Control and energy analyses of a driving force-based aromatic mixture distillation columns sequence

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Abstract. To minimize the energy usage of distillation systems, past researchers have developed algorithms that exploit the driving force of distillation, which is the difference in vapour and liquid fractions due to relative volatilities. So far, little is known about the degree of controllability of the energy efficient solutions. This paper aims to ascertain that idea by applying a simple methodology on a common mixture as the case study. The methodology is made up of four stages: (1) feed information gathering, (2) sequence determination, (3) energy analysis and (4) controllability analysis. The controllability was analysed in terms of input-output interaction and resiliency using RGAno and MRI, respectively. From the application, it has been found that the sequence determined using driving force algorithm is the most optimal sequence overall, measured by the use of a multi-objective function.

1. Introduction

Distillation systems are known to be widely used for the separation of liquids and vapours, despite their large energy requirement. To avoid unnecessary waste of energy, extra attention has to be given during the synthesis and design phase of distillation systems. One way of obtaining an energy efficient design with reliable certainty has been proposed by Gani and Bek-Pedersen [1]. They have introduced a design algorithm that is centred around the concept of driving force. The driving force of interest is defined as the difference between the vapour composition and liquid composition of a component in a mixture that is caused by the volatility of that component relative to the other components in the mixture. In mathematical terms, it can be expressed as such:

\[ F_{Dj} \cdot y_j \cdot x_j \cdot \frac{x_{ref}}{1 + x_j (\sigma_j - 1)} - x_j \]  

(1)
Where $F_{D_i}$ is the driving force of component $i$, $y_i$ is the vapour composition of component $i$, $x_i$ is the liquid composition of component $i$, $\alpha_{ij}$ is the relative volatility between component $i$ and $j$. Soon after, Bek-Pedersen and Gani [2] presented several algorithms including the algorithm for distillation system synthesis. This synthesis algorithm is based on a graphical representation of the driving force concept. The graphical representation consists of curves, from which an energy efficient sequence of distillation columns can be determined according to the peaks of the curves. Being energy efficient would not matter much if a system is hard to control. In addition, good controllability could lead to further energy savings, as much as 15% [3]. Regarding controllability, researchers have found that a binary system [4] and quaternary systems [5][6] that were designed and synthesized at maximum driving force had better controllability their alternatives. To further establish the capability of the driving force concept on providing energy efficient and controllable solutions, it is aimed to analyse a driving force-based quintenary mixture separation process.

2. Methodology
The methodology used for this study consists of four hierarchical stages: (1) feed information gathering, (2) sequence determination, (3) energy analysis and (4) controllability analysis. The simplified view of the methodology is displayed in Figure 1 below.

![Figure 1. Simplified view of the used methodology.](image)

Information essential to the methodology is gathered in the first stage. The pieces of information include feed flowrate, feed composition, feed condition and vapour-liquid equilibrium data. The information regarding the feed is required for the simulations in Stage 3 and 4 whilst the equilibrium data is needed in Stage 2 when the driving force curves need to be plotted.

After the required information has been gathered, Bek-Pedersen and Gani’s [2] S2 algorithm is applied to synthesise an energy efficient distillation columns sequence. The sequence is based on a set of driving force curves, which can be plotted using the gathered vapour-liquid equilibrium data. This ordering of separation that is based on the curves’ peak should ensure the energy efficiency of the resulting distillation columns sequence, as suggested by Bek-Pedersen and Gani [2]. From this point forward, the sequence determined using the algorithm will be called the driving force sequence.

Then, in Stage 3, the driving force sequence is simulated along with other possible conventional distillation columns sequences to obtain their energy consumptions. This is done to verify the claim made by Bek-Pedersen and Gani [2] regarding their S2 algorithm.

Out of all the sequences available, only three are chosen for Stage 4, which are the ones with the lowest energy consumption. Even though the rest might have acceptable controllability, their poorer energy efficiencies would not make them the optimal choices overall. For the three sequences, their controllability is analysed in terms of input-output pair interaction and resiliency.
For the interaction part, relative gain array number \((RGA_{no})\) is applied [7]. It quantifies the relative gain array \((RGA)\) proposed by Bristol [8] into a single number, instead of a matrix of numbers. This makes comparison between different distillation systems easier. The smaller the \(RGA_{no}\), the less interaction the sequence has. The following equation relates \(RGA_{no}\) to \(RGA\), and \(RGA\) is calculated from the steady state process gain matrix \(K_P\).

\[
RGA_{no} = \|RGA - I\|_{\text{man}}
\]  \hspace{1cm} (2)

For resiliency, Morari resiliency index \((MRI)\) [7] is used to quantify the sequences’ resiliency towards disturbance where a bigger number indicates better resiliency. \(MRI\) is the smallest singular value \((\sigma^*)\) of the matrix of singular values \(S\). Matrix \(S\) is obtained from the singular value decomposition of the process gain matrix \(K_P\), along with unitary matrices \(U\) and \(V\). Equations (3)-(5) display the mathematical relations.

\[
MRI = \sigma^*\]
\[
S = \begin{bmatrix}
\sigma^* & 0 & 0 & 0 \\
0 & \sigma_2 & 0 & 0 \\
0 & 0 & \sigma_3 & 0 \\
0 & 0 & 0 & \sigma_v
\end{bmatrix}
\]  \hspace{1cm} (4)

\[
K_P = USV^T
\]  \hspace{1cm} (5)

To determine the optimal sequence, the trade-off between energy and controllability have to be taken into account thus both need to be considered simultaneously. Therefore, the following multi-objective function is used.

\[
\min J = w_1 P_1 + w_2 P_2 + w_3 \left(\frac{1}{P_3}\right)
\]  \hspace{1cm} (6)

Where \(w_1\), \(w_2\) and \(w_3\) are the weight factors assigned to objective function terms \(P_1\), \(P_2\) and \(P_3\), respectively. \(P_1\) corresponds to the energy consumption, \(P_2\) to the interaction and \(P_3\) to the resiliency. The distillation columns sequence with the smallest multi-objective function value \(J\) is the most optimal sequence in terms of energy, interaction and resiliency.

3. Results

3.1. Stage 1: Feed information gathering

The case study for this paper was taken from Kiss et al. [9]. It was a mixture containing 12.32 wt % \(n\)-pentane, 20.42 wt % benzene, 26.87 wt % toluene, 27.36 wt % xylene and 13.03 wt % trimethylbenzene. As it was unclear which xylene and trimethylbenzene were used in their study, \(m\)-xylene and 1,3,5-trimethylbenzene were assumed for this study. Also assumed was the feed condition and pressure, which were saturated liquid and 1 atm respectively. The feed’s flowrate was 12,500 kg/hr. The vapour-liquid equilibrium data required was taken from Aspen HYSYS’s V10 database.
3.2. Stage 2: Sequence determination
From the application of the S2 algorithm, the following curves in Figure 2 were obtained.

![Figure 2. Driving force curves of the case study.](image)

From the curves, it can be seen that the curve with the highest peak corresponds to the separation of n-Pentane and Benzene. Therefore, the separation of n-Pentane and Benzene was conducted first as they had the largest driving force among the possible separations. The proceeding separations followed the order of the curves, from the one with the second highest peak to the one with the lowest peak. According to Bek-Pedersen and Gani [2], this sequence is near-optimal if not optimal in terms of energy consumption. This would be verified in Stage 3. Figure 3 shows the driving force sequence in this study, which is also commonly known as the direct sequence.

![Figure 3. Driving force sequence.](image)
3.3. Stage 3: Energy analysis

Table 1 shows the energy consumption of the top three energy efficient sequences.

| Sequence                | Energy consumption (kW) |
|-------------------------|-------------------------|
| Driving force           | 7,105.59                |
| BC-splitter-direct      | 6,916.77                |
| CD-splitter-direct      | 7,564.26                |

It can be seen that the driving force sequence is near-optimal in terms of energy consumption, as predicted. Figures 4 and 5 show the other two energy efficient sequences.

Figure 4. BC-splitter-direct sequence.

Figure 5. CD-splitter-direct sequence.
3.4. Stage 4: Controllability analysis

First, the input-output pairing of the sequences was determined. Customarily, the top product composition is controlled by manipulating the reflux flow whilst the bottom product composition is controlled by manipulating the flow of steam into the reboiler. Thus, for the steady state controllability analysis in this study, such pairing was used. Then, gain matrices of the sequences were calculated and scaled to later provide a more accurate results without the interference of different units during calculation. The scaled gain matrices were subsequently used for the calculation of the \( RGAno \) and \( MRI \). Tables 2 and 3 show value of \( RGAno \) and \( MRI \) of each sequence.

| Sequence          | \( RGAno \) |
|-------------------|-------------|
| Driving force     | 24.01       |
| BC-splitter-direct| 129.79      |
| CD-splitter-direct| 11.87       |

| Sequence          | \( MRI \)  |
|-------------------|-------------|
| Driving force     | 0.00062     |
| BC-splitter-direct| 0.00003     |
| CD-splitter-direct| 0.00010     |

For this study, all objective function terms are weighted equally (weight factors assumed as unity) because there was no preference towards any objective function term. As the three objective function terms had different units and range of values, each term will be normalized with respect to its maximum value.

| Sequence          | \( P_1 \) | \( P_2 \) | \( P_3 \) | \( J \)  |
|-------------------|-----------|-----------|-----------|--------|
| Driving force     | 0.9394    | 0.1850    | 0.0442    | 1.1686 |
| BC-splitter-direct| 0.9144    | 1.0000    | 1.0000    | 2.9144 |
| CD-splitter-direct| 1.0000    | 0.0915    | 0.2725    | 1.3640 |

Based on Table 4, the driving force sequence has the smallest objective function value among the three sequences. Thus, it can be said that the sequence that was synthesized at maximum driving force is the most optimal one in terms of energy consumption, input-output interaction and resiliency.

4. Conclusion

A four-stage methodology has been used to analyse the energy consumption, input-output interaction and resiliency of a driving force-based distillation columns system. The system has been compared to two distinct alternatives and it has been found that the system has the best overall performance. This finding further strengthens the idea that by using the driving force synthesis algorithm, an energy efficient and controllable sequence can be easily obtained with no use of simulation and optimisation as the algorithm only uses graphical representation. With further study, a reliable, easy and time-saving method for designing distillation columns systems may be available for industries in the future. Other interested researchers could analyse the controllability of complex and intensified distillation systems that are based on the driving force concept in their future works.
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