RESEARCH ARTICLE

Interaction and performance analysis of a ternary mixture distillation process

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Abstract

The objective of this study was to analyse the controllability of a driving force-based distillation columns sequence for the separation a benzene, toluene, and p-xylene mixture. Primarily, a methodology for this study was constructed, which consisted of five hierarchical stages. In the first stage, all possible distillation columns sequences were synthesised. Then, the sequences were simulated under steady state conditions using Aspen HYSYS in the second stage. In the third stage, the input-output interactions of the sequences were analysed by using relative gain arrays (RGA). In the fourth stage, controller parameters were determined. Finally, in the fifth stage, the controllers' responses were analysed using MATLAB. From this study, it was found that the driving force-based distillation columns sequence has better overall controllability than an alternative sequence.

Keywords: Driving force algorithm, relative gain array, aromatic mixture

INTRODUCTION

The distillation system is among the most used separation processes in the chemical industry and most energy consuming unit operations (Lucero-Robles *et al*., 2016). It is known to be accountable for up to 50% of the operating costs of a plant because of its large energy consumption *(*Kiss *et al*., 2012). One of the approaches known to minimise the consumption is by properly sequencing the distillation columns in the distillation system, as different sequences require different amounts of energy. An old and well-known method of sequencing is based on heuristics. Heuristics are guidelines that can be followed directly and require no calculations. A list of them can be found in the work of Floquet *et al*. (1994). A more recent one is based on thermodynamics insight and proposed by Bek-Pedersen and Gani (2004). Their approach is known as the 'driving force method', which is based on the driving force resulted from the difference between the vapour phase and the liquid phase of a component *i* in a system. The difference is actuated by a difference in volatilities between component *i* and other components in a mixture. This approach has the advantages of being simple and easy as the distillation columns sequence is determined graphically. The approach can be seen applied in many studies, including those related to process synthesis and design (Pérez-Cisneros and Sales-Cruz, 2017) and has been found to provide a solution that is energy efficient (Rahimi *et al*., 2017), and sustainable (Zaine *et al*., 2015), as compared to existing sequences. To maintain the energy consumption of a distillation system at a minimum, it must has good controllability. Not much is known about the controllability of the systems determined by the driving force approach, thus it is of interest to ascertain a driving force-based distillation columns sequence' controllability.

METHODOLOGY

The methodology applied for this study was consisted of five hierarchical stages. The overall view of the methodology could be seen in Fig. 1.
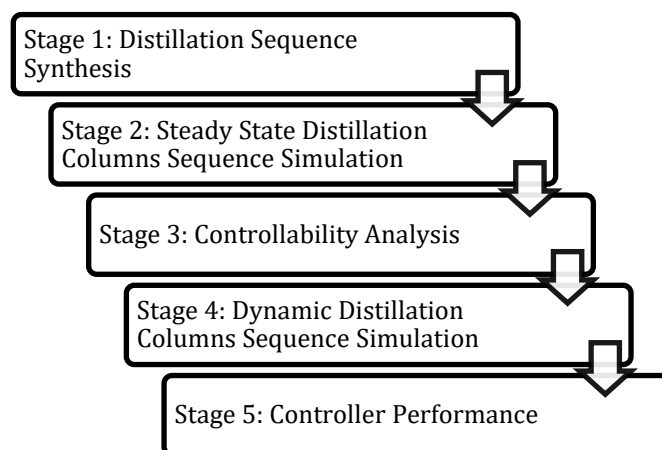

Fig. 1 Overall methodology of the controllability analysis.

To know whether the driving force-based distillation columns sequence has better properties, comparison with an alternative sequence has to be made. Thus, in the first stage, both the driving force sequence and an the existing sequence were synthesised. To

determine the driving force sequence, driving force curves must first be constructed. First, the feed components were listed in an increasing boiling point order. Then, the relative volatilities between the components in the list, α_{ij} were calculated. After that, the driving force equation, Eq. 1 was used to calculate the driving force values of each pair of component, D_{Fij}.

$$D_{Fij} = [x_i\alpha_{ij}/[1 + x_i(\alpha_{ij} -)]] - x_i \qquad (1)$$

Where, x_i is the composition of component i in liquid. The values of D_{Fij} are calculated from values of x_i ranging from 0 to 1. The obtained D_{Fij} values of each pair are then plotted against x_i to generate the curves. The driving force sequence is based on the curves of driving force values, where the peak of a curve determines its separation priority. The highest peak is corresponded to the first separation, followed by the second highest peak and so on. The alternative sequence is the sequence that is not the driving force sequence as for a three component case study, only two sequences are possible.

In Stage 2, the energy saving property of the driving force sequencing algorithm was verified. First, both the driving force sequence and the alternative sequence were simulated in Aspen HYSYS V10 using shortcut columns to determine their design variables such as the number of stages, feed stage, and distillate flow rate. Then, the obtained design variables were used in the simulation of both sequences using conventional distillation columns. From this simulation, their energy consumptions were tabulated and compared.

The objective of Stage 3 was to determine the interaction between input-output pairs of the sequences and compare the interactions of the sequences. The inputs and outputs are referred to manipulated and controlled variables, respectively. Typically, there are five inputs for a distillation column: condenser utility flowrate (F_C), reflux flowrate (F_{RF}), distillate flowrate (F_D), bottoms flowrate (F_B), and reboiler utility flowrate (F_{RB}). For outputs, there are the column pressure (P_C), reflux drum level (L_{RF}), column bottom level (L_{CB}), distillate product composition (X_D), and bottoms product composition (X_B). For this study, the following input-output pairings were used: F_C-P_C, F_D-L_R, F_B-L_{CB}, F_{RF}-X_D, F_{RB}-X_B. These selections were made because such pairings have been applied on many columns (Manikandan *et al.*, 2017). The first three of the used pairings were known as inventory controls and assumed to have and contribute no interaction in this stage. Only the pairs related to the product compositions were considered as they were usually the objective of control. To measure the magnitude of interaction of the remaining two input-output pairs in a sequence, the widely-applied relative gain array (RGA) was used. RGA uses steady-state process gains knowledge (Lau *et al.*, 1985) to determine the interactions. The closer the values in the array to 1 and 0, the less interaction can be inferred.

The objective of Stage 4 was to determine the PID controller parameters, namely controller gain (K_c), integral time (τ_I), and derivative time (τ_D), that would be used for the controllers in Stage 5. First, the process reaction curve method was used to obtain the controller gain, time constant, and time delay as the method was fairly simple and adequate for many applications (Marlin, 2000). The obtained process parameters were then used to calculate the PID controller parameters for each controller of both sequences.

In Stage 5, controllers' perfomance was determined based on Integral of Squared Error (ISE) and settling time. The objective of this stage was to determine on the how the distillation systems would behave under dynamic conditions. The ISE is a performance criterion that has been used for First Order Plus Time Delay (FOPTD) systems (Hussain *et al.*, 2014). It measures the deviation of the controller response from the steady state value, where larger ISE means larger deviation. Thus, controllers with smaller ISEs will be deemed having better controllability. Settling time is the time needed for the product purities to reach and remain inside a band whose width is equal to ±5% of the total change in product composition for 95% response time. In the end, both sequences' overall controllability was compared based on the steady state RGA and also the ISE and settling time.

RESULTS AND DISCUSSION

Stage 1: Distillation sequence synthesis

The feed mixture in this study, taken from Premkumar and Rangaiah (2009), consisted of benzene, toluene, and p-xylene with mol compositions of 0.33, 0.33, and 0.34, respectively. The feed would enter the first distillation columns as a saturated liquid at 100 kmol/hr and 10 atm. The number of possible unique ordinary distillation columns sequence for this study was obtained using Eq. (2), where n_s is the number of possible sequence and n is the number of products.

$$n_s = [2(n-1)]!/n!(n-1)! \qquad (2)$$

The number of possible sequences calculated was two. One of those sequences was determined using Bek-Pedersen and Gani's driving force-based sequencing algorithm (Bek-Pedersen and Gani, 2004). Fig. 2 shows the driving force curves for the ternary mixture. The graph was zoomed-in to highlight the difference of peaks.
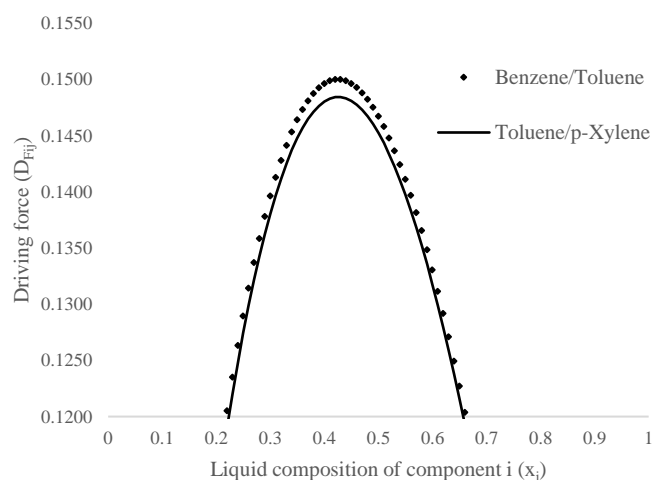

Fig. 2 Driving force curves of the ternary mixture.

From Fig. 2, it can be seen that the curve for the benzene/toluene separation was slightly higher than the curve for the toluene/p-xylene separation. Therefore, the driving force algorithm suggested that the first separation was between benzene and toluene, then followed by toluene and p-xylene. This separation sequence is also known as the direct sequence as components are separated in the order of increasing boiling points. The slight difference between the peaks showed that the ease of separation between the two separations might be similar, which might indicate similar energy consumption for the two separations in the sequence suggested by the algorithm. Fig. 3 shows the driving force sequence, which was synthesised based on the curves in Fig. 2 and Fig. 4 shows the indirect sequence, where the distillation system removed components in a decreasing boiling point order. The indirect sequence acted as the alternative sequence to the driving force sequence in this study.
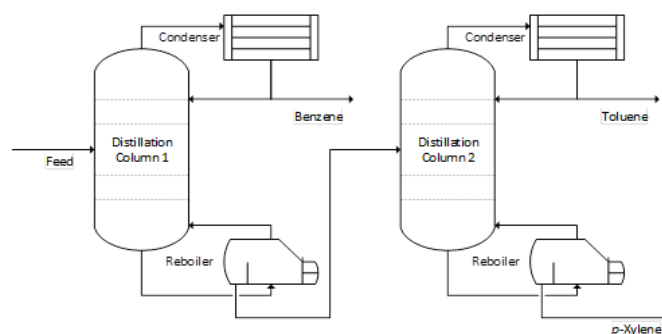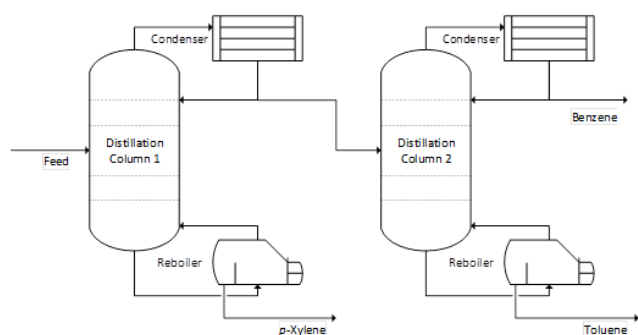

Fig. 3 Driving force sequence.

Fig. 4 Indirect sequence.

Stage 2: Steady state distillation columns simulation

The driving force and indirect sequences were simulated and the energy consumptions of each Distillation Column 1 (DC1) and Distillation Column 2 (DC2) were recorded. The duties are displayed in Table 1.

Table 1 Energy consumption of both sequences.

Sequence	DC 1 duty (kW)	DC 2 duty (kW)	Total duty (kW)
Driving force	1,891.10	1,912.44	3,803.54
Indirect	2,438.55	1,624.80	4,063.35

Based on Table 1, the first column of the driving force sequence consumed less energy than the first column of the indirect sequence; the energy consumptions were opposite for the second column of the sequences. It can be seen that the energy consumptions of the driving force sequence's columns did not differ as much as the indirect sequence's column. This finding was in line with the inference made from the curves in Fig. 2 where the similar-height peaks might indicate similar energy consumption between the two separations. Although the driving force sequence achieved energy saving only for the first column, its overall energy consumption proved that the driving force algorithm was successful in determining the most energy efficient distillation columns sequence for the benzene, toluene, and p-xylene mixture.

Stage 3: Controllability analysis

For this case study, there was one pair from each sequence that did not control the purity, rather, the impurity was controlled. The one pair in the driving force sequence controlled the benzene impurity in the bottom stream of the first column and another pair in the indirect sequence controlled the p-xylene impurity in the distillate of the first column. Before the RGA of each sequence was calculated, the steady state gain matrix of each sequence was calculated. Then, MATLAB was used to derive RGAs from the gain matrices. Fig. 5 and 6 show the RGA values of the driving force and indirect sequences, respectively. X_{D1} and X_{B1} denote DC1's product composition in the distillate and bottoms, respectively, while X_{D2} and X_{B2} denote DC2's product composition in the distillate and bottoms, respectively, F_{RF1} and F_{B1} denote DC1's reflux and reboiler utility flowrates, respectively, while F_{RF2} and F_{B2} denote DC2's reflux and reboiler utility flowrates, respectively.

$$\begin{matrix} & X_{D1} & X_{B1} & X_{D2} & X_{B2} \\ F_{RF1} & \begin{bmatrix} 0.0036 & 0.9964 & 0.0000 & 0.0000 \\ F_{B1} & 0.9964 & 0.0036 & 0.0000 & 0.0000 \\ F_{RF2} & 0.0000 & 0.0000 & 1.0000 & 0.0000 \\ F_{B2} & 0.0000 & 0.0000 & 0.0000 & 1.0000 \end{bmatrix} \end{matrix}$$

Fig. 5 Driving force sequence's RGA.

$$\begin{matrix} & X_{D1} & X_{B1} & X_{D2} & X_{B2} \\ F_{RF1} & \begin{bmatrix} -8.8247 & 9.8247 & 0.0000 & 0.0000 \\ F_{B1} & 9.8247 & -8.8247 & 0.0000 & 0.0000 \\ F_{RF2} & 0.0000 & 0.0000 & -7.9878 & 8.9878 \\ F_{B2} & 0.0000 & 0.0000 & 8.9878 & -7.9878 \end{bmatrix} \end{matrix}$$

Fig. 6 Indirect sequence's RGA.

From Fig. 5 and 6, the four values on the top left corner of the RGAs represented the interaction between the input-output pair of the first column while the four values on the bottom right corner of the RGAs represented the interaction between the input-output pair of the second column. It can be seen that the larger top corner values and the bottom corner values of the driving force sequence were much closer to 0 and 1 than indirect sequence's values, indicating that there was less interaction between the input-output pairs of the driving force sequence than the indirect sequence. Less interaction means whenever an output value moves away from its set point, there is less interference from other input-output pairs when corrective action is taken. In terms of input-output interaction, the driving force sequence has better controllability.

Stage 4: Dynamic distillation columns sequence simulation

Both sequences were simulated dynamically using Aspen HYSYS V10. First, the driving force sequence was sized using Aspen HYSYS' tray sizing utility, which included column diameter and column pressure drop. The settling time for the condensers and reboilers were set at 5 min. Then, controllers were installed in the sequence according to the pairing set for the controllability analysis in Stage 3, with the exception of the impurity of the first column of both sequences. The simulation was run in an open-loop fashion with no controller action, except for the actions to control the inventories. After the simulation has reached a steady state, a step change was introduced to one of the inputs and it was let to run until a new steady state was achieved. At the new steady state, the effect of the input change on its corresponding output was noted. Then, the process reaction curve method was used to calculate the process parameters, which then were used to calculate the PID controller parameters. The same procedure was repeated for other controllers of the driving force sequence and then was carried out on the controllers of the indirect sequence. Tables 2 and 3 show the calculated controller parameters.

Table 2 PID parameters of driving force sequence.

Controller	Kc	τ_I	τ_D
Benzene purity	88.30	516.19	88.63
Toluene purity	108.60	597.82	102.52
p-Xylene purity	114.25	502.54	85.67

Table 3 PID parameters of indirect sequence.

Controller	Kc	τ_I	τ_D
p-Xylene purity	75.27	527.08	89.00
Benzene purity	226.10	421.75	73.97
Toluene purity	391.80	459.66	76.04

Stage 5: Controller performance

The ISE and settling time analyses were both carried out using MATLAB, under two conditions. The first condition was when the set-points, i.e. the product purities were altered and the second condition was when the feed flowrates were changed. Fig. 7 and 8 show the settling times due to set-point change and feed disturbance, respectively.
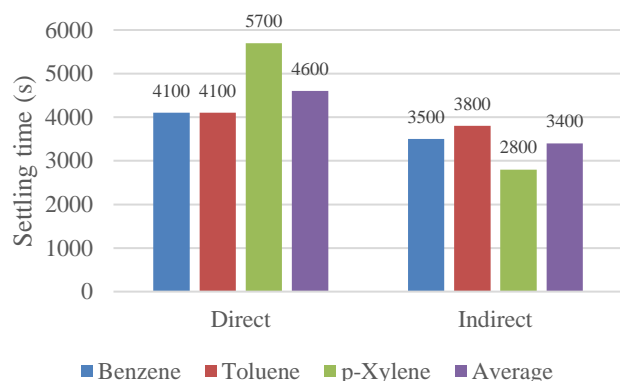
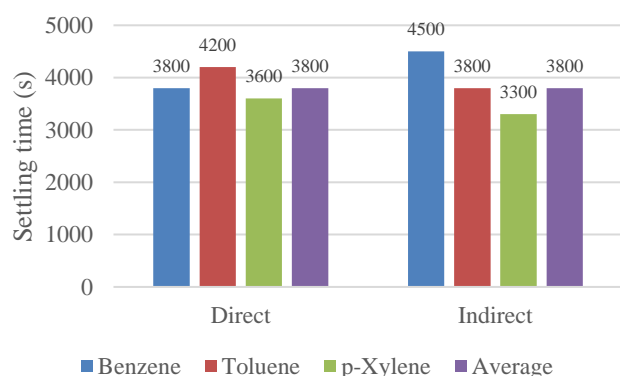**Fig. 7** Settling time due to set-point change.

Fig. 8 Settling time due to feed disturbance.

Based on Fig. 7 and 8, it can be seen that the indirect sequence has a smaller average settling time compared to the driving force sequence. This was because the settling time for each component in the indirect sequence has smaller settling time than the components in the driving force sequence. The longer settling times of the driving force sequence was not probably due to controller interactions as the controller interactions of the driving force sequence was significantly lower than that of the indirect sequence. This could probably be attributed to slow controller action. The calculated tuning parameters for the driving force sequence's controllers might not be the most optimal values. Similar could be said for the settling times due to disturbance. The driving force sequence was not any better than the indirect sequence as its average was the same as the indirect sequence's average settling time. This might also due to the slow controller action that was the result of inaccurate tuning.

Aside from settling time, the sequences were also compared based on their ISE values and Table 4 and 5 show the average ISE values for each sequence under set-point change and feed disturbance.

Table 4 Average ISE values due to set-point change.

	Driving force	Indirect
Average ISE	0.3262	253.4000

Table 5 Average ISE values due to feed disturbance.

	Driving force	Indirect
Average ISE	32.1333	89.2333

From Table 4 and 5, it can be seen that the driving force sequence has a lower average ISE than the indirect sequence for both set-point change and feed disturbance. This showed that although the driving

force sequence took a longer time to settle, the controller responses did not deviate far from the steady-state value of the product purities. This also showed that settling time performances did not reflect the error values and that both analyses were crucial when determining the control performance of a distillation sequence.

CONCLUSION

The controllability of a driving force-based distillation columns sequence has been successfully analysed by using a five-stage methodology. The results showed that the driving force sequence, which was also known as the direct sequence, was more controllable than the indirect sequence based on the input-output interactions, error values, but it was otherwise in terms of settling time. Although the driving force sequence has a slightly longer settling time, it was better than the indirect sequence in the other remaining aspects. For the separation of a benzene, toluene, and p-xylene mixture, this methodology was capable in providing an energy efficient and controllable solution. Future studies may include analysis of different separation units such as the flash column.

ACKNOWLEDGEMENT

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