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Modeling and Nonlinearity Studies of Industrial i-Butane/n-Butane Distillation Column

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Abstract: The dynamic and nonlinearity of the distillation column often become major constrain in selecting an appropriate control system in achieving the desired product purity. The aim of this research is to study the level of nonlinearity of the industrial i-Butane/n-Butane distillation column in order to propose a suitable controller. This will serve as a preliminary study in order to develop a robust controller for the column based on its degree of nonlinearity. In this study, the steady state model of the column is developed using commercial process simulator, Aspen Plus software and then validated with the industrial data available in the literature. Then, the model is exported to Aspen Dynamic and linked with Matlab Simulink for the dynamic study purpose. The nonlinearity analysis i.e. asymmetric response, harmonic response, input multiplicity and output multiplicity is done in order to study the nonlinearity level of the column. Based from the study, the industrial column under consideration can be categorized as a strong nonlinearity system and the development of a nonlinear controller is needed for the column.

Key words: Industrial distillation column, nonlinearity study, simulation, dynamic model, multiplicity study

INTRODUCTION

Distillation is the most widely used application in the industrial separating liquid mixtures. It is estimated that 95 percent of the separation processes for the refining and chemical industries in the world is using distillation column (Enagandula and Riggs, 2006). In the refinery process, distillation process is used to separate the long chain of hydrocarbons according to its boiling point and usage. One of the process is the debutanizer process which is to separate C4 from the feedstock. The process is then continued until it separates i-butane and n-butane. Distillation columns is known to exhibit nonlinear dynamic behavior due to their nonlinear vapor liquid equilibrium relationships, the complexity of column configurations (e.g., side streams and multiple feeds) and high purities of product (Luyben, 1987). The column dynamics condition is a result of a combination of very fast vapor flow rate changes, moderately fast liquid flow rate changes, slow temperature changes and very slow composition changes (Luyben, 2002). In order to achieve targeted product specification, the distillation column must be monitored and controlled at its optimum conditions. Based on Shinskey (1984), the distillation control is a challenging process due to: (1) inherent nonlinearity of the distillation, (2) multivariable interaction, (3) the non-stationary behavior and (4) the severity of disturbances. Besides that, Luyben (2006b) has mentioned that although there are many different types of control structure for distillation column, the selection of the best control structure is not as simple as some paper claim. There are several factors that influence the control selection process such as components volatilities, product purities, reflux ratio, column pressure, and cost of energy, column size and composition of the feed. Therefore, in order to perfectly control the distillation column, the knowledge of the process dynamic and understanding its behavior is required in order to develop the best nonlinear model for the column. Nevertheless, the complexity and difficulty of the nonlinear model had been a major constrain in building a reliable nonlinear model based control strategies (Pearson, 2006; Qin and Badgwell, 2003).

Pearson (2003) has noted that the complexity of the nonlinear model development arise from two major facts that is the fact that model utility can be measured in several, usually conflicting ways and the fact that the class of nonlinear model does not exhibit the unity that the class of linear models does. From the point of measuring model utility, there are four important indicators; they are the approximation accuracy, the physical interpretation, suitability for control and ease of development. Fundamental model are generally perform far better than empirical model in term of accuracy and physical interpretation. However, they are not very attractive in term of development ease and controllability. On the other hand, low order model (i.e., first order and

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second order) which is much more popular in process control application usually unable to approximate a wide range of qualitative behavior. For the model unity, the nonlinear models do not convert freely between themselves like linear models does due to the structural heterogeneity that those nonlinear model exist. This gives different model development technique is required for different type of nonlinear model. Henson (1998) had stated that the nonlinear model should be as simple as possible, less computational load and can retain the most of nonlinear characteristic of the system if to be used for control purpose. In order to decide which nonlinear model to be used, it is important to study the system nonlinearity behavior in order to determine its degree of nonlinearity. Pearson (2003) had laid down the nonlinear criteria to identify the degree of nonlinearity of the process. According to him, the asymmetric response to symmetric input changes (ASYM), generation of harmonics in response to sinusoidal input (HARM) and observation of Input Multiplicity (IM) is considered as mildly nonlinear behavior, whereas, Output Multiplicity (OM), generation of sub-harmonic response (SUB) and highly irregular response (CHAOS) is categorized as strongly nonlinear behavior. Finally, the input-dependent stability (IDS) behavior is known to be intermediate nonlinearity. Desoer and Wang (1980) have used approximated linearized system to measure the nonlinearity of input-output mapping of the system.

Harris *et al.* (2000) proposed an approach to compute the nonlinearity by using functional expansions. The method gives upper and lower boundary for degree of nonlinearity. Hahn and Edgar (2001) used a new approach using Gramian based approach to quantify the nonlinearity of the process. It is based on the comparison of controllability and observability Gramian that is linearized with discrete empirical Gramian from data of the nonlinear process.

In this study, the steady state model of the industrial i-Butane/n-Butane distillation column is developed using commercial process simulator, Aspen Plus software and then validated with the industrial data available in the literature. Then, the nonlinearity of the industrial column is evaluated based on the criteria proposed by Pearson (2003) which is based on the analysis of asymmetric response, harmonic response, input multiplicity and output.

Table 1: Plant stream data after reconciled (Ilme *et al.*, 2001)

Components	Feed	Top	Bottom
Propane (wt %)	1.54	4.94	2
i-butane (wt %)	29.5	94.2	0.3
n-butane (wt %)	67.7	0.2	98.1
Isobutene (wt %)	0.13	0.23	0.08
1-butene (wt %)	0.2	0.41	0.1
Neopentane (wt %)	0.11	0	0.17
Isopentane (wt %)	0.77	0	1.12
n-Pentane (wt %)	0.08	0	0.11
Total Flow rate (kg h^{-1})	26122	8123	17999

Table 2: Plant specification (Klemola and Ilme, 1996)

Column height (m^2)	51.8
Column diameter (m^2)	2.90
Number of tray	74
Weir length side (mm)	1.859
Weir length center (mm)	2.885
Liquid flowpath Length	0.967 m^2
Active area (m^2)	4.9
Downcome area (side) (m^2)	0.86
Downcomer area (centre) (m^2)	0.86
Tray spacing (m)	0.6
Hole diameter (mm)	39.0
Total hole area (m^2)	00.922
Outlet weir height (mm)	51.0
Tray thickness (mm)	2.0
Number of vales per tray	772.0
Free fractional hole area (%)	18.82

Table 3: Operation data (Klemola and Ilme, 1996)

Column top pressure (kPa)	92838.0
Reflux temperature (°C)	18.5
Column Top pressure (kPa)	658.6
Pressure drop per tray (kPa)	0.47
Feed pressure (kPa)	892.67
Boiler duty (MW)	10.24

INDUSTRIAL CASE STUDY

The industrial column case study is taken from Klemola and Ilme (1996) and Ilme *et al.* (2001). This column is used in a refinery plant to separate n-butane and i-butane from an upstream process. The liquid feed is containing approximately 29.4 wt.% of i-butane, 67.7 wt.% of n-butane, 1.5 wt.% of propane and 1.0 wt.% of pentanes.

The rest of the feed contains 0.5 wt.% of C4 olefins. The n-butane and i-butane is considered as the light key and heavy key component. The reconciled feed, distillate and bottoms data is shown in Table 1. The data need to be reconciled to meet the material balance requirement and the C4 olefins which are present in small concentration are lumped into i-butene and 1-butene. The column is 2.9 m in diameter and using 74 valve trays of Glitsch Ballast two-pass type V-1 valve. The feed is introduced onto tray 37. Specification details of the plant are shown in Table 2. The rest of the operation condition is shown in Table 3.

MATERIALS AND METHODS

The steady state distillation column condition is modeled based on Peng-Robinson thermodynamic property using Aspen Plus version 20.0 software. Peng-Robinson method is selected due to its ability to describing the state of hydrocarbon based components

Table 4: Stream validation results

	Distillate			Bottom		
Components	Actual	Simulation	Error %	Actual	Simulation	Error %
Propane wt.%	0.0494	0.0495	-0.202	0.000	0.000	0.00
i-butane wt.%	0.942	0.942	0.00	0.00300	0.00300	0.00
n-butane wt.%	0.00200	0.00168	16.0	0.981	0.981	0.00
Isobutene wt.%	0.00230	0.00311	-35.2	0.000800	0.000480	40.0
1-butene wt.%	0.00410	0.00412	-0.488	0.00100	0.00104	-4.00
Neopentane wt.%	0.000	0.000	0.00	0.00170	0.00160	5.88
Isopentane wt.%	0.000	0.000	0.00	0.0112	0.0112	0.00
n-Pentane wt.%	0.000	0.000	0.00	0.00110	0.00116	-5.46
Total Flowrate (kg/h)	8123	8123	0	17999	17999	0

according to the Aspen Plus property method guide. The data is first normalized before entering the software. The model is using tray efficiency at 110% based on the ratio of ideal stages to the number of real stages that can accomplish the same separation and from analysis based on several column efficiency method (Ilme *et al*., 2001).

The stream validation result with the normalized stream data can be seen at Table 4. From the result, it is observed that the key component streams produced from the model developed is matched perfectly with the literature referred. However, the error for some component streams is a bit high due to its small concentration in the process which hardens the process simulator to estimate them accurately. Their errors are not significantly affecting the process as their percentage in the feed stream is only 2.8%. The validation for the tray temperature result can be verified at Fig. 1. It show that all the tray temperatures selected are comparable with the industrial data. All the results achieved indicate that model developed is acceptable and can be used for further studies.

Afterward, the validated model is then updated into the dynamic state using Aspen Dynamic. Here, the sump and reflux drum dimension is based on the heuristic assumption to set up a 5 min of liquid holdup while the vessel is at 50% full when entering and leaving the vessel (Luyben, 2006a). The hydraulics and pressure drop within the stages is calculated by rigorous tray correlations provided in Aspen Plus. Then, the Aspen Dynamic model is interface with the Matlab Simulink software for the dynamic study by using dynamic data exchange block provided by Aspen Plus for distillation system. The dynamic and nonlinear behavior study of the system were then carried out which was based on the study of Pearson (2003). The following responses are used identify the degree of the nonlinearity for the process:

Asymmetric behavior: A system which shows asymmetrical response for the symmetrical input can be classified as a nonlinear. In this study, a step test is applied to the system by giving positive and negative step change. The step test is done through two manipulate variables i.e. reboiler duty and reflux flow rate and on two disturbance variables i.e., feed flow rate and composition of n-butane in the feed stream. Both reboiler duty and reflux flow rate were changed only +2% and -2% from its nominal condition due to constraint from the column high reflux ratio and reboiler duty in order to maintain its distillate flow rate. On the contrary, both disturbance variables were changed until +5% and −5% of their steady state values.

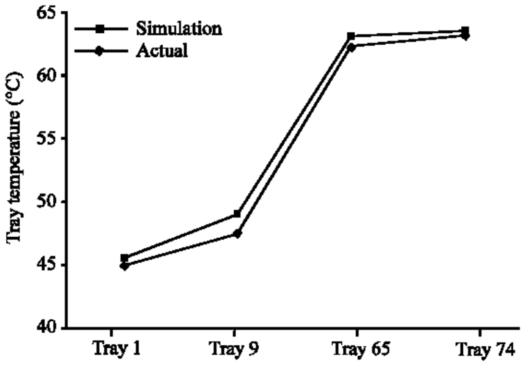

Fig. 1: Tray temperature validation

Harmonic response: Periodic input can also be used to determine the nonlinearity of the system. Although this type of response is uncommon in process application, it can be used in order to know more about the presence and nature of the system. In fact, some chemical process application shows some improvement by using periodic input (Khinast and Luss, 2000). The periodic input used in this study is the sine wave which was generated in Matlab Simulink. The bias of the sine wave used in this response test is the steady state condition of the process.

This is due to the Aspen Dynamic model cannot receive null input like normal sinus wave x-axis. By using the steady state value as the new sinus x-axis, the periodic response of the system can be studied. The amplitude used is +2% and -2% of the nominal condition of the reboiler duty and reflux flow rate. The frequency of the wave is selected as 1 and the angular phase is set to null.

Input multiplicity: The input multiplicity is the existence of several steady states input for a fixed set of output. The input multiplicity of a system can be considered as mild nonlinearity behavior. In this case, method proposed by Zheng *et al.* (1998) is adopted. The tray temperature is selected as the parameter that will show the multiplicity over a range of manipulated variables values (i.e. reboiler duty and reflux flow rate). First, the tray temperature location is observed based on tray temperature profile.

Here, the tray is referred as a stage which follows the Aspen Plus model specification. A stage number in Aspen Plus model is equal to number of tray plus 1 (Tn+1) due to the first stage is considered as the condenser. The Singular Value Decomposition (SVD) analysis is done in order to select the most sensitive tray temperature location (Luyben, 2006b). Based on this tray temperature location, the manipulated variables is varied over a selected range to observe the process for multiple steady state points which can be regarded as multiplicity behavior.

Output multiplicity: The output multiplicity is the existence of several steady state output for a fixed input. This criterion is associated with system with strong nonlinearity behavior. The study of output multiplicity is referring to a study from Guttinger *et al.* (1997). The output multiplicity can be determined by tracking two steady state branches via extending the parameter from different operating condition where only one steady state is existed. The selected operating parameter is used for tracking while the others are fixed. In this study, the selected operating condition is vary from higher to lower and lower to higher using multiple step staircase in order to obtain a variation of the operating parameter from different steady state values. The output multiplicity existed when the two steady state output branch is overlapping with each other for the same operating parameter condition.

Since this column operates at a high reflux ratio and reboiler duty, most of the operating parameter deviation using reflux flow rate and reboiler duty in this study is limited to within 2% changes. This is to ensure that the column is operating at the optimum and reasonable condition.

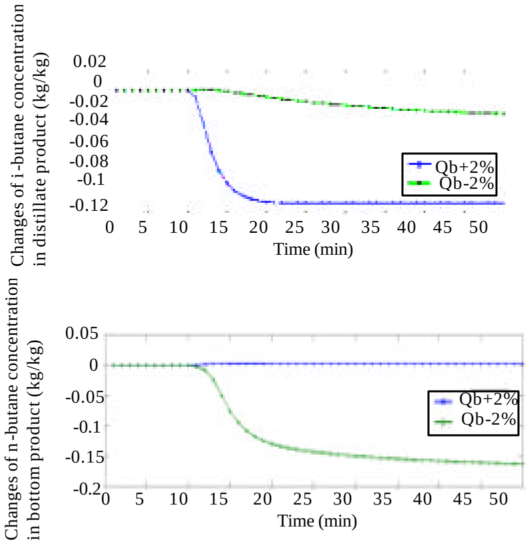

Fig. 2: The response of top product composition (top) and bottom product composition (bottom) with +2% and -2% of reboiler duty

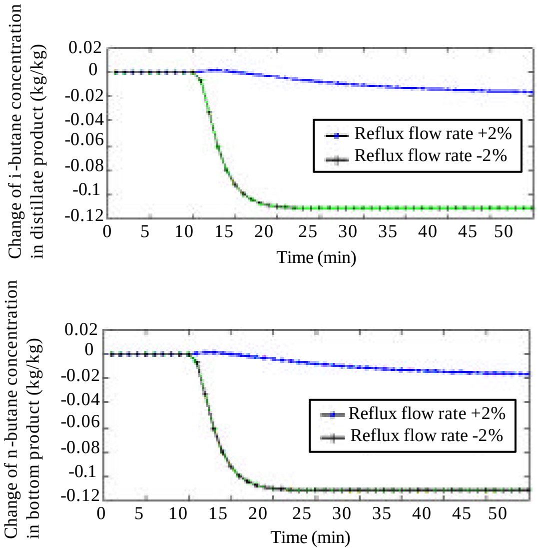

Fig. 3: The response of top product composition (top) and bottom product composition (bottom) with +2% and -2% of reflux flow rate

RESULTS AND DISCUSSION

The identification of nonlinearity and dynamic behavior of the system is important in choosing the best structure of the nonlinear model. The selection of input and output for the nonlinear model is also depending on the severity of the input change towards the output. Here, the results from the nonlinearity test will be discussed according to its category.

The results for asymmetric behaviors are shown from Fig. 2-5. In Fig. 2, (top) the reboiler duty effect on top compositions is not symmetrical. The positive step of

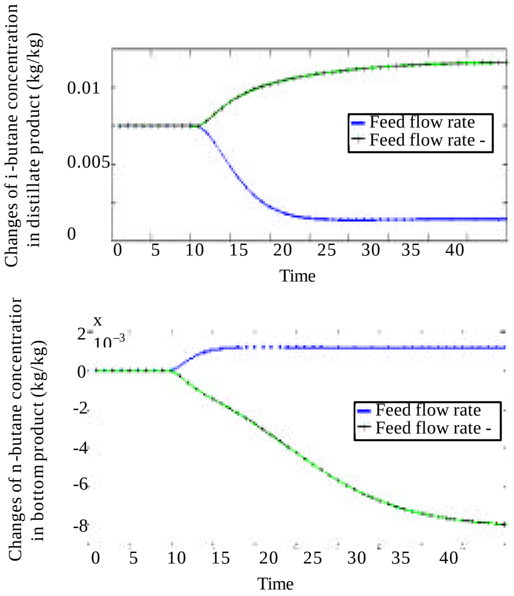

Fig. 4: The response of top product composition (top) and bottom product composition (bottom) with +5% and -5% of feed flow rate

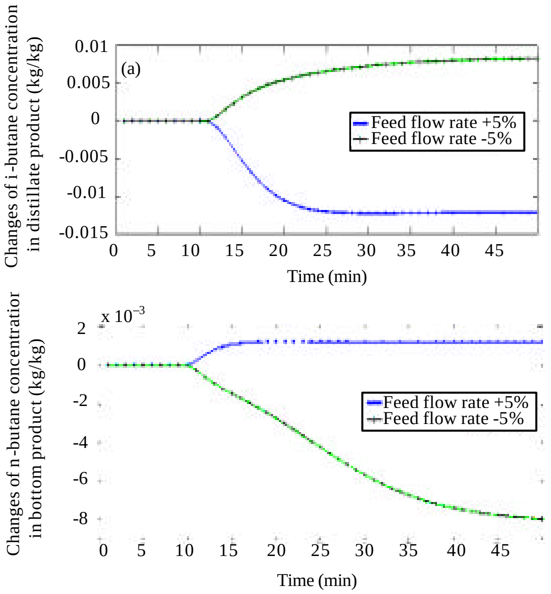

Fig. 5: The response of top product composition (top) and bottom product composition (bottom) with +5% and -5% of feed n-butane concentration

reboiler duty gives more significant effect than the negative step in the top composition profile. The positive step change in reboiler duty rate for top product has increased the vapor flow rate in the column, simultaneously decrease vapor-liquid ratio inside the column, which lead to increasing of impurity level of i-butane product. Figure 2 (bottom) shows the effect of the reduced reboiler duty has increased the vapor/liquid traffic inside the column which has caused a raise in the impurity level in the bottom product. The bottom response also shows the same asymmetric behavior. The effect of the reflux flow rate steps change to the top and bottom composition also produce non symmetrical line response as shown in Fig. 3. The negative step change in top composition has decreased the reflux flow rate which at the same time, results to poor vapor-liquid contact in the rectifying section and in return, reduces the distillate purity. On the contrary, the increase in reflux flow rate will lead to an increase in total liquid flow rate in the rectifying section thus eventually decreases the purity of the bottom product. Similarly, the nature of the responses portrayed by the system indentifies the nonlinearity of the process. From Fig. 4, the change of feed flow rate in both top and bottom composition show the deviation of symmetric behavior. Higher flow rate will increase the top product purity as the composition of i-butane in the feed is also increase. This will increase the volume of i-butane inside the column. For the dramatic effect on the bottom product composition, the feed flow rates is known to have more dynamic effect on bottom product composition compare to the top product composition, if the feed is a saturated liquid (Cantrell *et al*., 1995). The effect of concentration of n-butane in the feed towards the top and bottom product purity is shown in Fig. 5. Based on the results, the system shows asymmetric response towards the steps inputs as well. The increased of n-butane composition in the feed flow rate has resulted a decreased in i-butane purity in the distillate. In contrast, the concentration of n-butane in the bottom product has increased with the increase of n-butane at the flow rate input. This is obvious due to the much richer feed of n-butane will favor on the n-butane purity separation. Based on all the results of steps change in the column, the system can be said to exhibit asymmetrical responses which can be classified as a mild nonlinearity system.

In the harmonic response behavior study, Fig. 6 shows the effect of periodic reboiler duty input and Fig. 7 shows the effect of periodic reflux flow rate input towards distillate flow rate. The graphs were normalized by dividing the results with their means in order to get standard values for data that have different scales. From the results, it obviously shows that both output from reboiler duty and reflux flow input have same period, T with its input. This is called the harmonic generation (or superharmonic generation) response, i.e., a response that undergo shape wave changes without altering the periodicity. If the output period increased from the input

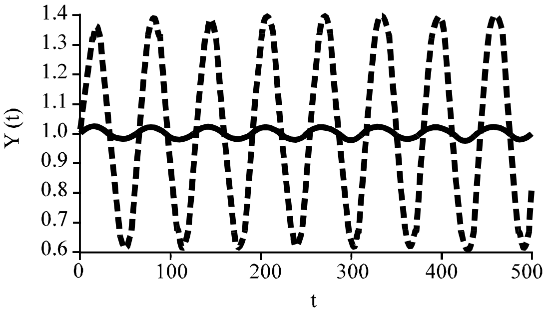

Fig. 6: The effect of periodic reboiler duty input towards distillate flow rate; dotted line is distillate flow rate and solid line is sine input after normalize

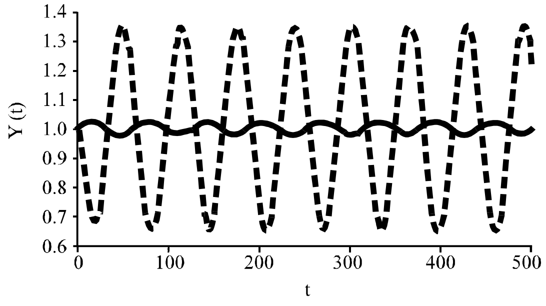

Fig. 7: The effect of periodic reflux flow rate input towards distillate flow rate; dotted line is sine input and solid line is distillate flow rate after normalize

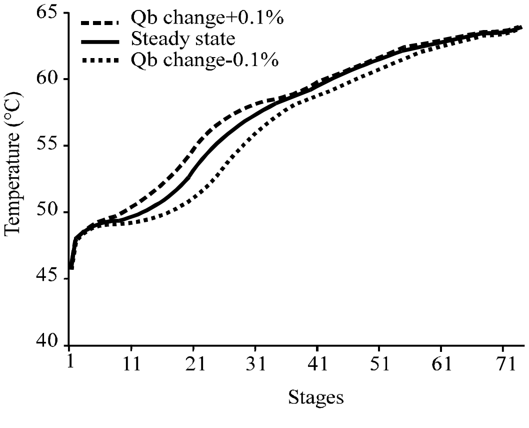

Fig. 8: Tray temperatures profile with reboiler duty (Q_b) +0.1% and -0.1% change

period by nT, where n is the integer larger than 1, then this sinusoidal response is called subharmonic response which is a strong nonlinearity condition (Pearson, 2003). However, from this analysis, the process only show the superharmonic behavior response which indicates that the system is mild nonlinear.

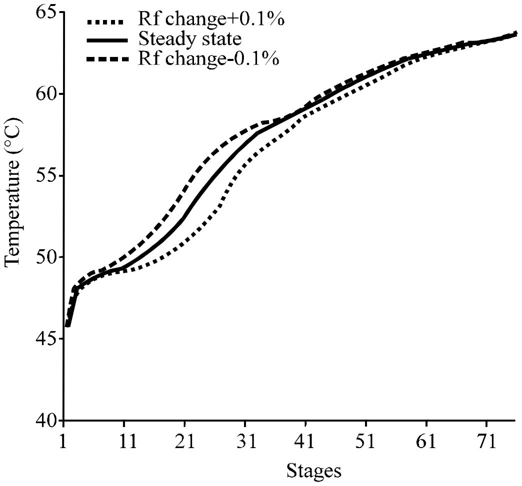

Fig. 9: Tray temperatures profile with reflux flow rate (R_f) +0.1% and -0.1% change

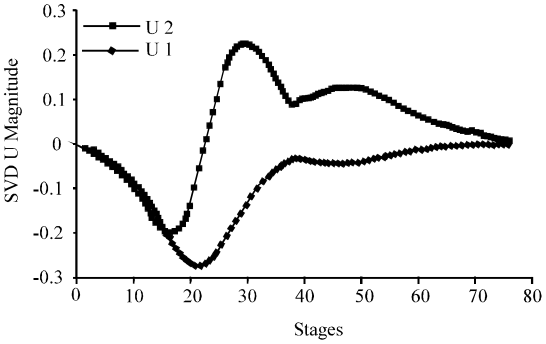

Fig. 10: The SVD analysis result; U1 (reboiler duty) and U2 (reflux flow rate)

The input multiplicities exist if the same outputs are obtained from different values of operating parameter. In this case, the method from Zheng *et al.* (1998) is referred to search and determine the input multiplicity. Figure 8 and 9 show the steady state stage temperature profile for 0.1% change in reboiler duty and reflux flow rate. The variation from steady state values is regarded as the column temperature sensitivity towards the manipulated variables. The variation values from both temperature profiles are used in SVD analysis to find the most sensitive stage location. In the SVD analysis, the U1 (reboiler duty) and U2 (reflux flow rate) profile are plotted against column stages as shown in Fig. 10. Based on the graph, stage 21 shows the highest magnitude for U1 and stage 30 for U2. The tray with the largest magnitude of U indicates locations in the column that can be most sensitive and effective to be controlled. These stages temperature are used to find the multiplicity when there is

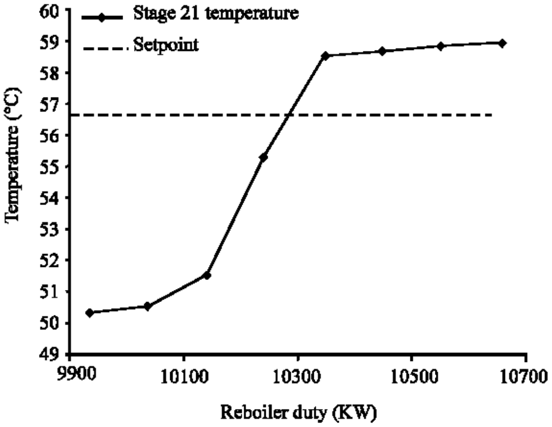

Fig. 11: Temperatures Stage 21 vs. reboiler duty

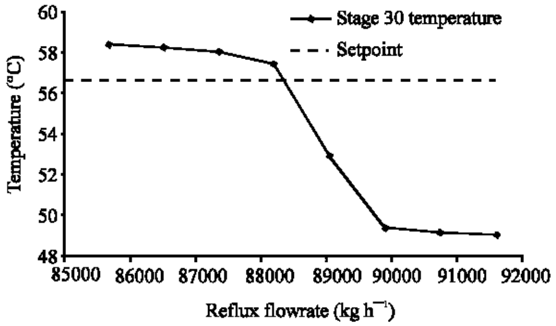

Fig. 12: Temperatures Stage 30 vs. reflux flow rate

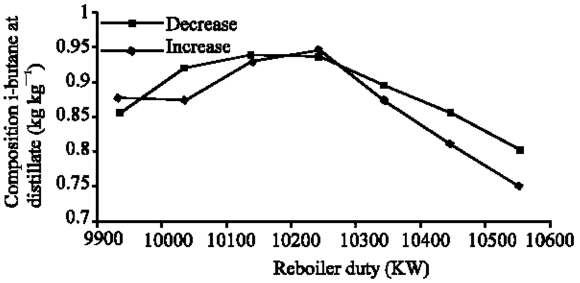

Fig. 13: The *i*-butane composition vs. reboiler duty from two different steady state lines

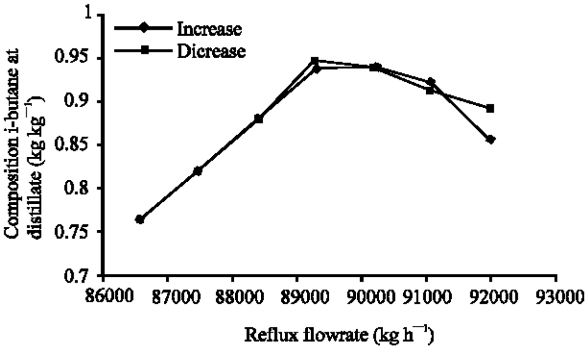

Fig. 14: The *i*-butane composition vs. distillate flow rate from two different steady state lines

more than one temperature steady state point over a range of the manipulated variable. Generally, the steady state tray temperature in a column increased when the reboiler duty increased. Figure 11 plots stage 21 temperature verses reboiler duty. Obviously, temperature from stage 21 varies when the reboiler duty is varied. Subsequently, Fig.12 shows the stage 30 temperature versus reflux flow rate. The behavior of the reflux flow rate is opposite of the reboiler duty due to the increase of the reflux ratio that will increase the volume of the composition in the column. Thus, at a fixed reboiler duty, the stage temperature will drop as more heat is needed to heat up the increasing volume of components in the column. Based on this phenomenon, the column did not exhibit any input multiplicity as there are no multiple steady state temperature occurred in both situation.

The output multiplicity exists if different outputs (e.g., product composition or temperature) are produced from the same set of operating parameters (e.g., reboiler duty and reflux flow rate). In this study, i-butane composition at distillate is plotted against reboiler duty as shown in Fig. 13 and also against reflux flow rate as shown in Fig. 14. The increase line is referred to the increased trend from lower to higher values and vice versa. Based on Guttinger *et al*. (1997), if the both parameters are overlapped with each other, than the output multiplicity is existed. Based on the observation, this overlapping phenomenon occurs in this system for both conditions. In Fig. 13, most of the composition of i-butane overlapped at the same reboiler duty value based on two separate steady state lines. These steady state lines are plotted based on increasing steady state values and decreasing steady state values. The increasing steady state values were obtained from a series of increasing step tests. After a step was introduced into the system, a new steady state values would be generated. Then, a new increased step test would be introduced to find the latest steady state value. This process was continued until several steady state values were acquired. The procedure was the same for the decreasing steady state values except for the step testvalues, which is in this case, was decreasing. Although the composition of i-butane is same at both line for nominal reboiler duty of 10240 KW, the variation that had occurred prior and later between the two steady state lines are still significant. Normally, the top composition is increased as the reboiler duty increased because higher portion of components are heated up and going to the top. This will lead more components to evaporate and

Table 5: Nonlinearity response result summary

Type of behavior	Existence	Degree of nonlinearity
Asymmetric response	Yes	Mild
Superharmonic response	Yes	Mild
Input multiplicity	No	Mild
Output multiplicity	Yes	Strong

come out as distilled product. This trend will increase the top product recovery and at the same time reduce its purity. As for Fig. 14, i-butane composition shows good agreement with both reflux flow rate lines prior to the nominal condition. After the nominal value of the column reflux flow rate at 89261 kg h^{-1}, both lines started to diverge and splitting, which will signify more than one steady state over a selected reflux flow rate. Higher reflux flow rate will tend to increase the liquid flow rate in the rectifying section and increase the bottom product flow rate stream. Eventually, both of the product purity will be affected if the bottom product flow rate keep increasing. The presence of output multiplicity in the system shows the strong nonlinearity behavior of the system.

The results of all tests conducted are summarized in Table 5. Based on all the tests that have been carried out, it can be concluded that the industrial column separating of i-butane/n-butane is behaved as a strong nonlinearity system despite the existing of two mild nonlinearity characteristics. Consequently, the test of the nonlinearity should be done begin from the behaviors of strong nonlinearity to mild nonlinearity. By that, if the process produces high nonlinearity behavior, than the system can be considered as strong nonlinearity with the mild nonlinearity tests can be disregard.

CONCLUSION

Model of industrial column to separate i-butane/n-butane has been developed using Aspen Plus and then validated with industrial data available in literature. The nonlinearity study of the industrial distillation column was carried in Matlab Simulink integrated with Aspen Dynamic. Four types of response i.e., asymmetric, harmonic, input multiplicity and output multiplicity have been observed. All the tests conducted were aimed to classify the degree of nonlinearity of the process under consideration. It was observed that the industrial i-butane/n-butane distillation column exhibit a strong nonlinearity behavior. Generally, most researchers just apply the asymmetric behavior test to determine the nonlinearity of the column as it is the simplest test. However, the extent of the degree of the nonlinearity is still remains unknown as it is not covered by the test. Therefore, it is encouraging to perform the nonlinearity test accordingly, to further study the nonlinearity of the distillation process. Hence, this can bring more information for the selection of the rigorousness of the nonlinear model needed for the distillation column. From the results obtained, it can be concluded that the industrial distillation column under consideration can be categorized as strong nonlinearity system. Therefore, an advance model based controller using nonlinear model is recommended and further studied for implementation.

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