DEVELOPMENT OF INFERENTIAL MODEL FOR ADVANCED PROCESS CONTROL (APC) OF ISOPROPYL-ALCOHOL (IPA) – ACETONE COLUMN

By

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Dissertation submitted in partial fulfilment of the requirements for the Bachelor of Engineering (Hons) Chemical Engineering

MAY 2014

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the Chemical Engineering Programme Universiti Teknologi Petronas In partial fulfillment of the requirement for the Bachelor of Engineering (Hons) Chemical Engineering

Approved by,

(Dr Haslinda Bt Zabiri)

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CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and the original work contained herein have not been undertaken or done by unspecified sources or persons.

NUR AINNA EMIRA BINTI E.ZANI

ABSTRACT

This project focusing on separating Isopropyl-Alcohol (IPA) – Acetone mixtures into desired purity in distillation process unit. The experiment is conducted in Pilot Scale Distillation Unit in UTP Academic Block and simulation is prepared using Aspen HYSYS.

This project presents a development of inferential model to provide standard product estimator for distillate in distillation column. This model acts like a 'soft sensor' that is able to give product properties online like hardware sensors. It is developed by Microsoft Excel Solver using existing variables data from experiment.

Based on the analysis, performance of inferential model are good in predicting product composition with less error and high accuracy when compared with HYSYS simulation. Case studies were perform in changes of variables of reflux rate and steam rate.

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I hope that this project will be useful and contribute greatly to the industry in the future.

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NOMENCLATURE

RI	Refractive Index
PLS	Partial Least Squares
PCR	Principal Components Regression
SSE	Sum of squares of error
\mathbb{R}^2	Coefficient of determination
UTP	Universiti Teknologi PETRONAS

CHAPTER 1 INTRODUCTION

1.1 Background of Study

This project is related to distillation column focusing in developing a control model that can directly estimate product composition. Inferential model will be developed for this project incorporated the data from lab analysis. Isopropyl Alcohol (IPA) and Acetone are used as component mixture that need to be separated in binary distillation column. Mixture is distilled by boiling point of component. Fraction of lighter component (Acetone) in the top part of distillation column will be vaporized and stripped away from liquid phase. Meanwhile, heavier component (Isopropyl-Alcohol) will be moved from the bottom of the column.

This project seeks an online estimator for distillate composition of distillation column. Direct measurements for estimating product composition of distillation column is very crucial in order to maintain the quality specifications of product [1].

Inferential model is chosen as product estimator which will be developed for this project incorporated data from lab analysis. Inferential model is a process model which can estimate product composition from on-line measurement variables such as temperature, pressure and flow rate [2]. Since computer-based process control is extensively used in industry, existing data can be utilized to improve process operation.

Isopropyl-Alcohol (IPA) and Acetone mixtures are used as component mixture that need to be separated in binary distillation column. Mixture is distilled by boiling point of components where fraction of lighter component will be vaporized and tripped away from top of the column, while heavier component will be moved down to bottom part of the column [3].

In this research paper, author will analyze the performance of inferential model with simulated data. The author also will tested the effect of variable changes toward distillate composition. Two parameters that is tested as variables are reflux rate and steam rate. The tests need to be conducted in order to see how well the inferential model performed with changes of variables. Performance of inferential model developed will be asses by calculating coefficient of determination, R². Coefficient of determination is a statistical measure of how good the model approximates real data points.

1.2 Problem Statement

This project is concerned with a problem on how to enhance the performance of distillation composition control using inferential model. In current process industry, product composition is predicted based on tray temperature by assuming certain composition can be achieved given a certain temperature. However, due to disturbance that usually occurs during dynamic operation, temperature-based estimator is not always correct. Therefore composition based on temperature will not always guarantee the accuracy of the product. In conjunction to this problem, common approach by the industry is through laboratory analyzers such as gas chromatograph and refractometer which infrequent and long delays. By the delays, the possibility for the samples to be affected is higher.

Thus, the reliability of the product estimation is doubted as well. In addition to that, the most favorable alternative is to estimate product composition through inferential model that will be built in this project. The model also known as 'soft sensor'. Existing variables such as temperature, pressure and flow are often used to develop a model.

1.3 Objective of Study

Profit function of plant operation can be maximized by keeping product quality in acceptable range. However, the quality specifications can be easily monitored if it is available online. Therefore it is important to develop a system that can directly estimate product composition. The system also must work on real-time operating variables such as temperature, flow rate and pressure which influenced product quality. The aim of the project is to build a model that can measure product composition to cater delay from sample measurement. The model will be validated through simulation and lab analysis data.

1.4 Scope of Study

Isopropyl Alcohol (IPA) and Acetone is used in the experiment as binary component that need to be separated in distillation column. The project focuses in obtaining product composition of Acetone in distillate. The experiment is done simultaneously by varying the manipulated variables:

- i. Steam flow rate
- ii. Reflux flow rate

The output to be observed from manipulating the parameters is the product composition.

1.5 Relevancy of the Project

The project of developing an inferential model for product estimator which to be made for easy implementation, thus is very important for process operation. Even though the subject is not new, there will be always a plenty of study done to verify the accuracy of the model. One of the old researches by Wood and Berry in 1973 proved the accuracy of the model based on 8 tray column. However, this project in the other hand, is aim to develop a model for 15 tray column of pilot scale plant which doubled the size of model made by Wood and Berry. This project is also relevant in term of chemical engineering thermodynamics concept. Besides, the study of process control of distillation column is one of main focal area in Chemical Engineering industry.

1.6 Feasibility of the Project

This project is feasible as it deals with narrowed scope of experiment whereby only two parameters are tested. It is within capability to be executed with helps and guidance from the supervisor. It is positive that this project can be completed within the time allocated with the acquiring of equipment and materials needed. The scope of study of this project will be accomplished within time frame, which is two semesters.

CHAPTER 2 LITERATURE REVIEW

2.1 Concept of Distillation Process

Distillation is the most universal process used for separation of mixtures in chemical and petroleum industries [4]. Even though distillation process is often costly and energy consuming, it remains as the most general separation technology in industries. The boiled up mixture will be vaporized and richer component is stripped to the top of the column.

A typical distillation unit contains several major components such as trays, condenser, reboiler, reflux drum and a column [5]. Figure 1 displays major components in distillation unit.



Figure 1: Major components in distillation unit (Source: <u>http://lorien.ncl.ac.uk/ming/distil/distileqp.htm</u>)

Feed tray is usually somewhere in the middle of the column where liquid mixtures is fed. The tray divided a sections between rectifying (top) section and stripping (bottom) section. Feed flow down the column and being heat up by the reboiler. Bottom product is removed from the reboiler. Meanwhile, the heat supplied will generate vapor that will moves up the column and exists the top unit and then being cooled by condenser. The condensed liquid will be stored in reflux drum. Some of the liquid is recycled or reflux back into the column, or removed as distillate.

2.2 Inferential Model

Most petroleum and petrochemical industries lack of capability in obtaining real time measurement [6]. Common approach in industries, product measurement can only be identify by human procedures such as laboratory analysis data. However, laboratory analysis may contains error due to infrequent lab test especially for dynamic process operation which fast-acting process [7]. Meanwhile, the cost of installing hardware sensor may not relevant to plant operation and the sensor may suffers from long measurement delays [8]. In order to achieve a certain product specifications, the product must be measured in real time, which is difficult. In recent years, industry has started to develop methods through mathematical inference model to produce an estimate product quality, based on regression analysis [9]. There are several regression models have been develop throughout the years include Kalman-Bucy Filter, Brosilow Estimator, Principal Component Regression (PCR) and Partial Least Square (PLS).

A soft sensor based on Kalman-Bucy Filter is introduced by Kalman and Bucy in 1961 [10]. The model is an estimator based on dynamic process plant [11]. However, plenty of reports on the use of the model based Kalman Filters for composition estimation of distillation process. Complexity and model uncertainty in recognize weight of disturbance and noise are main drawbacks of this model.

Meanwhile in process control, Weber and Brosilow proposed a composition estimators called Brosilow Estimator. Secondary measurement is used to estimate disturbance. Disturbance contributes less in process control application are their justifications. Even though Brosilow scheme seems have found to be used in industry, it is still may not work well for ill-conditioned plants duet to measurement noise, model error and poor numerical properties caused by colinearity [12].

Further on, Principal Component Regression (PCR) estimator based on principal component analysis (PCA) have been proposed. PCR does not have the same flaws as Brosilow Estimator. Direct relationship is derived between input and output of PCR. According to Ahmed and Zhang (2003), model based on software sensors are developed from available data.

In earlier study, it was found that the Brosilow Estimator performed better than a regression estimator. However, they used simple least-square estimator which suffers from the same poor numerical properties.

In recent years, a study was done by Zamprogna, Barolo and Seborg to shows that soft sensor is developed based on Principle Component Regression (PCR) and Partial Least Square (PLS). Temperature measurement is use as base for create product composition profile. Result from the study proves that precise estimation for product composition can be obtained from PLS [13]. From the result obtained, using few temperature measurements as input provide effective estimation. However, some issues addressed in the research includes effect of measurement inputs and effect of noise in model. Even though the study convey that benchmarks for proper data selection is based on optimal number and location of temperature measurements, apparently there is no report has been made prior application of PLS regression.

Most inferential researches rely on regression and steady state data. However, the reliability of measurements are not constant even at steady state or dynamic because it is not designed for disturbance. Furthermore, since model based on regression analysis requires all inputs to be independent thus they are commonly inferior to first principle model. Hence, first principle model is believed to be the most feasible control strategies to cater this problem.

2.2.1 First Principle Model

The inferential model can also be obtained through first principle method. Advantages of using first principle model compared to regression model are listed as below [14]:

- Regression model requires independent inputs which impossible for real time operation. First principle can be develop using at least knowledge to approach input independence.
- Large volume of laboratory data is needed for empirical model therefore poor quality data also will be used.
- iii. Only minor changes are necessary for first principle model if there are modifications to the process, but empirical model would have to be redeveloped from scratch.

Thus, first principle model are better by definition but need to be proof whether they exist [15]. Mathematical format must be programmed to the computer in order to ensure first principle model work. Even though models are frequently developed, but plant operation has not been using it widely until today.

Effective approach in sustaining the composition control of distillation unit is through inferential temperature control [16]. From economic viewpoint, this method requires less maintenance and installation cost rather than using on-line analyzers such as gas chromatograph. In addition, the model will reduce the flaws of measurement during dead time and thus reliability of the result is achieved [17]. Since column pressure also plays significant effect to tray temperature, thus most system and feedback control should use simple linear correction pressure-compensated temperature [18].

CHAPTER 3 RESEARCH METHODOLOGY

3.1 Project Activities

3.1.1 Literature Review

- For FYPI and FYPII, understanding on the concept of distillation concept and comparison between result from simulation, experiment and modeling must be done.
- Review on literature is done to understand the inferential model and effect of parameters adjusted

3.1.2 Experiment

- Experiment is conducted in Advanced Process Control (APC) distillation column in UTP Academic Block and parameters is determined.
- Chemicals and equipment required for the experiment is prepared and experiment is done.

3.1.3 Data Collection

- From the experiment conducted, the samples are withdrawn.
- The samples are analyzed using refractometer to observe the composition of distillate.

3.1.4 Simulation

• Simulation is done by Aspen HYSYS by manipulating the operating parameters.

3.1.5 Modeling

• First principle based inferential model will be used, applying chemical engineering fundamentals.

3.1.6 Conclusion

• The data obtained from experiment and simulation will be compared with inferential model

3.2 Gantt Chart and Milestone

The activities and targets for Final Year Project have been set to ensure the smoothness of the project and shown in Table 1 and Table 2. The Gantt Chart (FYPII only) and milestones (FYPII) are tabulated in table below:

No	Detail/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Chemical preparation for experiment														
2	Conducting experiment of Isopropyl Alcohol (IPA) - Acetone distillation process														
3	HYSYS simulation														
4	Inferential model development														
5	Validating the model with experimental data and HYSYS														
6	Case study														
7	Preparation of dissertation and technical paper														
8	Preparation of VIVA														

Table 1: Project Activities and Gantt Chart of Final Year Project

Table 2: Milestone of FYP II

No	Detail	Month
1	Completion of experiment of Isopropyl Alcohol (IPA) - Acetone distillation process	June 2014
2	Completion of HYSYS simulation	July 2014
3	Completion of inferential model development	July 2014
4	Completion of validating the inferential model	July 2014
5	Completion of case study validation	July 2014
6	Completion of final year project	August 2014

3.3 Experiment and Modeling Methodology

3.3.1 Experimental Approach



Figure 2: Distillation unit process operation

A. Chemical preparation for distillation column

Isopropyl Alcohol (IPA) and Acetone is fed to the column with ratio 70:30. Flash drum of 240L will contain mixtures of IPA (70%) and Acetone (30%). Equation below is used to calculate the amount of IPA and Acetone to be fed into the feed tank.

 $\rho_{(IPA)}$ = Density of Isopropyl Alcohol (IPA) = 0.768 kg/L

 $\rho_{(\text{Acetone})}$ = Density of Acetone = 0.791 kg/L

Let x = Isopropyl Alcohol (IPA)

Let y = Acetone

Let z = IPA-Acetone

$\mathbf{x} = (0.7/\rho_{(\mathrm{IPA})})\mathbf{z}$	Equation [2]
$y = (0.3/\rho_{(Acetone)})z$	
$z = (\rho_{(\text{Acetone})}/0.3)y$	Equation [3]
Substitute Equation [3] into Equation [2],	
x/y = 2.348	Equation [4]

Substitute Equation [4] into Equation [1], Therefore amount of IPA and acetone to be fed are Acetone = y = 71.68LIPA = x = 168.32L

After calculation has been made, IPA and Acetone is ready to pump into feed tank.

B. Starting-up the distillation column

After the feed mixtures has completely pump into feed tank,

- i. Checking initial valve positions.
- ii. Start-up reboiler.
- iii. Distillation column will operate until steady state temperature profile is achieved.

C. Switching to steady state continuous operation

- i. Feed is introduced into distillation column.
- ii. Adjust control valve for steam supply and two product streams is kept continuously and steady state temperature profile is observed.

iii. After achieve steady state mode, samples is taken from sampling points to be analyzed.

D. Shutting down the distillation column

After finishing the experiment, distillation unit is shut down carefully to avoid any damage to the instruments or injury to operators.

3.3.2 Simulation

A simulation of the distillation process was conducted using Aspen HYSYS using the same base steady-state condition as in experiment. The column consists of 15 trays and the diameter and height of the column is 0.15 m and 5.50 m respectively. The information on the dimension of the distillation column is obtained from actual distillation column used in the experiment. Feed stream enter at Tray 7 and feed composition is 30 weight percent of acetone and 70 weight percent of isopropyl-alcohol (IPA). Schematic diagram of the distillation column is illustrated in Figure 3. The steady state condition used for simulation is tabulated in Table 3.



Figure 3: Schematic diagram of distillation process

Feed		
F	0.5	L/min
Composition	0.3	Acetone
	0.7	Isopropyl Alcohol
Reflux Drum		
L	0.7	L/min
D	0.3	L/min
Т	72.7	°C
Р	101.3	kPa
Reboiler		
V	20	kg/hr
В	0.2	L/min
Т	80.5	°C
Р	101.3	kPa

Table 3: Base steady-state condition

3.3.3 Inferential Modeling

Operational variables data obtained from experiment is used to develop an inferential model. The inferential model will predict product composition of distillate. Microsoft Excel Solver is utilized during the development of inferential model. Below is suggested methodology for inferential modeling is illustrated in flow chart (Figure 4).



Figure 4: Flow chart of inferential model development

An equation to calculate pressure-compensated temperature is used and the obtained temperature is used to calculate the product composition which is acetone composition. Temperature is often used as process variable to calculate stream compositions rather than complex analyzer systems because it is easy and inexpensive way of composition controls. However, temperature control can suffer from pressure variations in column, as column temperature can change due to variations in column pressure at fixed position. Below is the equation that give correlation between column pressure and control temperature taken from Riggs (2006):

 $T_{pc} = T_{meas} - K_{pr}(P-P_o)$ Equation [5]

Where,

 $T_{pc} = pressure-compensated temperature$

 $T_{meas} = measured temperature$

 K_{pr} = pressure correction factor

P = operating pressure

 $P_o =$ reference pressure

K_{pr} is estimated by

$$K_{\rm pr} = \frac{Ti(P_1) - Ti(P_2)}{P_1 - P_2}$$
(2)

Where,

Ti = temperature of tray i predicted by column simulator

The pressure-compensated temperature calculated in Equation [5] is used to calculate the distillate composition by this following equation:

 $X_D = -aT_{pcC} + bT_{pcR} + C$ Equation [7]

Where,

XD = distillate composition

TpcC = pressure-compensated temperature of 'To Condenser' stream

TpcR = pressure-compensated temperature of 'Reflux' stream

a, b, and C are the coefficients to be obtained from Microsoft Excel Solver

To calculate product composition, two (2) pressure-compensated temperature value is needed. According to Riggs (2006), the chosen tray temperature can be insensitive to changes in product impurity levels if a single tray temperature is used in inferring the product composition.

Sum of squared errors (SSE) is calculated using formula below:

$$SSE = \sum_{n=1}^{N} (x(n) - \hat{x}(n))^2$$
 (4)

Where,

x = measurement of the product composition

 \hat{x} = estimated value

N = number of measurements

CHAPTER 4

RESULT AND DISCUSSION

This section is divided into three parts; experiment, simulation and modeling.

4.1 Experiment Results

Eight (8) step changes has been achieved for this experiment, where total eight (8) samples of distillate product collected at top part of distillation column for each step change. The samples is then analyzed by refractometer to obtain refractive index. Formula to calculate composition from refractive index is shown as below:

Let P = mole fraction of Isopropyl-Alcohol (IPA)

Let Q = (1-P) = mole fraction of Acetone

Let p = refractive index of Isopropyl-Alcohol (IPA)

Let q = refractive index of Acetone

Let r = refractive index of Isopropyl-Alcohol (IPA) – Acetone obtained from sample

(P)(p) + (Q)(q) = r Equation [9]

Two parameters is observed in this experiment, 1) Reflux flow rate versus distillate composition and 2) Steam flow rate versus distillate composition. Data obtained from experiment is shown in Table 4.

Time (pm)	Reflux rate (LPM)	Steam rate (LPM)	T1 (°C)	T ₂ (°C)	P1 (kPa)	P2 (kPa)	XD
12.28	0.2	13.00	69.96	69.01	103.50	101.31	0.5485
12.51	0.3	11.84	67.97	67.19	103.50	101.31	0.5802
1.05	0.4	11.55	65.92	65.22	103.50	101.31	0.6055
1.20	0.5	9.48	64.07	63.20	103.50	101.31	0.6207
1.35	0.6	7.41	61.82	60.97	103.50	101.31	0.6561
1.50	0.7	7.03	59.93	59.17	103.50	101.31	0.6858
2.05	0.8	6.40	58.29	57.65	103.50	101.31	0.7133
2.20	0.9	6.15	57.40	56.56	103.50	101.31	0.7384

Table 4: Data obtained from experiment of distillation process

4.2 Inferential Model

Inferential model were developed using Microsoft Excel Solver. All calculations has been done in spreadsheet. By using equations stated in Chapter 3, inferential model for product composition of distillate were built based on coefficients calculated by Microsoft Excel Solver.

$$X_D = 0.114 TpcC + 0.131 TpcR + 1.65$$

The model developed in this project gives the most satisfying result in terms of sum of squared errors (SSE) and coefficient of determination (R^2). Comparison of errors and R^2 will be discussed in the next section. The acetone composition predicted by model is shown in Appendix.

4.2.1 Model Validation

HYSYS simulation data has been used as base to validate results from experiment result data and inferential model. Figure 5 displays graph of temperature versus distillate composition.



Figure 5: Graph of temperature versus Acetone composition

From Figure 5, it is observed that all three methods (experiment, HYSYS, and inferential model) follows same trend which shows the higher the temperature at top of the column, the lower the Acetone composition. The result is expected since Acetone boiling point is 56°C. As the temperature increases, Acetone is already extracted on trays thus Acetone composition on top of the column will decrease.

Coefficient of determination, R^2 has been made between HYSYS and inferential models of distillate. It has been used to assess how well the inferential model predict

product composition. R^2 lies between 0 to 1. The higher the value of R^2 , the better the prediction becomes. R^2 is calculated based on formula below.

$$R^2 = 1 - \frac{SSE}{SST} \tag{6}$$

Where,

SSE = residual sum of squares SSR = regression sum of squares SST = SSE + SSR

Maximum value of R^2 is 1 which means perfectly fit (for HYSYS). Meanwhile, R^2 obtained for the inferential model is 0.947. The higher the coefficient of determination, the higher the accuracy of model obtained. Therefore, inferential model shows a good estimation ability towards Acetone composition.

The errors between inferential model and experimental data is calculated using sum of squared errors (SSE) formula below:

$$SSE = \sum_{n=1}^{N} (x(n) - \hat{x}))^2$$
 (7)

SSE is minimized using Microsoft Excel Solver, where Solver iterates the value until it can reach the lowest possible value of SSE for experimental data and predicted data.

SSE calculated is simultaneously find values for predicted composition based on experimental data.

4.2.2 Case Studies

A. Changes in Reflux Flow Rate

The case study was performed between HYSYS simulation, experimental and inferential model of distillate. The variable to be manipulated is reflux flow rate. The purpose of this case study is to observe how well the inferential model can predict product composition of distillate by varying the reflux flow rate. In this project, reflux flow rate was manipulated between 0.2 LPM to 0.9 LPM. Figure 6 displays the effect of different flow rate to estimated product composition.



Figure 6: Graph of reflux rate versus Acetone composition

Based on Figure 6, the predicted composition by inferential model managed to follow the same trend line as HYSYS value although inconsistency occurs. The relationship between distillate composition and reflux rate shows that by increasing the reflux rate, the composition of Acetone composition in distillate will increases. Since the distillate rate is kept constant, and only reflux rate is being manipulate thus the reflux ratio is higher if reflux rate is higher. Therefore, the result is expected because higher reflux ratio is desired to produce a higher concentration of Acetone in the distillate. Thus, from the graph it was found that inferential model has done well to cooperate changes in reflux flow rate.

B. Changes in Steam Flow Rate

The case study was also performed between HYSYS simulation, experimental and inferential model of distillate. The variable to be manipulated is steam flow rate. The purpose of this case study is to observe how well the inferential model can predict product composition by different steam flow rate. Since steam flow rate is varied simultaneously with reflux rate, thus value of steam flow rate recorded was between 6.15 LPM to 13 LPM. Figure 7 shows the changes of product composition by various steam flow rate.



Figure 7: Graph of steam flow rate versus Acetone composition

According to Figure 7, it is observed that predicted composition by inferential model shows same trend line as HYSYS and experimental data. The amount of Acetone in distillate decreases as steam flow rate increases. The result is expected since the increasing value of steam flow rate causes the temperature in the column increases thus some of Acetone is extracted earlier in trays before it stripped away from top of the column. The graph is well explained of the concept of distillation unit. Thus, it can be concluded that inferential model has done well to predict product composition.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATION

5.1 Conclusions

Inferential model has been developed to predict product composition in distillate. The inferential model was built under steady-state category. The coefficient of determination, R^2 calculated shows the performance of the model developed are good and the predicted composition is reliable.

Case studies have been carried out to observe the effect of predicted composition by inferential model towards changing of variables. By testing both case study, it was found that inferential model cooperate well with changes of reflux rate and steam flow rate. The predicted composition by modeling displays same trend as HYSYS and experimental data.

As a conclusion, this project is beneficial as it deals with alternative way of getting product composition directly from distillation unit. By keeping composition of product in acceptable range, product quality can be maintained significantly and profit function can be optimized. Furthermore, inferential model is believed to be one of the effective method to predict product composition as it is suitable for fast-response dynamic process and the cost is inexpensive compared to others online analyzer such as gas chromatograph.

5.2 Recommendations

As a recommendation, a future work may be done to study other parameters to know which the best variables is in order to estimate product composition in distillation column. In addition, since the data obtained from experiment is limited thus modeling shows a very good result. However, limited data shall not concludes overall performance of the modeling itself. Therefore, may be more data (hundreds) should be obtained from the experiment in order to have more accurate result for modeling.

This project shows a good progress and expected results are obtained from the runs of experiments conducted.

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APPENDIX

Reflux rate (LPM)	Steam rate (LPM)	T ₁ (°C)	T ₂ (°C)	P1 (kPa)	P2 (kPa)	Kpr	P (kPa)	Po (kPa)	T _{pcR} (°C)	T _{pcC} (°C)	Xd	X _D (model)	SSE
0.2	13.00	69.96	69.01	103.50	101.31	113.97	101.31	101.30	68.82	67.87	0.5485	0.5451	1E-05
0.3	11.84	67.97	67.19	103.50	101.31	104.02	101.31	101.30	66.93	66.15	0.5802	0.5563	0.0006
0.4	11.55	65.92	65.22	103.50	101.31	98.32	101.31	101.30	64.94	64.24	0.6055	0.5816	0.0006
0.5	9.48	64.07	63.20	103.50	101.31	104.35	101.31	101.30	63.03	62.16	0.6207	0.6382	0.0003
0.6	7.41	61.82	60.97	103.50	101.31	101.27	101.31	101.30	60.81	59.96	0.6561	0.6755	0.0004
0.7	7.03	59.93	59.17	103.50	101.31	95.10	101.31	101.30	58.98	58.22	0.6858	0.6961	0.0001
0.8	6.40	58.29	57.65	103.50	101.31	88.09	101.31	101.30	57.41	56.77	0.7133	0.7088	2E-05
0.9	6.15	57.40	56.56	103.50	101.31	96.15	101.31	101.30	56.44	55.60	0.7384	0.7518	0.0002
					,	TOTAL							0.0021