Comparison and improvement of driving force-based distillation columns system designs

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Abstract. The aim of this paper is to compare two driving force-based approaches for designing distillation column systems. A new methodology intended as a comparison tool is presented, where a distillation column system designed at maximum driving force is compared with a distillation column system designed at driving force that corresponds to the feed composition of the light component. In addition, a simplified Kirkbride equation is proposed to improve the existing feed location determination. The methodology is made up of four hierarchical stages; (1) identification of process mixture, (2) determination of driving force sequence, (3) design using driving force method and (4) energy analysis. The steps to sequence and design the systems as well as to analyze their performance in terms of energy usage were applied on an aromatic mixture separation case study. The findings show that by using this study’s approach, the design variables obtained resulted in a system that achieves better purity (near-optimal), is more accurate and more energy efficient that an existing system, with 9.34% less energy used.

1. Introduction
Distillation is a highly energy-intensive unit operation and yet is most frequently used for liquid-vapor separation processes. Over the years, continuous modifications and optimizations have been carried out to design more energy-efficient distillation systems to reduce the energy and costs of the processes. Compared with other methods, driving force proposed an integrated solution that is capable of synthesising and designing distillation columns sequences based on a graphical representation of the maximum driving force point. The graphical representation is similar to the McCabe-Thiele method. However, instead of plotting vapor composition (yi) against liquid composition of light component (xi), the driving force graph is constructed by plotting driving force value (FDi) against liquid composition of light component (xi). The method was developed by Gani and Bek-Pedersen [1] and is defined as in equation (1).
Where \( \alpha_{ij} \) is the relative separable factor of a binary pair. The method’s concept is to design a distillation system which operates at the maximum driving force. When the FD\(_i\) approaches maximum the energy required to achieve a separation is at minimum, whereas when the FD\(_i\) approaches zero the separation becomes more difficult and energy usage will also increase [2]. The findings of other researchers in this field [3-5] also proved that the design obtained by using this method operates with lower energy usage than other methods.

Recently, a new approach to design non-reactive and reactive distillation columns systems using combined Gibbs energy and driving force method was proposed by Sales-Cruz et al. [6] and Lopez-Arenas et al. [7]. For saturated liquid feeds, this approach locates the feeds’ light component composition on the x-axis of the driving force graph and adjusts the thermal feed condition to satisfy the maximum driving force point to obtain the design variables required. The adjustment of thermal feed condition may be possible for binary mixtures but not for multicomponent mixtures because heaters would be required between each distillation column to fulfill the thermal feed condition.

Hence in this study, a comparison was carried out to determine the effects of the design variables obtained at the maximum driving force point and at the feed composition-based driving force point (without adjustments on the thermal feed condition). The basis for designing systems is still the same as the design procedure proposed by Bek-Pedersen and Gani [2], with the exception of the location of the design point and feed stages of mixture. The resulting distillation systems were compared in terms of product purity and energy usage.

2. Methodology
The methodology consists of four stages; identification of process mixture, determination of driving force sequence, design using driving force method, and energy analysis. The simplified overall methodology is displayed in figure 1.

![Figure 1. Overview of the simplified methodology as a comparison tool.](image)

Stage 1 deals with the identification of process mixture and data gathering for the design of distillation column systems using the driving force method. The feed and product information such as flow rate, composition, pressure, temperature and desired purity of product was gathered. The thermodynamic model used to simulate the process was taken from a previous research of similar process.
In stage 2, the driving force method was used to determine the driving force sequence based on the feed and product streams information gathered. The algorithm proposed by Gani and Bek-Pedersen [1] was used to design the sequence of distillation columns based on driving force curves. Initially, the components to be separated were listed in decreasing volatility order and binary mixture splits were defined. The driving force curve of a split was plotted using equation (1). The split of the binary mixture with the highest driving force value was separated first followed by the second highest, and the rest.

In stage 3, distillation systems based on the driving force method was designed according to two approaches. The first approach as shown in figure 2a was taken from Bek-Pedersen and Gani [2], where the design point is at the maximum value of driving force on the driving force curve ($FD_{max}$). The second approach as shown in figure 2b was designed at a point on the driving force curve that corresponds to the light component’s feed composition ($X_{feed}$). A simplified Kirkbride equation as shown in equation (2) was added to the latter approach to determine the feed location (NF) since Bek-Pedersen and Gani’s [2] approach is not accurate, especially when the feed mixture has high relative volatilities as well as the composition of the light components is significant.

$$N_P = \frac{N}{\left(\frac{X_{feed}}{1-X_{feed}}\right)^{4.9} + 1}$$

Where N is the number of stages of distillation column.

Then, both of the obtained systems were simulated using rigorous distillation column design in Aspen HYSYS process simulator to verify the designs variables obtained using Excel from the previous steps in terms of product purity and to determine energy usage.

Finally, in stage 4, the simulated systems were compared in terms of energy usage. The system that operated with less energy was preferred since it was more economical.
3. Results and discussion
Comparison of the approaches was carried out using an aromatic case study because the separation of aromatic mixtures is common, hence making this study relevant for industrial application [8].

3.1. Stage 1: Identification of process mixture
A case study of an aromatic mixture of six components that consisted of 10 mol% Methylcyclopentane (MCP), 10 mol% Benzene, 10 mol% Methylcyclohexane (MCH), 10 mol% Toluene, 10 mol% m-xylene and 50 mol% o-xylene was taken from Zaine et al. [3]. The feed flowrate was at 1000 kmol/hr at a temperature of 30 ºC and a pressure of 2 atm. The desired purity of product for all components were set at 99.9 %, as in Zaine et al.[3]. Previous studies used Antoine fluid package as the thermodynamic model in the simulator. However, to rely solely on this fluid package would lead to inaccurate results since there was an azeotrope point in the MCP-benzene mixture. Hence, the Antoine fluid package was selected without analyzing the MCP-Benzene separation.

3.2. Stage 2: Determination of driving force sequence
The components of the feed in Stage 1 were listed in decreasing volatility order. Pairs of adjacent components were defined as binary mixtures; they were MCP/Benzene (A/B), Benzene/MCH (B/C), MCH/Toluene (C/D), Toluene/m-xylene (D/E) and m-xylene/o-xylene (E/F). Once the splits had been determined, driving force curves were plotted using Microsoft Excel to determine the maximum driving force point of each curve in the graph. The driving force curves are illustrated in figure 3.

![Figure 3. The driving force curves of the aromatic mixture.](image)

Based on the curves in figure 3, D/E had the highest maximum driving force point and would be separated first, followed by B/C, C/D, E/F and lastly A/B. However, for this case, A/B would not be separated to ensure valid comparison.
3.3. Stage 3: Design using driving force method

The distillation column for the separation of D/E was selected first according to driving force sequence. Then, the design variables required for the distillation column were determined using Bek-Pedersen and Gani’s [2] and this study’s approaches. Next split was selected and the previous steps were repeated. The design variables obtained are shown in Table 1 and Table 2 and were used for the rigorous simulation in Aspen HYSYS. Both systems were simulated using similar fluid packages and reflux ratio of 1.2Rmin was used. The obtained product purities of the systems are shown in Table 3.

| Split   | Number of Stages | Feed Stage | Reflux Ratio (mol) |
|---------|------------------|------------|--------------------|
| D/E     | 48               | 25         | 1.6778             |
| B/C     | 63               | 37         | 2.7090             |
| C/D     | 129              | 67         | 9.5230             |
| E/F     | 220              | 92         | 17.2790            |

| Split   | Number of Stages | Feed Stage | Reflux Ratio (mol) |
|---------|------------------|------------|--------------------|
| D/E     | 48               | 24         | 1.2452             |
| B/C     | 63               | 32         | 2.2519             |
| C/D     | 129              | 65         | 9.1286             |
| E/F     | 220              | 123        | 49.0523            |

Based on Table 3, the purities obtained using this study’s approach is closer to targeted purities than the Bek-Pedersen and Gani’s [2] approach. This indicates that the latter approach is more accurate than the previous approach.
3.4. Stage 4: Energy analysis

Table 4 summarizes the energy usages that were obtained from Aspen HYSYS, with respect to both approaches.

| Split | Bek-Pedersen and Gani’s [2] approach | This study’s approach |
|-------|--------------------------------------|-----------------------|
|       | Condenser  | Reboiler  | Condenser  | Reboiler  |
| D/E   | 9.10       | 15.87     | 7.63       | 14.40     |
| B/C   | 5.87       | 5.97      | 5.14       | 5.24      |
| C/D   | 8.57       | 8.56      | 8.25       | 8.24      |
| Total Energy (MW) | 53.94 | 48.90 |
| Savings (%) | 9.34 |

Based on Table 4, it can be said that the system designed based on this study’s approach combined with the Kirkbride equation in this study is more accurate and operated at lower energy than the Bek-Pedersen and Gani’s [2] approach. The energy usage for the E/F split was not taken into account in the analysis since the purity of E and F from the Bek-Pedersen and Gani’s [2] approach deviated too far from the targeted purity.

4. Conclusion

A comparison between two different approaches to distillation columns system design was conducted. To compare those approaches, a systematic methodology was proposed and tested on an aromatic mixture case study. The energy analysis reveals that this study’s approach combined with a proposed feed location determination equation produced a more energy efficient and accurate result than the Bek-Pedersen and Gani’s [2] approach. The system obtained from this study’s approach was able to attain an energy saving of 9.34 %. It can be concluded that the distillation columns system designed using this study’s approach that was based on the driving force method is more accurate and economical than the previous approach. Further studies should be done using different case studies to further test and verify the effectiveness of this study’s approach combined with a proposed feed location determination equation. In addition, the use of different types of distillation column can be further studied to replace the current columns’ number of stages, which were quite high.

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