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Controllability and Performance Analysis of Quaternary Aromatic Distillation Columns Sequence

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The purpose of this study is to show the application of a four-stage distillation columns sequence controllability analysis framework on a Benzene, Toluene, Ethylbenzene, and o-Xylene (BTEX) mixture. The controllability aspects of interest are the stability of distillation sequences, the error values of controller responses, and the settling time of the responses. In order to perform the analysis, a four-stage framework was developed. In the first stage of the framework, the driving force-based BTEX distillation columns sequence was simulated, along with other sequences for comparison purposes. In the second stage, the stability of the sequences was analysed based on Condition Numbers (CN) and minimum singular values obtained through Singular Value Decomposition (SVD). In the third stage, the sequences were simulated under dynamic conditions. In the fourth and final stage, the controller responses were analysed based on the Integral of Squared Error (ISE) criterion and settling time. The results show that the driving force sequence has several advantages over other sequences in terms of theoretical control properties and ISE.

1. Introduction

Distillation is a separation method that is widely used in the process industries such as chemical and petrochemical industries (Osuolale and Zhang, 2015). The distillation process is known to be responsible for almost 95% of all fluid separation in the chemical industry and around 3 % of world's energy consumption is directed to distillation units (Hernández et al., 2005). Separation of a multicomponent mixture is usually carried out by arranging multiple distillation columns in series, and the most notable sequences of such series are the direct and indirect sequence (Uwitonze et al., 2016). The concept of the driving force was introduced by Bek-Pederson and Gani (2004) to aid in the selection of an energy efficient distillation process. The concept is defined as the difference in composition of a component *i* between the vapour phase and the liquid phase, which is caused by a volatility difference between component *i* and other components in the mixture. The concept is defined mathematically as Eq(1) where F is the driving force, y_i is the vapour composition of i, x_i is the liquid composition of i, and α_{ij} is the relative volatility between components i and j.

$$F = y_i - x_i = \frac{x_i\alpha_{ij}}{1+x_i(\alpha_{ij}-1)} - x_i \quad (1)$$

According to Bek-Pederson and Gani (2004), the optimal sequence with the most energy efficient can be determined from their driving force algorithm, where the sequence determination involve the construction of driving force curves. The algorithm begins by arranging the components in a mixture in an increasing boiling point order. Then, the relative volatility between each pair of adjacent components is calculated. Using Eq(1), the driving force F for a pair of adjacent components is calculated for a range of values of x, which is from 0 to 1. The resulting values of F for each x are then plotted against x, thus creating a graph known as the driving force curve. The number of curves will always be one less than the number of components in a mixture. The

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height of a curves' peaks indicates the ease of separation of each curve's corresponding pair of components. The higher a driving force curve's peak, the easier it is to separate its corresponding pair. The driving force algorithm has been proven to give a result that has good sensitivity (Nordin et al., 2015). Aside from sensitivity, the sequence derived from the algorithm has also shown to be sustainable (Zaine et al., 2015). Another important property for distillation systems is its controllability. Controllability is important to set a stable operating condition and regulate the conditions so that products always meet the required specifications (Dumpa et al., 2016). Currently, there is little known about the controllability of the driving force sequences, thus it is the objective of this study to determine the controllability of a sequence derived from the driving force algorithm.

2. Methodology

2.1 Overall framework

Figure 1 shows the overview of the framework used for this study. The framework consists of four hierarchical stages.

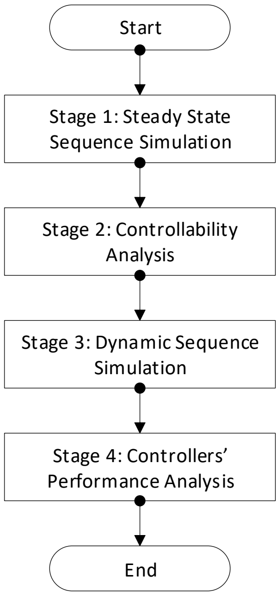

Figure 1: Framework overview

2.2 Stage 1: Steady state sequence simulation

In the first stage of the framework, sequences will be synthesised and simulated. In this study, sequence synthesis is defined as the process of determining a unique separation order that will make up a distinct distillation columns sequence. First, a case study, which is defined as the chemical mixture consisting of multiple components, will be selected from available literature and will be the feed mixture for the distillation columns sequences in this study. Then, the driving force sequencing algorithm will be used to determine the driving force sequence, which is the focal point of this study. Alternative sequences will also be determined for comparison purposes. The determinations will then be followed by a simulation of the sequences using Aspen Hysys V9 (2015). The sequences will first be simulated using short-cut columns to obtain design variables such as the feed stage, reflux ratio, and number of stages. The sequences will then be simulated using rigorous columns which are required for the proceeding analyses and the obtained design variables will also be used here.

2.3 Stage 2: Controllability analysis

In the second stage, gain matrices will be generated. Positive and negative increments will be made to each input in a sequence and its effect on the outputs will be recorded. A gain matrix will be calculated by dividing the change in output by the change in input, for every input and output considered. The inputs considered for this study were the reflux flow rate and the reboiler duty of each column of every sequence. The outputs considered are the top and bottom composition of every column of every sequence. Then, the gain matrices obtained will be inputted into MATLAB R2017a (2017) software to calculate the U, S, and V matrices. The three matrices will be obtained through Singular Value Decomposition (SVD). Eq(2) shows the MATLAB command to compute the three matrices, where U, S, and V are the matrices and K is the gain matrix.

$$[U, S, V] = svd(K) \tag{2}$$

Out of the three matrices, the S matrix is the only matrix of interest as it has the maximum singular value and the minimum singular value, which will be used to calculate the Condition Number (CN).

2.4 Stage 3: Dynamic sequence simulation

In the third stage, all sequences will be simulated dynamically using Aspen HYSYS V9 (2015). The purpose of the simulations is to obtain the process parameters, which are process gain (K), time constant (τ), and time delay (θ) of every input-output pair. Perturbations will be introduced to the systems during simulation and the resulting process reaction curves will be plotted. From the curves, process gains, time constants, and time delays will be calculated and the first order plus time delay (FOPTD) models will be developed. Eq(3) shows the general form of an FOPTD model.

$$FOPTD = \frac{Ke^{-\theta s}}{\tau s+1} \tag{3}$$

2.5 Stage 4: Controllers' performance analysis

The process parameters and FOPTD models obtained from the previous stage will be used to model the controllers. Modelling of the controllers will be done using Simulink programme under the MATLAB R2017a (2017) software. Each model requires an FOPTD model and also a controller gain (K_C), an integral time constant (τ_I), and a derivative time constant (τ_D). The K_C, τ_I, and τ_D can be calculated using the Eq(4), (5), and (6) (Kumar and Garg, 2015).

$$K_C = \frac{1}{K_P}\frac{\tau}{\theta}\left(\frac{4}{3} + \frac{\theta}{4\tau}\right) \tag{4}$$

$$\tau_I = \theta\frac{32 + {}^{6\theta}/_{\tau}}{13 + {}^{8\theta}/_{\tau}} \tag{5}$$

$$\tau_D = \theta\frac{4}{11 + {}^{2\theta}/_{\tau}} \tag{6}$$

After the models have been developed, they will be tested for settling time and error. The error calculation will be based on the integral of the squared error (ISE) criterion. The settling times and errors will be calculated under two circumstances: set-point change and feed flow rate change.

3. Result and Discussion

3.1 Case Study

The case study chosen for this study is a four-component mixture that consists of Benzene, Toluene, Ethylbenzene, and o-Xylene. The mixture enters the distillation system as a saturated liquid at 1 atm. The flow rates and composition are shown in the Table 1.

Table 1: The properties of feed composition for BTEX

Component	Molar flow rate (kmol/h)	Volumetric flow rate (m^3/h)	Mol fraction
Benzene	25	2.2135	0.25
Toluene	25	2.6476	0.25
Ethylbenzene	25	3.0506	0.25
o-Xylene	25	3.0053	0.25

3.2 BTEX sequence based on Driving Force

From the feed mixture information, the driving force curves were plotted. Figure 2 shows the driving curves for the BTEX separation. From the curves, the curve representing the separation of Benzene/Toluene has the highest peak, followed by the peaks of Toluene/Ethylbenzene and Ethylbenzene/o-Xylene. Therefore, the first separation of the driving force sequence is between Benzene and Toluene, followed by Toluene and Ethylbenzene and Ethylbenzene and o-Xylene.

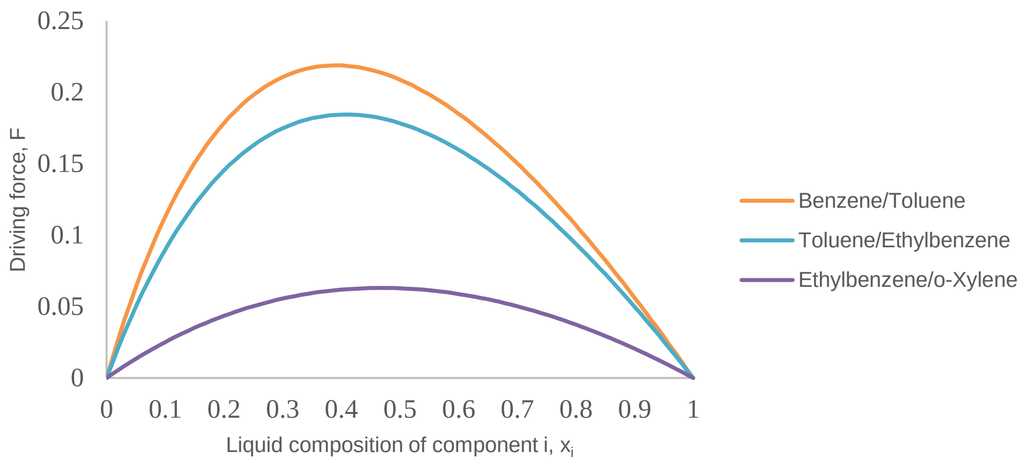

Figure 2: Driving Force curves for set of binary components at uniform pressure

The obtained driving force sequence is also commonly known as the direct sequence, which is shown in Figure 3. The sequences were first modelled based on the shortcut method primarily to obtain the number of stages and the feed stage. After the design variables were obtained, the sequences were simulated using rigorous distillation columns, which are depicted in Figures 3, 4, and 5.

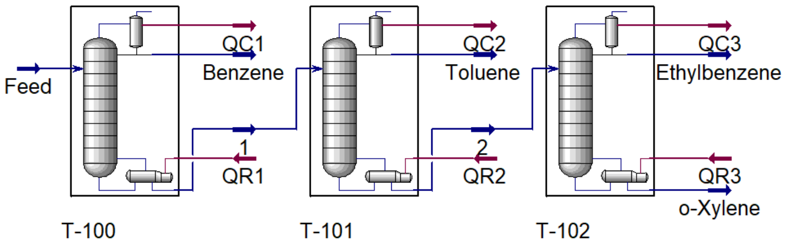

Figure 3: The driving force sequence

The number of alternative sequences was calculated using the following Eq(7), where n is the number of products and n_s is total number of possible sequence.

$$n_s = \frac{[2(n-1)]!}{n!(n-1)!} \quad (7)$$

The total number of possible sequence was five which means that there were four differently-arranged alternatives to the driving force sequence. Two of the four sequences had no converged solutions during the simulations, therefore only two alternative sequences were considered for further analyses. The two sequences were the direct-indirect and splitter sequence, which are shown in Figure 4 and 5.

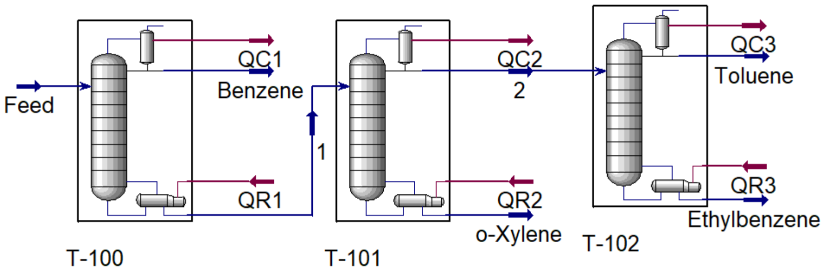

Figure 4: The direct-indirect sequence

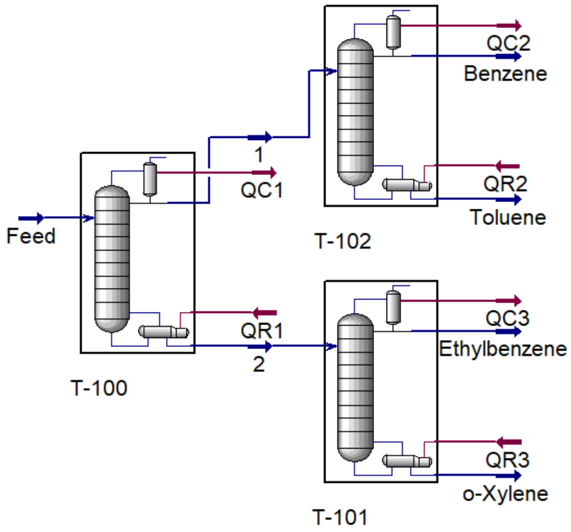

Figure 5: The splitter sequence

3.3 Controllability analysis

Table 2 shows the average CN and minimum singular value of each sequence. The CN and minimum singular value were first calculated with positive and negative increments. Then, the average of the two values were calculated for comparison.

Table 2: Average CNs and minimum singular values of each sequence

	Condition number	Minimum singular value
Driving force	29.6069	0.6220
Direct-indirect	31.6786	0.5165
Splitter	81.3813	0.6121

Based on Table 2, the sequence with the best CN is the driving force sequence, as it has the smallest CN. The sequence with the best minimum singular value is also the driving force sequence, as it has the largest minimum singular value. These results indicate that the driving force sequence should be the most stable out of the three sequences as the CN and the minimum singular value qualitatively indicate the stability of a sequence based on the magnitude of the value. Stability increases as the CN decreases and minimum singular value increases. Low CN and high minimum singular value may also indicate good dynamic performance under feedback control (Segovia-Hernandez et al., 2006).

3.4 Controller performance analysis

Table 3 and 4 show the average ISE and settling time due to set point change and feed disturbance.

Table 3: Average ISE and settling time due to set point change

	Driving force	Direct-indirect	Splitter
Average ISE	3.6×10^{-11}	6.1×10^{-9}	4.9×10^{-11}
Average settling time, min	850	212.5	425

Table 4: Average ISE and settling time due to feed disturbance

	Driving force	Direct-indirect	Splitter
Average ISE	4.7×10^{-10}	5.22×10^{-9}	8.6×10^{-9}
Average settling time, min	775	225	437.5

From the tables, the driving force sequence has the lowest average ISE value under both conditions when compared to the direct-indirect and splitter sequences. Its smallest ISE values illustrate that the desired output value does not differ much with the actual output value. Although it has the smallest error, the driving force sequence has the slowest settling times compared to the other sequences. The direct-indirect sequence which has the largest error has the fastest settling time in both cases. It can be said that the theoretical control properties predicted using the CN and minimum singular value do not entirely reflect the actual dynamic performance as the driving force sequence does not have the best settling time.

4. Conclusions

A systematic framework to analyse the controllability of driving force sequences was developed and tested on a four-component, BTEX mixture. Based on the results, the driving force proves to be the best sequence in terms of CN, minimum singular value, and ISE as it has the smallest CN, largest minimum singular value, and smallest error. It can be concluded that for this BTEX mixture, the driving force algorithm provides a viable choice because of its several advantages. Further study on driving force sequence's controllability at different operating conditions would be needed.

Acknowledgments

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