

## Economic, Feasibility, and Sustainability Analysis of Energy Efficient Distillation Based Separation Processes

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The aim of this paper is to develop and carry out additional analyses aside from economics in designing distillation columns which are feasibility and sustainability analyses. The analyses' results for an existing design and driving force method-based design were compared. First, an existing design was simulated using Aspen HYSYS process simulator to determine its energy usage. In the next stage, an optimal sequence was determined using a driving force graph developed using Excel. Then, a suitable equipment was selected to replace the existing design and the new design based on the driving force method was simulated using the same process simulator. Lastly, the three analyses were carried out for both designs to determine which design is better in terms of feasibility, sustainability, and economics. A case study of aromatic compounds (Methylcyclopentane (MCP), Benzene, Methylcyclohexane (MCH), Toluene, m-Xylene, and o-Xylene) obtained from a literature was used where the driving force method was applied to determine the sequence for the separation of the aromatic mixture. However, the individual columns were designed using the short-cut design method. This study applied the driving force method for both sequencing and designing to compare the existing design with the new design to determine which method leads to better results from the analyses. The analyses results' show that the new design surpasses the existing design in feasibility, sustainability, economic analyses and a total annual cost (TAC) of up to 7.11 % can be saved annually.

### 1. Introduction

Distillation can be considered as the most popular vapour-liquid separation process that is widely used industrially to separate various chemicals, most commonly petroleum products. Distillation utilizes the volatilities of the components to be separated through multiple stages of evaporation and condensation to attain the desired product purity (Galli et al., 2017). The capability to obtain near-pure products makes distillation the most preferable choice over other types of separation process. However, a design that focuses only to achieve the best product quality may consume a huge amount of energy and may utilise a taller distillation tower. Over the years, continuous research was carried out to further modify and improve the system to improve its efficiency. The driving force method can be considered as one of the most popular methods to improve distillation system and was introduced by Gani and Bek-Pedersen (2000). By using this method, the sequence and design of distillation columns can be determined easily and the design obtained should operate at an optimal or near optimal efficiency with respect to energy usage. Despite that, an optimal distillation column design should not just focus on energy and cost factor but also include other aspects such as feasibility and sustainability into the design. Hence, this study integrated three different types of analysis which are feasibility, sustainability, and economic into the design of distillation systems using the driving force method. The feasibility analysis referred here is from economic point of view related to the optimal number of stages and reflux ratio range. High number of stages and reflux ratio will increase investment and operating cost of the plant. The sustainability analysis focuses on the material and energy consumption of the process.

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## 2. Methodology

### 2.1 Simplified framework

Figure 1 shows the overview of the simplified framework with four hierarchical stages used in this study. At the end of the framework, three different types of analysis will be used to determine whether the driving force method applied here has any impact on other aspects aside from energy consumption.

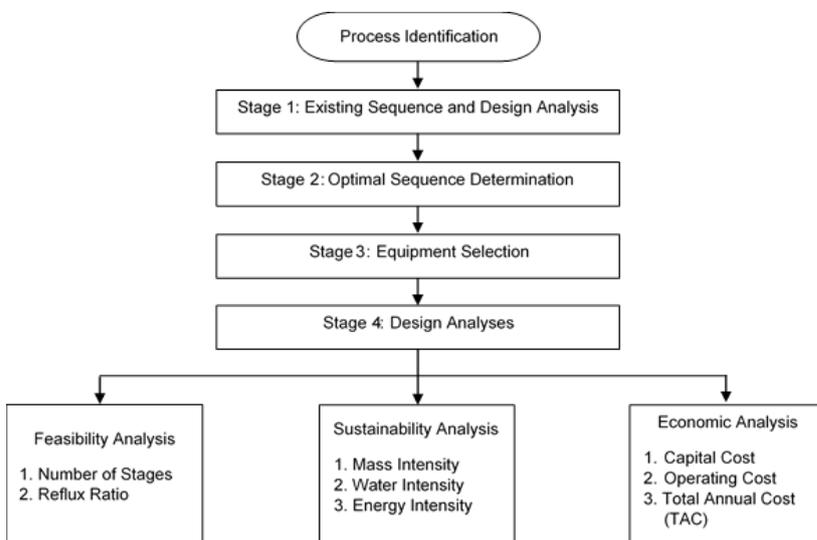


Figure 1: Overview of the simplified framework of energy efficient distillation-based separation processes

### 2.2 Stage 1: Existing sequence and design analysis

In stage 1, feed information such as temperature, pressure, feed composition, and feed flow rate of the base case mixture is gathered. A suitable fluid package is determined for the process selected if the fluid package used by the previous research is not available or not appropriate. For the base case used in this study, it was identified that the previous researcher used the ideal gas law thermodynamic model, which is not suitable for highly non-ideal liquid mixture. According to Chukwu (2008), the activity coefficient thermodynamic model is often used to represent highly non-ideal liquid mixtures for pressures up to 10 bars. Hence, a thermodynamic model with activity coefficients such as NRTL and UNIQUAC is selected whenever a highly, non-ideal liquid mixture such as an azeotrope mixture is present. However, the parameters required by those thermodynamic models may be not available sometimes, which in turn may lead to inaccurate results; in this case, an equation of state (EOS) is used instead. Design variables such as the number of stages, reflux ratio, and feed location of the base case are determined using the short-cut design method as used by the referred study. The sequence used by the base case is also determined, whether it is direct, indirect, direct-indirect, or other configurations. The data collected are used in Aspen HYSYS process simulator to determine the energy usage of the existing design and then the energy usage is recorded for comparison purposes.

### 2.3 Stage 2: Optimal sequence determination

To apply the driving force method, initially, the components to be separated in stage 1 are listed according to their boiling point. Each listed component then is defined as a binary pair with its adjacent components. A driving force curve is constructed for each binary pair where the y-axis shows the driving force values (DF) and the light component's compositions is shown on the x-axis of the graph. The sequence which has a higher DF is separated first, followed by the next one until the last curve (Gani and Bek-Pedersen, 2000).

### 2.4 Stage 3: Equipment selection

The equipment selection in this study was limited to distillation-based equipment such as ordinary distillation columns, extractive distillation columns, and flash columns. Even though the flash column is the most economical operation unit compared to the other two, it can only be used for components that have a very high relative volatility. Hence, ordinary distillation column is usually selected and used in industrial practices. However, the presence of azeotropes and close boiling point mixtures makes the ordinary distillation an infeasible option and extractive distillation is selected instead. After the equipment is selected, design

variables such as reflux ratio and number of stages are easily determined from the driving force graph. A step-by-step method to design an extractive distillation column can be found in the work of Zubir et al. (2017). Information on the optimal sequence from stage 2 and the design variables from this stage are simulated using Aspen HYSYS simulator to determine the energy usage of the proposed design.

## 2.5 Stage 4: Design analyses

### 2.5.1 Feasibility analysis

Feasibility analysis of distillation columns can be divided into two parts in this study. The first one is to determine whether the column has a feasible number of stages and the second part is to determine whether the design operates within an optimum reflux ratio range. According to Seader et al. (2009), the maximum allowable height of column should be around 200 ft or 61 m. In addition, Couper et al. (2012) stated that the maximum height of column should be less than 175 ft or 53 m due to its foundation and wind load considerations. When calculating a distillation column's height, a space at the bottom and top for reboiler return and vapor release should be considered as well. This study assumes a 1.8 m height for the sump at the bottom and a 1.2 m of disengagement height at top of the column. The actual height of the column can be calculated using Eq(1).

$$\text{Column Height, } H = (N_{\text{actual}} - 1) \times \text{Tray Spacing} + \text{Height of Sump} + \text{Disengagement Height} \quad (1)$$

According to Couper et al. (2012), the most common tray spacing used is 20 – 24 in. or 0.508 – 0.610 m. By using a tray spacing of 0.508 m with a column height of 61 m, the maximum allowable number of stages calculated is limited to 115 stages in this framework. Hence, columns with a larger number of stages than this value are considered infeasible. The optimal reflux ratio (RR) range is between 1.1 to 1.5 times the minimum reflux ratio ( $R_{\text{min}}$ ) (De Haan and Bosch, 2013). A column that operates outside the feasible reflux ratio range will cause a dry up of liquid or vapour at a certain number of trays and will affect the separation process. Even though the number of stages and reflux ratio can be manipulated to achieved desired separation, it should be noted that it must be operated within optimal range as mentioned above.

### 2.5.2 Sustainability analysis

The sustainability analysis employed here was developed by Nordin (2015) and is called 'two-dimensional (2-D) sustainability index, which takes into account both material and energy consumption of the designs. The design with a lower index is preferred since it is more sustainable and more energy efficient.

### 2.5.4 Economic analysis

Economic analysis is the most common analysis carried out by previous researchers. For this study, the capital and operating costs were determined using Aspen Economic Analyzer. The total annual cost (TAC) was calculated based on an equation from Zhu et al. (2017) with an assumed payback period of 3 y.

## 3. Result and discussion

### 3.1 Case study

A case study from Zaine et al. (2015) which consists of six components (Methylcyclopentane (MCP), Benzene, Methylcyclohexane (MCH), Toluene, m-xylene and o-xylene) was used and listed according to their boiling point as shown in Table 1. The feed flowed at 1,000 kmol/h at 2 atm and 30 °C.

Table 1: Feed information of aromatic mixture (Zaine et al., 2015)

Feed Component	Composition (mol %)	Boiling point (K)
MCP (A)	0.1	344.96
Benzene (B)	0.1	353.24
MCH (C)	0.1	374.05
Toluene (D)	0.1	383.75
m-xylene (E)	0.1	412.25
o-xylene (F)	0.5	417.55

Initially, the existing design and sequence was analysed and simulated using Aspen HYSYS process simulator. It was identified that the existing design had the optimal sequence since it was designed using the driving force method but the individual columns' design was carried out using the short-cut method. The process flow diagram (PFD) of the existing design is displayed in Figure 2 and the design variables obtained from the short-cut method used on the existing design are shown in Table 2. Since an azeotrope point was

detected between MCP and Benzene, an activity coefficient thermodynamic model was selected. The parameters for the NRTL model are available for this separation, thus they were used to simulate both existing and proposed design.

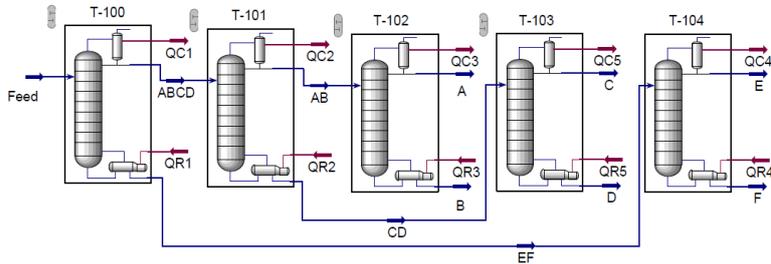


Figure 2: PFD of the existing design

Table 2: Design variables of existing design

Operating Variables	T-100	T-101	T-102	T-103	T-104
	Ordinary Column				
Number of stages	35	46	121	118	172
Feed stage	18	23	61	59	114
Feed (kmol/h)	1,000.0	399.9	200.0	199.9	600.1
Min. reflux ratio	1.1340	1.6845	7.5533	7.4176	33.6833
Reflux ratio (mol)	1.3608	2.0214	9.0640	8.9011	40.4200
Pressure (atm)	2	2	2	2	2

Compared to the existing design, the proposed design was developed using the driving force method for both sequencing and designing of the distillation columns. The PFD of the proposed design is illustrated in Figure 3 and the design variables obtained using the driving force method with substitution of three ordinary distillation column system with extractive distillation column system as proposed in stage 3 of the framework are shown in Table 3. The solvents used in this study were N-formylmorpholine (NFM) in MCP and Benzene separation (Brondani et al., 2015), N-methyl-2-pyrrolidone (NMP) from the separation of MCH from Toluene (Quijada-Maldonado et al., 2016) and 1-Nonanol from the separation of m-xylene and o-xylene (Berg, 1992). The listed solvents were used and tested by respective researchers and showed good results in their studies. Based on the results in Table 4, the proposed design has a significant increase in the purity of products for most components compared to the existing design, with the exception of a slight reduction of 2.6 % for m-xylene and 0.6 % for o-xylene.

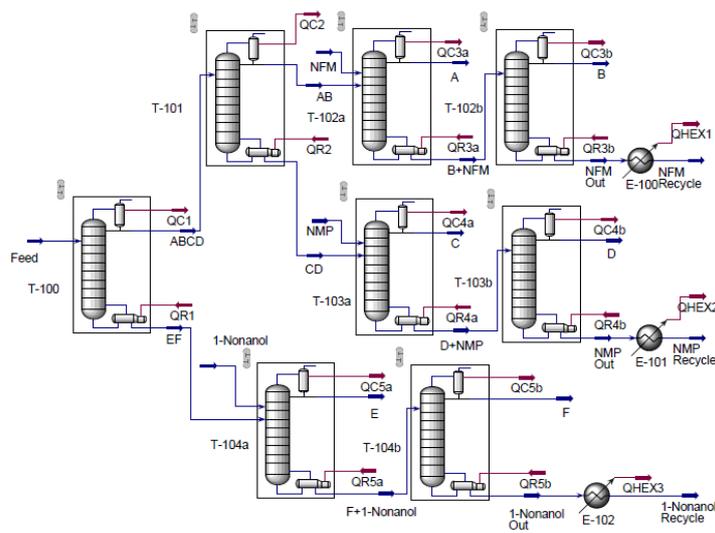


Figure 3: PFD of the proposed design

Table 3: Design variables of the proposed design

Operating Variables	T-100	T-101	T-102a	T-102b	T-103a	T-103b	T-104a	T-104b
Number of Stages	35	46	18	6	55	11	31	21
Feed Stage	21	26	12	5	31	8	20	14
Solvent Feed Stage	-	-	3	-	6	-	3	-
Solvent Temperature (°C)	-	-	95	-	95	-	95	-
Feed (kmol/h)	1,000.0	400.0	200.0	300.0	200.0	300.0	600.0	1,700.0
Solvent (kmol/h)	-	-	200.0	-	200.0	-	1200.0	-
Min. reflux ratio	1.7290	2.8159	1.6028	0.2790	3.9419	1.4359	1.8315	1.4753
Reflux ratio (mol)	2.0748	3.3791	1.9233	0.3348	4.7303	1.7231	2.1978	1.7704

Table 4: Products purity specifications for both existing and proposed designs

Equipment	Purity (mol %)								
	MCP	Benzene	MCH	Toluene	m-xylene	o-xylene	NFM	NMP	Nonanol
Zaine et al. (2015)	83.6	83.5	92.8	92.9	99.6	99.9	-	-	-
This study	99.9	99.8	99.9	99.8	97.0	99.3	99.9	99.9	99.8

### 3.2 Feasibility analysis

The design variables obtained for both designs were used to determine the feasibility of the designs. Based on Table 5, the existing design by Zaine and co-workers (2015) is infeasible for certain distillation columns due to the high number of stages. The number of stages for equipment labelled T-102, T103, and T-104 from the existing design exceed the feasible range even though the reflux ratio was increased up to  $1.5R_{min}$  to reduce the number of stages. Hence, the proposed design replaced the ordinary distillation system with an extractive distillation system which is more appropriate, uses less energy, and has fewer number of stages.

Table 5: Feasibility analysis comparison

Design Model	Equipment	Feasibility Status	
		Number of Stages (< 115 Stages)	Reflux Ratio (RR) ( $1.1R_{min} < RR < 1.5R_{min}$ )
Zaine et al. (2015)	T-100	Feasible	Feasible
	T-101	Feasible	Feasible
	T-102	Not feasible	Feasible
	T-103	Not feasible	Feasible
	T-104	Not feasible	Feasible
This study	T-100	Feasible	Feasible
	T-101	Feasible	Feasible
	T-102a	Feasible	Feasible
	T-102b	Feasible	Feasible
	T-103a	Feasible	Feasible
	T-103b	Feasible	Feasible
	T-104a	Feasible	Feasible
	T-104b	Feasible	Feasible

### 3.3 Sustainability analysis

Table 6 illustrates the sustainability comparison between the existing design and the proposed design. The proposed design has a lower total sustainability index, which means it is more sustainable compared to the existing design. In addition, according to the result, there is a huge difference on the energy consumption of both designs where the proposed design used energy more efficiently compared to the existing design.

Table 6: Sustainability analysis comparison

Design Model	Material Consumption		Energy Consumption	Total
	Mass Intensity Index	Water Intensity Index	Energy Intensity Index	
Zaine et al. (2015)	1.09	0.32	5.43	6.84
This study	1.01	0.32	1.72	3.05

### 3.4 Economic Analysis

Based on Table 7, savings up to 11.40 % for capital cost and 5.83 % for operating cost were obtained for the proposed design. Using a payback period of 3 y, a saving up to 7.11 % can be attained annually.

Table 7: Economic analysis comparison

Design Model	Capital Cost (USD)	Capital Savings (%)	Operating Cost (USD/y)	Solvent Start-up Cost (USD/y)	Operating Savings (%)	TAC (x 10 <sup>6</sup> USD/y)	TAC Savings (%)
Zaine et al. (2015)	23,029,500	11.40	25,713,900	-	5.83	33.39	7.11
This study	20,401,800		22,371,800	1,843,143.83		31.02	

## 4. Conclusion

A systematic framework to design energy efficient distillation-based separation processes was proposed and tested with an aromatic mixture case study. By using this framework, the proposed design operated within feasible number of stages and reflux ratio ranges. The sustainability analysis reveals that the proposed design is more sustainable and more energy efficient compared to the existing design. Lastly, the design obtained is more economical with a Total Annual Cost (TAC) saving of 7.11 %. It can be concluded that the proposed design that was based on the driving force method is more economical, more feasible, and more sustainable than an existing design. Further studies should be done using different case studies to further test and verify the effectiveness of the driving force approach using the three analyses.

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