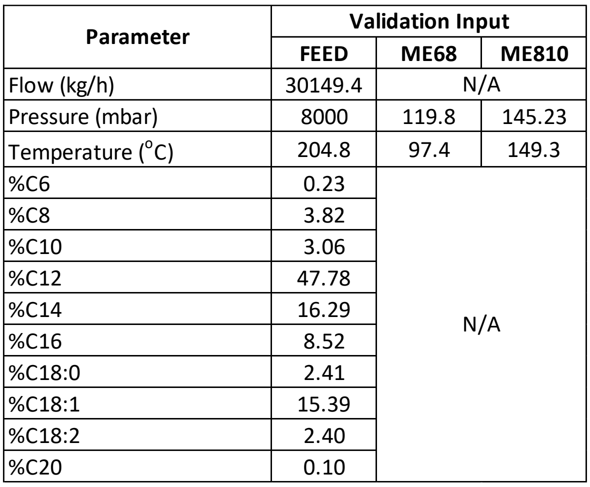


Parameter	RadFrac		Actual Composition	
	ME68	ME810	ME68	ME810
%C6	64.01	0.09	63.52	0.13
%C8	35.98	57.11	36.35	57.6
%C10	0	42.74	0.12	42.12
%C12	0	0.003	0	0.16

Figure 9. Comparison of RadFrac vs Factory Actual Product Composition
Source: By Researcher

Model Validation

The model obtained using the RadFrac operating unit will then be validated using the operating conditions and *feed* composition at different times, namely on June 28, 2023 which can be seen in **Figure 10.**

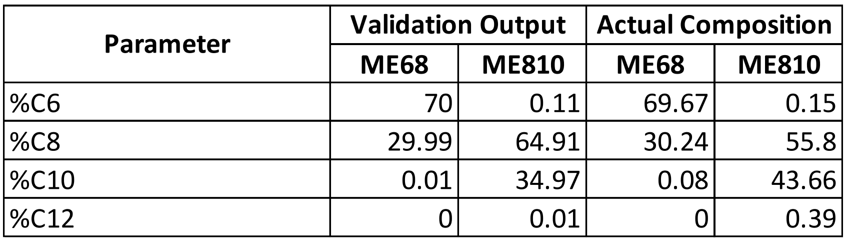


Parameter	Validation Input		
	FEED	ME68	ME810
Flow (kg/h)	30149.4	N/A	
Pressure (mbar)	8000	119.8	145.23
Temperature (°C)	204.8	97.4	149.3
%C6	0.23	N/A	
%C8	3.82		
%C10	3.06		
%C12	47.78		
%C14	16.29		
%C16	8.52		
%C18:0	2.41		
%C18:1	15.39		
%C18:2	2.40		
%C20	0.10		

Figure 10. Operating Conditions and Composition of Model Validation Feeds

Source: By Researcher

Based on the input **of Figure 10**, results were obtained in the form of product composition that is close to the actual composition of the factory on June 28, 2023. A comparison of the product composition and actual factory can be seen in **Figure 11.**



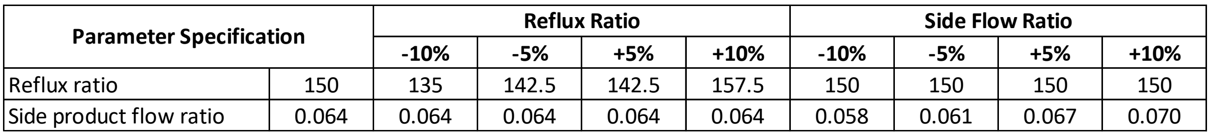
Parameter	Validation Output		Actual Composition	
	ME68	ME810	ME68	ME810
%C6	70	0.11	69.67	0.15
%C8	29.99	64.91	30.24	55.8
%C10	0.01	34.97	0.08	43.66
%C12	0	0.01	0	0.39

A. Process Simulation

Figure 11. Comparison of Product Composition Model Validation

Source: By Researcher

A valid model can then be used in conducting process simulations, while the process simulation carried out is by changing process variables such as the flow rate of by-products and *reflux ratio* to obtain a profile of the influence of operating conditions on the purity of the top product (C6-C8/ME68). The variation in the by-product flow rate and *reflux ratio* is in the range of +/- 10% of the initial parameters which can be seen in **Figure 11.**



Parameter Specification		Reflux Ratio				Side Flow Ratio			
		-10%	-5%	+5%	+10%	-10%	-5%	+5%	+10%
Reflux ratio	150	135	142.5	142.5	157.5	150	150	150	150
Side product flow ratio	0.064	0.064	0.064	0.064	0.064	0.058	0.061	0.067	0.070

Figure 11. Process Simulation Variations

Source: By Researcher

Based on the variations in the above parameters, simulation results were obtained in the form of the composition of the upper product (ME68) which can be seen in **Table 4.10.**

Parameter Specification			**Reflux Ratio**				**Reflux Ratio**			
			-10%		**-5%**		**+5%**		**+10%**	
Reflux ratio	150		135	135	142.5	142.5	157.5	157.5	165	165
Side product flow ratio	0.064		0.064	0.064	0.064	0.064	0.064	0.064	0.064	0.064
Composition	**ME68**	**ME810**	**ME68**	**ME810**	**ME68**	**ME810**	**ME68**	**ME810**	**ME68**	**ME810**
%C6	64.01	0.10	63.38	0.10	63.71	0.10	64.25	0.09	64.47	0.09
%C8	35.98	57.12	36.62	55.53	36.29	56.37	35.75	57.66	35.53	58.15
%C10	0.00	42.74	0.00	40.77	0.00	41.93	0.00	42.24	0.00	41.75

Figure 12. Comparison of Composition of Process Simulation Variations – *Reflux Ratio*

Source: By Researcher

Parameter Specification			**Side Flow Ratio**				**Side Flow Ratio**			
			-10%		**-5%**		**+5%**		**+10%**	
Reflux ratio	150		150	150	150	150	150	150	150	150
Side product flow ratio	0.064		0.058	0.058	0.061	0.061	0.067	0.067	0.070	0.070
Composition	**ME68**	**ME810**	**ME68**	**ME810**	**ME68**	**ME810**	**ME68**	**ME810**	**ME68**	**ME810**
%C6	64.01	0.10	63.98	0.10	64.00	0.10	63.97	0.09	63.98	0.09
%C8	35.98	57.12	36.02	63.26	36.00	60.00	36.03	54.00	36.02	51.12
%C10	0.00	42.74	0.00	36.63	0.00	40.00	0.00	40.79	0.00	38.73

Figure 13. Perbandingan Komposisi Variasi Simulasi Proses – *Side Product Flow Ratio*

Source: By Researcher

Based on the results obtained, a graph of the product composition and *process gain* value can be made to learn the ratio that most affects the composition of *methyl caproate products.* The product composition graph can be seen in **Figure 1.** and **Figure 2**, while the table of *process gain* composition to variation can be seen in **Table 12** and **Table 13.**

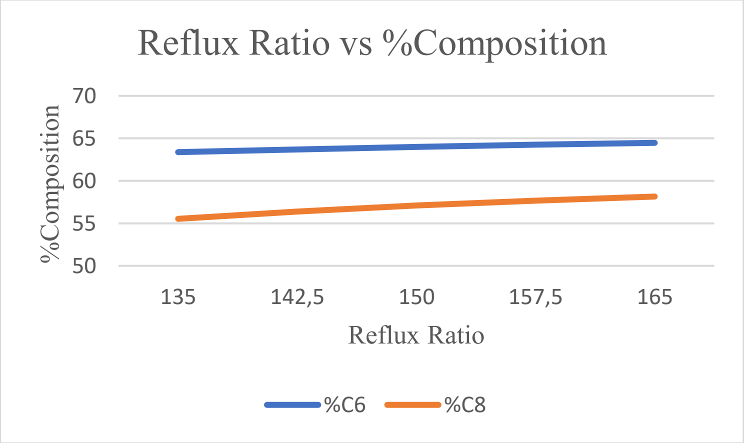


Figure 14. Graph of Reflux Ratio vs %Composition

Source: By Researcher

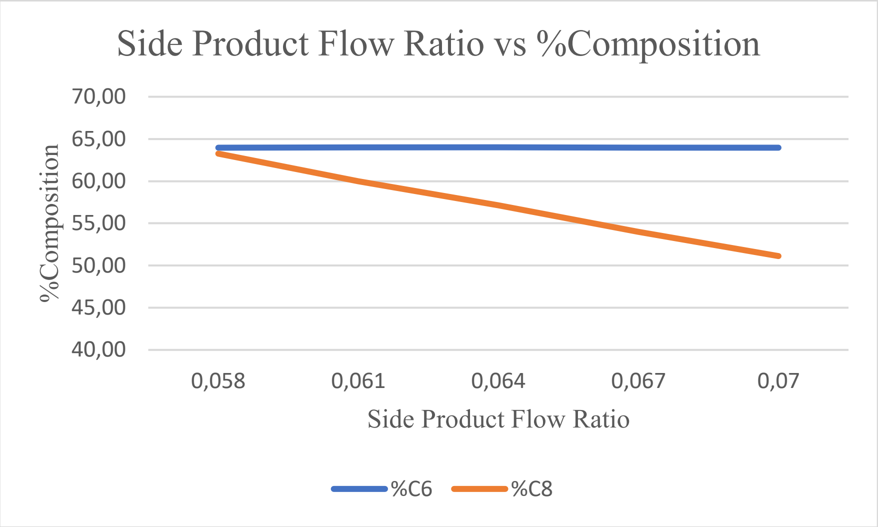


Figure 15. Graph Side Product Flow Ratio vs %Composition

Source: By Researcher

Reflux Ratio	%C6	%C8	Gain %C6	Gain %C8
135	63.38	55.53	5%	13%
142.5	63.71	56.37		
150	64.01	57.12		
157.5	64.25	57.66		
165	64.47	58.15		

Figure 16. Process Gain Reflux Ratio

Source: By Researcher

Side Product Flow Ratio	%C6	%C8	Gain %C6	Gain %C8
0.058	63.98	63.26	0%	61%
0.061	64.00	60.00		
0.064	64.01	57.12		
0.067	63.97	54.00		
0.07	63.98	51.12		

Figure 17. Process Gain Side Product Flow Ratio

Source: By Researcher

Based on the data above, changes in *the reflux ratio* affect the composition of *methyl caproate products* more than the *side product flow ratio*.

Potential Model Applications in Industry

The valid models obtained from this research and modeling have potential that can be applied in the following industries: Predict the composition of the product if there are changes in feed adjusted to the conditions and availability of raw materials. Provide the basis for determining standard operating procedures to factory personnel if there is a deviation in the composition of the products produced.

CONCLUSION

The research demonstrated that the use of *Aspen Plus* was accurate for modeling and simulating the fractionation process of *methyl caproate* in the first column of *methyl ester* separation, with optimal process parameters identified as a minimum reflux ratio of 150, a total of 32 stages, and the feed introduced at stage 23. The study found that among the various flow parameters, the reflux ratio had the most significant impact on the *methyl caproate* composition in the top product of the first fractionation column. For future research, it is suggested to expand the modeling to the subsequent columns in the fractionation train and to investigate the effects of additional process variables, such as temperature fluctuations and feed composition changes, to further optimize product quality and process efficiency.

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