

ROBUST AND OPTIMAL ENERGY-EFFICIENT DISTILLATION COLUMNS
SEQUENCE

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ABSTRACT

This thesis presents an integrated and simultaneous solution framework for obtaining a robust energy-efficient distillation columns sequence. Several methods for robust energy-efficient distillation columns sequence synthesis have been developed. The aim was to provide a distillation column sequence design with a reasonable energy consumption when exposed to disturbances. However, the capability of a robust energy-efficient distillation columns sequence in maintaining its energy changes at a minimum with respect to feed conditions has not been analyzed. As a result, the operability of a designed energy-efficient distillation columns sequence may be questionable. There is a clear need to develop a new integrated and simultaneous solution framework for designing a robust energy-efficient distillation columns sequence. Therefore, the objective of this study was to develop a new integrated and simultaneous solution framework for an energy-efficient distillation columns sequence by considering process sensitivity and economic analyses. In Stage 1, an existing sequence was simulated using Aspen HYSYS process simulator to obtain design variables. In Stage 2, the design of the distillation column sequence was considered through rigorous design at different design variables. In Stage 3, the process sensitivity of each design was analyzed and compared, where the feed conditions and reflux ratios were changed for each design, which represented different column designs. The economic and robustness analyses for the sequence were performed in Stage 4. The capability of the proposed methodology was tested using a case study to obtain a robust energy-efficient distillation columns sequence. A maximum energy saving of separation was obtained with return of investment and payback period about 796 % and 0.13 year respectively. All of these findings proved that the proposed framework is capable of solving problems in the energy-efficient distillation columns sequence for obtaining a robust energy-efficient distillation columns sequence in an easy, efficient, and systematic manner.

ABSTRAK

Tesis ini membentangkan penyelesaian kerangka yang bersepadu dan serentak untuk mendapatkan jujukan turus penyulingan yang cekap tenaga dan mantap. Beberapa kaedah sintesis telah dibangunkan untuk mendapatkan jujukan turus penyulingan yang cekap tenaga. Tujuannya adalah untuk memastikan jujukan turus penyulingan dengan penggunaan tenaga yang berpatutan apabila didedahkan dengan perubahan. Walau bagaimanapun, keupayaan jujukan turus penyulingan yang cekap tenaga untuk mengekalkan perubahan tenaga terhadap keadaan masukan masih belum dianalisis. Akibatnya, operasi reka bentuk jujukan turus penyulingan yang cekap tenaga boleh dipersoalkan. Oleh itu, penyelesaian kerangka yang bersepadu dan serentak adalah satu keperluan untuk dibangunkan bagi mendapatkan jujukan turus penyulingan yang cekap tenaga dan mantap. Objektif kajian ini adalah untuk membangunkan kerangka baharu yang bersepadu dan serentak untuk jujukan turus penyulingan yang cekap tenaga dan mantap dengan mengambil kira analisis kepekaan dan ekonomi. Pada Peringkat 1, turus penyulingan sedia ada disimulasikan menggunakan perisian simulasi proses Aspen HYSYS untuk mendapatkan pemboleh ubah reka bentuk. Pada Peringkat 2, jujukan turus penyulingan direka bentuk melalui cara pengubahsuaian pada pemboleh ubah reka bentuk yang berlainan. Seterusnya, Peringkat 3 menganalisis dan membandingkan kepekaan proses untuk setiap reka bentuk yang berbeza keadaan masukan dan nisbah refluks yang mewakili reka bentuk turus penyulingan yang berbeza. Kemudian, analisis kepekaan dan ekonomi untuk setiap reka bentuk jujukan turus penyulingan ditentukan pada Peringkat 4. Keupayaan kaedah yang dicadangkan telah diuji menggunakan kajian kes untuk mendapatkan jujukan turus penyulingan yang cekap tenaga dan mantap. Keputusan kajian penjimatan tenaga maksimum telah diperolehi dengan pulangan pelaburan dan tempoh bayar balik sebanyak 796 % dan 0.13 tahun. Kesemua penemuan ini menunjukkan kerangka yang dicadangkan mampu menyelesaikan masalah jujukan turus penyulingan untuk mendapatkan jujukan turus penyulingan yang cekap tenaga dan mantap dengan cara mudah, berkesan, dan sistematik.

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LIST OF ABBREVIATIONS

CC	-	Conventional Column
EEDCs	-	Energy-efficient Distillation Columns
MILP	-	Mixed-Integer Linear Programming
MIMO	-	Multi-input-multi-output
MW	-	Megawatts
RGA	-	Relative Gain Array
VLE	-	Vapour Liquid Equilibrium
VRP	-	Vapour Recompression System

LIST OF SYMBOLS

α_{ij}	-	Relative separability for component i with respect to property
D_x	-	Largest driving force
F_{ij}	-	Driving force for component i with respect to property j
N_F	-	Feed stage
N_s	-	Number of sequences
P	-	Pressure
RR_{\min}	-	Minimum Reflux Ratio
RR_{act}	-	Actual Reflux Ratio
T	-	Temperature
X_D	-	Desired purity of top composition
X_{Fi}	-	Feed mole fraction of the light component
x_i	-	Liquid phase composition
y_i	-	Vapour phase composition

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CHAPTER 1

INTRODUCTION

1.1 Background of the Study

Distillation is the most widely applied separation technology and continues as an important process for the foreseeable future in many process industries, including chemical, petrochemical, biochemical, and bioenergy among others. As reported by several researchers, distillation units have the highest energy consumption among other units in refineries (Kiss, 2013; Jiang & Agrawal, 2019) as distillation remains the most used separation method at an industrial scale. For example, almost 10% of the industrial energy consumption in the United States of America is from distillation columns (Jana, 2017).

With the recent strong upward trend in the cost of energy, there is considerable renewed interest in determining energy-efficient distillation column (EEDC) designs and multiple distillation column configurations. The price of energy has varied dramatically over the last few decades. This is a motivation for process plant designers to devise energy-saving strategies in the distillation column system design for satisfying a specific separation task.

Three main problems of conventional distillation columns are large size, high energy consumption, and high operating costs (Rix et al., 2019). Nowadays, some energy-saving technologies have been proposed to reduce the energy consumption of distillation processes based on process intensification, such as dividing wall columns, thermal coupling of columns, heat-integrated distillation columns, and heat pump-assisted distillation columns. This modification of distillation columns has the potential for a significant reduction of energy consumption.

The dividing wall column (DWC), for example, is one of the most appealing options to improve the existing distillation processes because it can help in enhancing thermal efficiency (Aurangzeb & Jana, 2016). It was reported that 25%–30% of energy saving could be achieved by implementing DWC (Kiss & Smith, 2020; Minh et al., 2015). The DWC technology can also be effectively combined with reactive distillation (Weinfeld et al., 2018) or heat pumping for improving energy saving up to 60% (Long & Lee, 2015).

Besides designing new distillation column configurations, an alternative and safe approach is to use the existing configuration and operate the plant more efficiently, possibly with some minor modifications. Several methodologies for designing energy-efficient separation processes have been proposed by researchers. The methodology for an EEDC sequence, which is based on the driving force method, was developed by Mustafa and co-workers. This methodology can increase energy saving for a distillation column sequence in an easy, systematic, and efficient way. They found that 16% energy saving could be achieved using the driving force method compared to the existing direct sequence for the alcohol separation process (Mustafa et al., 2014). Numerous studies have also concluded that energy consumption can be successfully reduced by changing the existing direct sequence into an energy-efficient sequence suggested by the driving force method. For instance, the EEDC separation was proposed by Zaine et al. (2015) for the multi-component aromatic mixture. The approach resulted in a 7% reduction in terms of energy consumption compared to the existing distillation column sequence. Meanwhile, further investigation on the EEDC sequence was conducted for azeotropic separation (Zubir et al., 2017). Their study showed that the operational cost was successfully reduced up to 7.61% with similar product purity.

Although several studies on the EEDC sequence have been successfully reported to save more energy consumption on a distillation column sequence, there are still less integrated, systematic, and simultaneous guides for finding the optimal solution for EEDC sequence problems that consider the criteria for process design and process operation (e.g., process sensitivity and process economics) simultaneously.

There is a clear need to develop a new integrated and simultaneous framework for designing a robust and optimal EEDC sequence.

In this study, the integrated approach is defined as finding the optimum interaction solutions between the energy consumption for the EEDC sequence and the process sensitivity simultaneously rather than separately. Meanwhile, the simultaneous approach is defined as both solutions for minimum energy consumption and process sensitivity can be obtained at a single point. The integrated and simultaneous approach in this study emphasizes the simultaneous solution to the problem of obtaining minimum process sensitivity with respect to energy changes and minimum energy consumption for a distillation column sequence. This simultaneous and integrated solution can be obtained at the maximum point of the driving force curve. At the maximum point of the driving force curve, multi-component distillation column separation has less energy consumption and also shows less energy changes when disturbance appears in the distillation column sequence.

1.2 Problem Statement

A distillation column is an important equipment in the process separation system and it plays a key role in the chemical processing industry. When more than two components are involved, a sequence of distillation columns is used for fractionating and producing eligible individual chemical products, such as hydrocarbons. Due to the combinatorial nature of synthesizing a distillation column sequence, the problem becomes more complex and the solution to synthesize an optimal distillation column sequence is hard to obtain when the number of components involved in the separation process increases. This phenomenon is directly shown in the equation to determine the number of different sequences (NS) of conventional distillation columns to separate final products (P) with the desired purity (Kao, 1995). Equation 1.1 is used to obtain some insights on the number of sequences for a conventional distillation column sequence.

$$N_s = \frac{[2(P - 1)]!}{P!(P - 1)!} \quad (1.1)$$

From Equation 1.1, the number of different sequences increases rapidly as the number of products increases gradually. It will be easier to find a possible number of sequences when there are only three products. The feed to the second column can be either the overhead or the bottoms from the first column. Therefore, there are only two possible sequences and the energy required for these two possible sequences can be easily analyzed. However, if the sequence has eleven products, the number of possible sequences should be around 16,796 sequences. In this case, lots of effort, time, and cost are required to analyze the energy consumption of every possible sequence. Therefore, finding an optimal solution in terms of selecting a possible sequence with the lowest energy consumption becomes complicated and tedious.

It should be noted that the number of possible sequences increases rapidly with an increasing number of components in the original feed. In addition, among those thousand possible sequences, there is a need to select one of the best sequences that uses minimum energy in an easy, efficient, and systematic way. Due to that, Mustafa et al. (2014) proposed a new systematic methodology that can design the existing direct sequence of distillation columns with minimum energy requirement in an easy, systematic, and efficient way without requiring any major modification to the existing sequence. Numerous studies have attempted to explore the application of the driving force method on the EEDC sequence that involved a number of components, for example, six components of aromatics separation process (Zaine et al., 2015a) with 7% energy saving and eleven components of hydrocarbon separation process (Zaine et al., 2015b) with 5% energy saving. However, the capability of the developed methodology is only limited in selecting a sequence with less energy consumption. Moreover, the capability of the EEDC sequence in rejecting the effect of disturbance (process sensitivity with respect to disturbance) or maintaining its energy changes at a minimum with respect to the disturbance (robustness) is still not thoroughly analyzed.

In recent years, several researchers have studied the effect of disturbances on the product qualities of distillation columns. According to Hamid et al. (2010), a distillation column designed at the maximum point of the driving force resulted in a

design with lower energy requirement and better performance in maintaining its product purities than any other points in the presence of disturbances. The finding by Hamid et al. (2010) is supported by Nordin et al. (2014), where they performed a controllability analysis for a single distillation column. They discovered that at point A (i.e., the maximum point at the driving force curve), the derivative value of the controlled variable (i.e., top and bottom product purities) with respect to disturbances is at a minimum. However, previous researchers only concentrated on the process sensitivity in terms of product purities with respect to disturbance changes for only a single distillation column design.

Technically, the separation process in a chemical plant consists of multi-components that require several distillation columns. In this study, it is important to analyze the process sensitivity of the designed EEDC so that the designed distillation column sequence is energy-efficient (requires less energy) and also robust in maintaining its less energy requirement in the presence of disturbances. It should be noted that finding an optimal solution in terms of selecting a possible sequence with the lowest energy consumption becomes complicated and tedious when the number of components is higher. In addition, it is also important to find the optimal solution for the robust EEDC. Combining the complexity and complicated EEDC problem together with the process sensitivity to identify robust EEDCs adds more weight to the existing problem.

From the process optimization point of view, adding process sensitivity analyses to the complex and complicated EEDC design causes a higher degree of non-linearity to the existing problem, which also increases the degree of difficulty of that problem. Therefore, another problem also needs to be importantly considered in this study, which is the capability of the solution framework to obtain a simultaneous optimal solution for a robust EEDC problem in an easy and systematic manner.

Therefore, it is important to design a robust EEDC sequence to ensure that the distillation column sequence design is energy-efficient and robust to meet its product specifications and maintain its energy-efficient performance in the presence of process disturbances at the early process design stage. It should also be noted that finding the

best solution to this robust EEDC sequence problem is not an easy and straightforward task. Therefore, there is an important need to synthesize and design a robust EEDC sequence in this study to develop an integrated and simultaneous solution framework. The problem statement of this study is summarized as follows:

Given a task involving a mixture of components that needs to be individually separated with desired product purities, it is desired to synthesize and design a robust and optimal EEDC sequence. In addition, it is also desired to systematically use the concept of the driving force method to synthesize and design a robust and optimal EEDC sequence.

1.3 Research Objective

Based on the above-mentioned problem statement, the main objective of this study is to develop a new solution framework for the EEDC sequence by considering the process sensitivity analyses in designing a robust and optimal EEDC sequence for maintaining energy changes when disturbances appear in the system in an easy, efficient, and systematic way.

In achieving the main objective, some specific objectives that need to be fulfilled have been planned, which are:

- (a) To design a robust and optimal energy-efficient distillation columns sequence.
- (b) To develop a new solution framework to evaluate the capability of the driving force distillation columns design concept in determining the optimal solution to the robust energy-efficient distillation columns sequence synthesis problem.
- (c) To verify the capability of the newly developed solution framework in solving robust and optimal energy-efficient distillation columns sequence problem.

1.4 Research Scope

To achieve the intended research objectives, the scope of research has been drawn as followed:

- (a) Studying the state-of-the-art development and technologies related to energy-efficient distillation columns (EEDCs) sequence synthesis, design, sensitivity, and identify gaps and potential improvement for EEDCs sequence design and process sensitivity analyses.
- (b) Developing a new solution framework for designing a robust and optimal EEDCs sequence. The development includes the inclusion of the process sensitivity analyses to the established EEDCs sequence methodology. Specific scopes include:
 - (i) Using a commercial process simulator (ASPEN HYSYS V9) to simulate the distillation columns sequence and analyze the energy requirement for each analyzed sequence.
 - (ii) Extending the established EEDCs sequence methodology by considering the different points at the driving force curves.
 - (iii) Extending the established EEDCs sequence by including process sensitivity analyses by modifying column process design values such as reflux ratio and feed stage location for improving further the potential of energy saving.
- (c) Evaluating the capability of the driving force distillation column design concept in determining the optimal solution to the robust EEDCs sequence synthesis problem. Specific scopes are:
 - (i) Using a commercial process simulator (ASPEN HYSYS V9) to simulate the distillation columns sequence and analyze the energy requirement for each analyzed sequence.

- (ii) Evaluating the capability of driving force concept for distillation column design in determining the optimal distillation column sequence which requires less energy for process sensitivity analyses.
- (d) Verifying the capability of the newly developed solution framework in solving the robust and optimal EEDCs sequence problem from different points on the driving force curves. To define the best parameter estimate.

1.5 Research Contributions

Through the work conducted in this study, several key contributions can be identified as follows:

- (a) A new integrated and simultaneous solution framework

A new integrated and simultaneous solution framework for designing a robust and optimal EEDC sequence developed in this study addresses the driving force approach for analyzing the EEDC sequence at different points of driving force curves. The inclusion of this approach in the framework leads to a more systematic and simultaneous EEDC sequence analysis. In addition, the solution framework also includes process sensitivity analyses for further improving the potential of energy saving of the EEDC sequence. The availability of systematic and simultaneous EEDC sequence analysis with process sensitivity analyses can provide an integrated and simultaneous framework for synthesizing and designing a robust and optimal EEDC sequence.

- (b) Determination of the optimal solution

The evaluation of the driving force concept in this study is able to provide users, such as process systems engineers or process plant managers, with valuable insights in determining the optimal solution to the robust EEDC

sequence problem. The use of the driving force graphical concept helps users in understanding how to synthesize and design the robust EEDC sequence in a manual but systematic manner. In addition, evaluating the capability of the driving force concept for distillation column design provides useful and informatics guidelines to users in identifying and modifying distillation columns for further improving the potential of energy saving using process sensitivity analyses.

(c) Commercialization value of research output

The developed framework, which is also a step-by-step algorithm, can be packaged into a commercial tool specialized in solving various robust and optimal EEDC sequence synthesis and design problems. The inclusiveness of the step-by-step algorithm into a commercial process simulator allows a large volume of data to be processed in a short time and helps to find the integration of the design decision for the multi-objective problem. This allows the design decision to be made easily and systematically without using rigorous analyses. This integrated analysis tool can help process systems engineers or process plant managers, as well as students and researchers in this area.

Several publications have been successfully produced from this study as a part of the intellectual contributions. The lists of publications and achievements that have been accomplished during the study period and the key contribution of the knowledge can be referred in the List of Publications.

1.6 Thesis Organization

This thesis comprises five chapters. Chapter 1 is the research introduction, highlighting the background of the study, problem statement, research objectives, scope, and contributions. Chapter 2 is the literature review where the state-of-the-art development and technologies related to EEDCs sequence synthesis and design are presented. In the same chapter, previous studies on the process sensitivity analyses

mainly for EEDCs design are also reviewed and analyzed to identify gaps and potential improvement for EEDCs sequence design and analyses. Chapter 3 describes the step-by-step of the new integrated and simultaneous solution framework for designing robust and optimal EEDCs sequence. The research findings, including case studies are reported in Chapter 4. Last but not least, Chapter 5 concludes all the research output from this study and recommends possible future work to be explored.

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LIST OF PUBLICATIONS

SCOPUS Indexed Publications

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