INTEGRATED FRAMEWORK FOR SYNTHESISING ENERGY-EFFICIENT DISTILLATION COLUMN SEQUENCE

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DEDICATION

This thesis is dedicated to my father, Zubir bin Mohd Said, who has always been supporting me from far away. It is also dedicated to my mother, Norliah binti Mahani, who is continuously by my side throughout this research. I pray for them to be always under His Protection.

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ABSTRACT

This thesis presents and describes the development and application of an integrated framework for the synthesis of energy-efficient distillation column sequences. The framework is generic and applicable to various types of distillation columns. It is unique in the sense that it integrates distillation column sequencing, selection and design with the graphical representation of the driving force method. The existing driving force method was improved to include the effect of feed composition and also several concepts from existing methods, which can improve the capability of the method in finding optimal solutions that are feasible, economical, energy-efficient and material-efficient. The framework consists of five stages: 1) energy analysis of the existing sequence, 2) determination of the driving force sequence, 3) design of the driving force sequence, 4) feasibility, energy intensity and material intensity analyses and 5) economic analysis. In Stage 1, an existing distillation column sequence was simulated using the Aspen HYSYS process simulator to obtain its energy usage. In Stage 2, the graph of the improved driving force method was used to determine an energy-efficient distillation column sequence, which was also simulated to obtain energy usage. Then, by using a similar graph, suitable unit operations (flash columns, ordinary distillation columns, or extractive distillation columns) for the sequence were selected and designed in Stage 3. This post-design driving force sequence was also simulated for the same purpose as in Stage 1. The analyses began in Stage 4, where the feasibility, energy intensity and material intensity of the distillation column sequences obtained in Stages 1, 2 and 3 were compared. Feasibility was determined based on the reflux ratio range, distillation column height and product purity whilst energy and material intensities were based on mass, water and energy indexes. Finally, in Stage 5, an economic comparison based on capital, operation and total annual costs was employed. The framework was successfully tested on five different case studies with different objectives to test and verify the methodologies used in the framework. The application of the overall framework showed that energy savings of up to 32.94 % could be achieved whilst operating within the feasible range. The energy and material intensities were also reduced by up to 59.31 %, indicating lesser amount of energy and material used for the framework's sequence. The capital and operation costs were also reduced, as much as 35.05 % and 30.88 %, respectively, which led to 31.71 % lower total annual cost, compared with the sequences obtained by previous studies.

ABSTRAK

Tesis ini membentangkan dan menerangkan perkembangan dan penerapan kerangka bersepadu untuk sintesis jujukan turus penyulingan cekap tenaga. Rangka kerja ini bersifat generik dan boleh digunakan untuk pelbagai jenis turus penyulingan. Rangka kerja ini adalah unik kerana ia menggabungkan penjujukan, pemilihan, dan reka bentuk penyulingan dengan perwakilan grafik dari kaedah daya pacu. Kaedah daya pacu yang sedia ada telah ditambah baik untuk merangkumi pengaruh komposisi suapan dan juga beberapa konsep dari kaedah yang sedia ada yang dapat meningkatkan kemampuan kaedah itu dalam mencari penyelesaian optimum yang dapat dilaksanakan, menjimatkan, cekap tenaga dan cekap bahan. Kerangka kerja ini terdiri daripada lima tahap: 1) analisis tenaga dari jujukan yang sedia ada, 2) penentuan jujukan daya pacu, 3) reka bentuk jujukan daya pacu, 4) analisis kebolehlaksanaan, intensiti tenaga dan intensiti bahan, dan 5) analisis ekonomi. Dalam Tahap 1, turus penyulingan sedia ada disimulasikan menggunakan simulator proses Aspen HYSYS untuk mendapatkan penggunaan tenaganya. Dalam Tahap 2, graf kaedah daya pacu yang ditambah baik digunakan untuk menentukan jujukan turus penyulingan yang cekap tenaga, yang juga disimulasi untuk mendapatkan penggunaan tenaga. Kemudian, dengan menggunakan graf yang sama, operasi unit yang sesuai (turus kilat, turus penyulingan biasa, atau turus penyulingan penyarian) untuk jujukan dipilih dan direka bentuk dalam Tahap 3. Jujukan daya pacu pasca reka bentuk ini juga disimulasikan untuk tujuan yang sama seperti dalam Tahap 1. Analisis bermula di Tahap 4 dimana kebolehlaksanaan, dan intensiti tenaga dan intensiti bahan jujukan turus penyulingan yang diperoleh di Tahap 1, 2 dan 3 dibandingkan. Kebolehlaksanaan ditentukan berdasarkan julat nisbah refluks, ketinggian turus penyulingan, dan kualiti produk sementara intensiti tenaga dan bahan berdasarkan indeks jisim, air, dan tenaga. Akhirnya, di Tahap 5, perbandingan ekonomi berdasarkan modal, operasi, dan jumlah kos tahunan digunakan. Rangka kerja ini berjaya diuji pada lima kajian kes yang berbeza dengan objektif yang berbeza untuk menguji dan mengesahkan metodologi yang digunakan dalam rangka kerja tersebut. Penerapan keseluruhan rangka kerja menunjukkan bahawa penjimatan tenaga hingga 32.94 % dapat dicapai sementara beroperasi dalam lingkungan yang boleh dilaksanakan. Intensiti tenaga dan bahan juga dikurangkan sehingga 59.31 % menunjukkan jumlah tenaga dan bahan yang lebih sedikit digunakan oleh jujukan rangka kerja. Modal dan kos operasi juga dikurangkan, masing-masing sebanyak 35.05 % dan 30.88 %, yang membawa kepada jumlah kos tahunan 31.71 % lebih rendah, berbanding dengan jujukan oleh kajian-kajian sebelumnya.

TABLE OF CONTENTS

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Background of the Study

The synthesising of process flowsheets involves creating and identifying feasible alternatives, together with determining and selecting the optimal design variables and operating conditions. The objective of an integrated design approach is to consider aspects such as process synthesis, process design and process feasibility simultaneously. Many aspects need to be considered in choosing the layout of unit operations, and appropriate decisions have to be made during the process synthesis and process design stages (Montastruc *et al.,* 2019). In general, process flowsheets can be divided into three important parts which are reaction system, separation system and integrated mass and energy network. The focus of this study is on the separation system, specifically the distillation column.

Distillation columns are the most common unit operations used in industrial separation systems, despite being energy-intensive (Kiss *et al.*, 2012). They are energy-intensive because distillation processes repeatedly vaporise and condense mixtures to achieve desired separation targets (Bennett, 2014). Because of this, extensive research has been carried out to improve the energy efficiency of distillation columns (Shahruddin *et al.,* 2017). By improving energy efficiency, the economic performance of distillation columns can be improved through the reduction of energy consumption and utility usage.

Another factor that may affect the energy consumption of distillation columns is the number of products. In industrial practices, multicomponent separation systems are very common (Gooty *et al.,* 2018). When designing multicomponent distillation columns, important criteria such as separation sequence, column selection, and column design can affect energy consumption (Zubir *et al.,* 2019). Typically, heuristics are used on existing distillation column sequences to solve problems related to those issues (Leeson *et al.*, 2017). Heuristics are very useful since they do not require any mathematical and computational skills from the user (Leeson *et al.*, 2017). However, this method may be difficult to be applied by fresh process designers since it relies heavily on the user's experience (Vasudevan *et al.*, 2012). Because of this, tasks such as sequencing, selecting, and designing distillation column sequences of the same feed mixture and product quality may produce varying results. Other methods may be used for this case; however, the existing methods are usually only limited to a specific task.

Therefore, an integrated framework that integrates sequencing with selecting and designing distillation columns is necessary to improve the energy efficiency, feasibility, and economics of distillation column sequences. This framework will benefit plant operations as well as contribute to one of the sustainable development goals of the United Nations, which is to achieve sustainable consumption and production by reducing material consumption and promoting energy efficiency.

1.2 Problem Statement

Distillation columns are the most common separation unit used in industries and are responsible for 95 % of the energy in chemical industries (Chaniago *et al.*, 2015). Due to this, continuous research efforts have been carried out to improve the energy efficiency of distillation columns (Shahruddin *et al.*, 2017). These efforts can be divided into three main areas which are the sequencing of distillation columns, the selection of proper types of distillation unit, and the design of the distillation columns.

For multicomponent distillation processes, there many ways to sequence distillation columns. Different sequences lead to different energy consumptions (Thompson and King, 1972). The heuristic method, which is considered as the simplest and earliest method to sequence distillation columns has been developed by many researchers to determine the optimal sequence of distillation columns (Hendry *et al.*, 1973). This method has been widely applied since it does not involve any complex calculation or specific skill (Leeson *et al.*, 2017). According to Turton *et al.* (2012), there are hundreds of heuristics; some are general, and some are specific, with respect to different applications. This method is very useful to process designers, especially when sophisticated computers are not available. However, the output from this method may vary as it depends on the user's experience (Vasudevan *et al.*, 2012). For example, one heuristic states that the component with the largest mole fraction needs to be separated first whilst another states that sequencing should be done in the order of decreasing relative volatility. Experienced users may able to make a decision based on their experience, but it is difficult to be applied by inexperienced users such as fresh process designers, students or researchers related to this area.

Compared to heuristics, the trial-and-error method may be another option, as stated by Peters *et al.* (2003) and Li *et al.* (2009), where the best way to evaluate is by listing all potential separation techniques and carry out several tests. This method might give effective results, but it is very time consuming, especially when the selection of distillation column types in a sequence needs to be considered as well. For example, as shown in Figure 1.1, there are 81 possible separation units and sequence combinations for the separation of five components, with respect to three different types of separation units (flash, ordinary, and extractive distillation columns). This trial-and-error method may not feasible due to the many combinations that need to be individually tested.

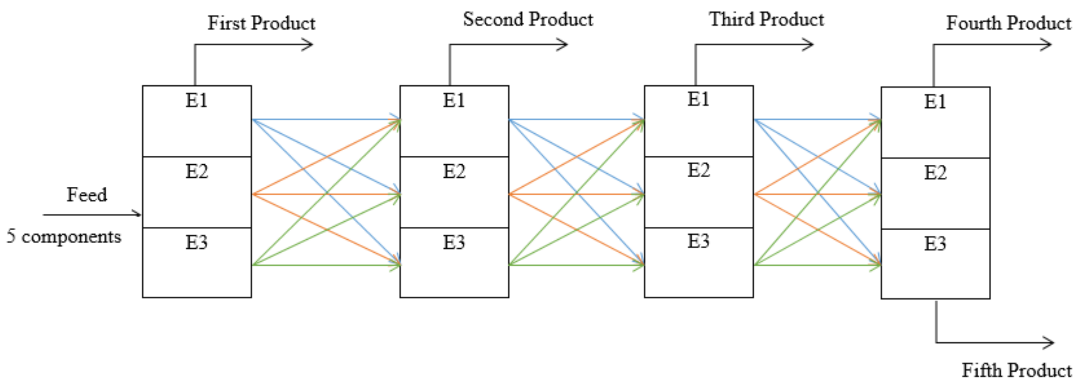

Figure 1.1 A superstructure for the separation of five components using three types of distillation-based operation units, where E1: Flash; E2: Ordinary distillation column; and E3: Extractive distillation column

For the design of individual distillation columns, the McCabe-Thiele method (McCabe and Thiele, 1925) was the first and the most commonly used method for designing distillation columns (Haydary, 2019). The method uses a simple graphical approach to design a binary distillation column before it was later improved by the Fenske-Underwood-Gilliland (FUG) method (Fenske, 1932; Underwood, 1949; Gilliland, 1940), which is also known as the shortcut design method (Masoumi and Kadkhodaie, 2012). The advantage of the shortcut method is that performance screening in terms of the minimum number of stages or minimum energy demand (MED) can be made easily (Skiborowski *et al.*, 2013). However, their design procedures are only for ordinary distillation columns that are used to separate ideal or near-ideal mixtures (Kiss *et al.*, 2012; Górak and Sorensen, 2014).

Compared to the McCabe-Thiele and shortcut methods, the driving force method introduced by Gani and Bek-Pedersen (2000) can be used to design ordinary distillation columns as well as sequence them. The concept of this method is to maximize the 'driving force' when sequencing and designing distillation columns. The 'driving force' can be defined as the difference in composition between vapour and liquid; the higher the driving force, the less energy is required to achieve separation (Bek-Pedersen and Gani, 2004). However, Gani and Bek-Pedersen (2000)'s approach does not take into account the effect of feed composition in synthesising distillation column sequences, which may result in higher energy consumption and operation cost for certain cases, as shown by Zubir *et al.* (2020).

Even though there are other methods to synthesise, select, and design distillation columns, they do not cover those aspects simultaneously as do the heuristic and driving force methods. Despite being commonly used, heuristics are sometimes contradictory, making it difficult for inexperienced users to identify optimum distillation column sequences (Turton *et al.*, 2012). For the driving force method, there is still room for improvement since this method has no guideline for the selection of distillation columns. In addition, the driving force method of Gani and Bek-Pedersen (2000) needs to include the effect of feed composition during the sequencing and designing of distillation column sequences.

In order to solve the problems, an integrated framework for synthesising energy-efficient distillation column (EEDC) sequences based on the driving force method is presented in this study. This framework would close a gap in the driving force method area by integrating sequence synthesis with separation unit selection and individual column design within a single framework, with Aspen HYSYS and Microsoft Excel as tools. The existing driving force method is also improved to include the effect of feed composition when synthesising EEDC sequences. Also, the framework would ease users during the design phase as it is integrated with essential distillation column analyses. In this way, the framework would produce output that is energy efficient, feasible and economical.

1.3 Research Objectives

Based on the problem statement mentioned in the previous section, the main objective of this study is to develop an integrated framework for synthesising energy-efficient distillation column sequences. The sub-objectives that need to be fulfilled as parts of the main objective are:

(a) To improve and apply the driving force concept in locating the optimal design solution with respect to energy consumption during the synthesise of distillation column sequences.

(b) To integrate feasibility, energy intensity, material intensity and economic analyses within the integrated framework.

(c) To validate the improved driving force concept within the integrated framework in improving feasibility, energy intensity, material intensity and economic performance of distillation column sequences through several case studies.

The ‘energy-efficient distillation column sequence’ can be defined as ‘a distillation column sequence that has near-optimal if not optimal energy usage (energy requirement) for a particular separation’. The ‘feasible design’ term used in this study is defined as a column design that can attain the desired purity within feasible design limitations such as the reflux ratio and the number of stages. ‘Energy intensity’ and ‘material intensity’ use some metrics as an indicator of energy consumption and material consumption of distillation columns, respectively. Lastly, ‘economical’ is defined as a design with the lowest total annual cost that is based on capital and operating cost estimations.

1.4 Research Scope

The literature was reviewed to find research gaps. On the sequencing, selection, and design of distillation columns, many methods are available but none, except for the heuristic method, covers all three aspects within a single framework. In this study, a heavier focus is put on the synthesis of conventional distillation column sequences (non-intensified), which covers the determination of energy-efficient sequences, the selection of separation units, and the design of individual columns based on the driving force approach and heuristics. In achieving the intended research objectives, the scope of research has been drawn as follows:

(a) Review state-of-the-art and potential improvements related to non-intensified energy-efficient distillation column (EEDC) sequence synthesis, as well as studies on driving force-related process feasibility, energy intensity, material intensity and economics.

(b) Improve and apply the driving force concept in tasks involved in synthesising EEDC sequences. Specific scopes are:

   i. Improving and applying the concept of driving force in determining the optimal sequence of distillation columns that requires the least energy.

ii. Use a graphical representation of the improved driving force concept to distinguish between the selection of conventional flash columns, ordinary distillation columns, and extractive distillation columns.
iii. Design selected columns using the graph used for the selection.

(c) Develop an integrated framework for synthesising EEDC sequences based on the improved driving force concept. The development includes adding process feasibility, material and energy intensity, and economic analyses to the established EEDC sequence methodology. Specific scopes include:

i. Use commercial process simulators such as Aspen HYSYS V10 to simulate distillation column sequences and analyse their energy consumption.
ii. Apply Microsoft Excel-based analyses such as feasibility analysis, energy intensity analysis, material intensity analysis and economic analysis on analysed sequences.
iii. Extend the established EEDC sequence methodology by considering process feasibility analysis.
iv. Extend the established EEDC sequence methodology by considering energy intensity and material intensity analyses.
v. Extend the established EEDC sequence methodology by considering simple economic analysis.

(d) Verify the capability of the framework by conducting feasibility, energy intensity, material intensity, and economic analyses on various case studies. Specific scopes include:

i. Analyse the feasibility criterion, which involves distillation column height, optimum reflux ratio range and product purity.
ii. Analyse the energy and material criteria, which involve energy intensity and material intensity analyses.
iii. Analyse the economic performance, which involves capital cost, operating cost, and total annual cost.

1.5 Significance of the Study

The integrated framework developed in this study will benefit industrial and research communities as it addresses several vital gaps regarding the synthesising of distillation column sequences. The use of the improved driving force method in the framework would help users able sequence, select and design distillation columns through simple graphical representation. The resulting sequence will be feasible, energy-efficient and less expensive than sequences obtained from existing methods. The key contributions of this study are listed as follows:

(a) An integrated framework

The integrated framework for synthesising feasible and economical EEDC sequences developed in this research is applicable to ideal and non-ideal mixtures' separation problems, which is a substantial improvement. The framework would fill some of the gaps regarding the synthesising of distillation column sequences as separation sequencing, separation unit selection and individual column design are integrated into a single framework. Sequences synthesised using the framework are ensured to be feasible, energy and material efficient, and economical as the relevant analyses are integrated into the framework. The framework gives straightforward solutions, and the step-by-step process to obtain the solutions is shown in detail.

(b) Determination of the optimal solution

The improvement and application of the driving force concept in this study would provide valuable insights in determining the optimal solution to the feasible and economical EEDC sequence problem. The improvement made on the driving force method would further improve the potential for energy saving without sacrificing the separation specification target by considering the feed mixture condition during the synthesising of the distillation column sequence. The use of the graphical driving force concept would help users, especially fresh process designers, students or researchers in this area understand a manual but systematic (sequential) way of synthesising EEDC sequence.

(c) Commercialization value of research output

The developed integrated framework, which is also a step-by-step algorithm, can be packaged into a commercial tool that specializes in solving various EEDC sequence synthesis problems. The addition of the step-by-step algorithm into a commercial process simulator would allow large volumes of data to be quickly processed and would help in finding the integration of design decisions for multi-objective problems. The non-trial-and-error approach of the framework will allow easy decision making without further rigorous analyses.

1.6 Thesis Organization

The overall content of this thesis can be divided into five chapters:

Chapter 1 begins with the background of the study, followed by the problem statement, research objectives, research scopes, and the significance of this study. Chapter 2 discusses the state-of-the-art developments and technologies related to energy-efficient distillation column sequence synthesis, selection and design, as well as process feasibility, energy intensity, material intensity and economics. Chapter 3 shows the integrated framework for the synthesis of EEDC sequences with the integration of column sequencing, selection, and design. Analyses on process feasibility, energy intensity, material intensity, and economics are also integrated. Chapter 4 discusses the results obtained from the application of the integrated framework of various case studies. Lastly, Chapter 5 concludes the research and proposes several ideas that can be worked on in the future to improve the framework.

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