Faculty of Engineering and Science

Modelling and Optimization of Dividing-Wall Column: Stage-by-Stage Calculation Approach

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DECLARATION

To the best of my knowledge and belief, this thesis contains no material previously published by any other person except where due acknowledgement has been made.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any university.

Signature : _____

(TIONG CHING CHING)

Date : 31st August 2017

“Don’t think for one moment that your daydreams are beyond your power of accomplishment.”

Dr. Forest C. Shaklee

ABSTRACT

The dividing-wall column (DWC) has recently emerged as one of the very promising technologies in multi-component distillation processes. The DWC distillation has an advantage over the traditional series multi-column distillation (SMCD) technique in terms of its reduced capital and operating costs. Compared with the traditional SMCD technique, the installation cost for DWC is relatively small as it combines two conventional columns in series into a single column. However, the design and operation of a DWC are more complex than that of the traditional SMCD because the DWC involves a higher number of degrees of freedom. Although several academic groups have researched the design of DWC, most of the studies have been conducted based on a short-cut design approach. One major problem with the use of the short-cut design approach is that it can lead to an unrealistic oversimplification due to several assumptions made in the design, such as the approximation of a DWC by several conventional columns and constant relative volatilities. Such an oversimplification using multi-column approximation can reduce the accuracy of the model developed. Consequently, the design solution obtained based on the approximation may deviate far away from the real DWC situation. Thus, a more rigorous, stage-by-stage distillation model has been introduced in the design of DWC to give better predictions on the distribution of components and to obtain more realistic design outputs.

So far, most of the rigorous design procedures for the DWC have been performed via the use of rating methods which often requires a high number of degrees of freedom to initialize the design. Therefore, the rigorous design procedures have to be applied in conjunction with the short-cut or semi-rigorous methods. It is important to note that, one of the key challenges to applying the stage-by-stage model in the DWC design is the slow convergence at some selected locations, such as at the feed and side-stream trays. Another challenge is to integrate the process design of DWC with the internal column design in a single optimization framework. The current PhD study aims to address the aforementioned challenges in the design of DWC process. In this study, the stage-by-stage model calculation is performed on a whole DWC column without any need for approximating it by several columns. Matlab

programmes are written to perform all calculations involved. The case study considered in this work is limited to the hydrocarbon feed system.

One main contribution of this study is the development of two novel design algorithms to solve the dividing-wall column (DWC) stage-by-stage model. With the aid of these new algorithms, the design of DWC can be carried out independently without the requirement of input from the short-cut or semi-rigorous models as well as simulating of the rigorous model for rigorous study of the column. The first new design algorithm is proposed based on the Lewis-Matheson (LM) approach. This approach manages to reduce the design variables and improve the speed of convergence at the interlinking stages via modified theta method. To overcome the tedious and ad-hoc trial-and-error procedures commonly used to achieve convergence of solutions at selected locations, e.g., feed and side-stream trays, the second new design algorithm is proposed by introducing two tuning parameters to speed up the convergence rate. Another main contribution of the present work is the establishment of an optimization methodology combining both process and mechanical design aspects of DWC. The type of column used in this work is limited to tray column. The proposed methodology which adopts the aforementioned algorithm is able to address major physical constraints due to flooding and weeping phenomena in the entire DWC design. In the present study, total annualized cost (TAC) is adopted as the economic performance criterion in the optimization.

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LIST OF PUBLICATIONS

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ABBREVIATIONS

B	Bottom Product Stream
BTX	Benzene-toluene-xylene mixture
CAP	Capital Cost
CMO	Constant Molar Overflow
D	Distillate Stream
DWC	Dividing-Wall Column
F	Feed Stream
FTCDS	Fully Thermally Coupled Distillation System
HK	Heavy Key Component
LK	Light Key Component
LM	Lewis-Matheson Method
MK	Middle Key Component
OP	Operating Line
OPC	Operating Cost
PR	Peng-Robinson Equation of State
S	Side Stream
TAC	Total Annualized Cost
TCDS	Thermally Coupled Distillation System
VLE	Vapour-Liquid Equilibrium

CHAPTER 1: INTRODUCTION

This introductory chapter provides the motivation for the research study as well as an overview of the distillation. The chapter starts with the background of the distillation, which gives a look into the history of distillation and the major problems related to the applications of the distillation columns in the industries. Besides that, this section also describes the development of the distillation column with a focus on the multiple column case. Due to the low thermodynamic efficiency in the conventional distillation, several improved options proposed for the single column case and complex distillation arrangements are presented. This chapter also includes the problem statement, research objectives, research scope and the outline of the thesis.

1.1. Distillation Background

After several decades, the distillation process is still the most widely used separation and purification technology in chemical and allied industries. The art of distillation process dates back to at least the first century A.D. (Forbes, 1970). The separation principle of a distillation operation is based on the difference in the relative volatilities of the components involved in the given feed mixtures. To make a distillation process works, a significant amount of heat must be applied and removed to achieve the desired purity (Kiss, 2014). Unlike other separation methods, such as membrane separation and extraction, the distillation process in general can be considered as a very matured technology, which can provide high separation volume and purity, low capital investment, low operational risk and flexible in operation.

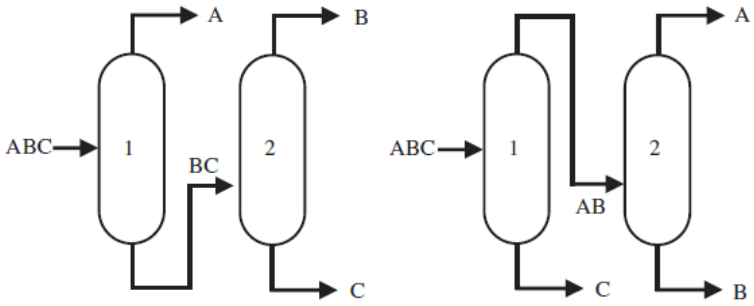
In the eleventh century A.D., the art of distillation was typically carried out batchwise using just a single stage in the production of alcoholic beverages in Italy (Forbes, 1970). Over the centuries, distillation has been applied commercially in sectors such as food and drink, paper and board, textiles, chemicals and crude oil. Recently, distillation has become extremely important in the global energy supply system and has undergone enormous development because of the petrochemical industry (Harmsen, 2010). Humphrey (1995) estimated that in the United States

alone, there are 40,000 distillation columns in operation that handle more than 90% of the separations and purifications.

Although distillation is the primary separation process used in the chemical processing industries today, its significant energy requirement is a major drawback (Schultz et al., 2002). In fact, distillation accounts for an estimated 3% of the total world energy consumption (Hewitt et al., 1999; Masoumi & Kadkhodaie, 2012) and uses up more than 50% of the plant operating cost (Kiss & Bildea, 2011). This large energy consumption is caused by the evaporation steps involved as over half of the process heat distributed to a plant is supplied to the reboilers of distillation columns (Kunesh et al., 1995). Moreover, distillation is also one of the most capital intensive process technologies because it utilizes the largest scale equipment (Dejanović et al., 2010).

The rising energy cost due to the oil crisis in the 1970s and 1980s, and stricter environmental regulations on fossil fuel use, have led to studies of new and efficient separation methods to reduce the significant operating costs and capital expenditures while increasing the production capacity (Malinen & Tanskanen, 2009; Ognisty, 2000; Olujić et al., 2009). A number of alternative approaches have been proposed to reduce the columns' energy consumption: for examples, application of other energy sources (e.g. solar energy), membrane distillation, HiGee distillation, cyclic distillation, heat pump technologies and configurations, process and column energy integration, and the design of new configurations (Christiansen et al., 1997; Kiss, 2014; Kiss et al., 2012; Linnhoff et al., 1983).

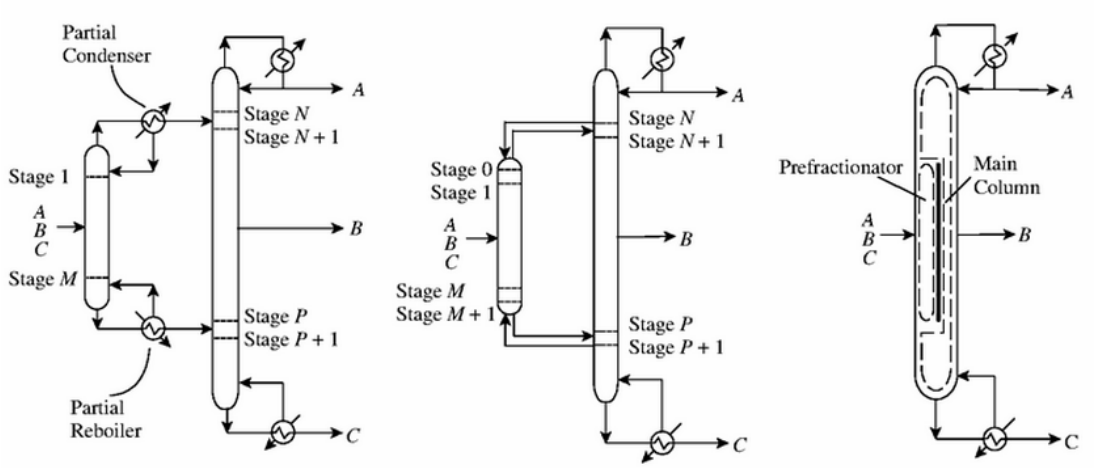
For the separation of multi-component mixtures, a sequence of distillation columns is frequently used. At least two columns are required for ternary separations. The well-known conventional arrangements for the separation of a three-component mixture are direct and indirect sequences, as shown in Fig. 1.1 (Yildirim et al., 2011). In every column, there is a reboiler and a condenser with the same number of product flows. The sequence illustrated in Fig. 1.1a is known as the direct sequence, in which the lightest component is separated as the overhead product in each column. Meanwhile, the indirect sequence shown in Fig. 1.1b separates the heaviest component as the bottom product in each column. These conventional columns often



(a) (b)

Figure 1.1 Direct (a) and indirect (b) sequence for separating a three-component mixture (ABC: A: light boiling component, B: middle boiling component, C: heavy boiling component)

(Yildirim et al., 2011)



(a) (b) (c)

Figure 1.2 (a) Prefractionator arrangement; (b) Fully thermally coupled distillation system (FTCDS) or Petlyuk column; (c) Dividing wall column (DWC)

(R. Smith, 2005)

require simple control and operation systems. However, they suffer from low energy efficiency because of the remixing effects by irreversible split (Asprion & Kaibel, 2010).

In order to reduce the energy consumption for the conventional distillation column arrangements, a non-conventional distillation column is proposed. The three well-known non-conventional distillation columns are: (1) prefractionator arrangement, (2) fully thermally coupled distillation systems (FTCDS) or Petlyuk column, and (3)

dividing wall column (DWC). The prefractionator arrangement is a three product system with two columns, a prefractionator and main column as shown in Fig. 1.2a. The prefractionator has its own condenser (partial) and reboiler, connected to the main column. Petlyuk column, as shown in Fig. 1.2b is an advanced form of prefractionator arrangement, where the prefractionator condenser and reboiler are replaced by extra plates. Owing to further development of the Petlyuk column, the DWC is introduced by integrating two distillation columns of a configuration into a single column shell. The configuration of the DWC is shown in Fig. 1.2c. This arrangement is thermodynamically equivalent to the Petlyuk column but is usually much cheaper (lower capital cost) due to the need for only a single column shell.

1.2. Problem Statement

Even though theoretical studies have shown the economic advantages of DWC, the widespread application of DWC in the industries is hindered by lack of reliable design methods and difficult controllability. The complexity in the design of the DWC is caused by the presence of a higher number of degrees of freedom than that in the conventional column. Several academic groups have researched this area in recent years. However, most of the studies are conducted based on a short-cut design approach (Dejanović et al., 2010; Yildirim et al., 2011). The main drawback of this design is the use of assumptions in the design, especially the assumption of constant relative volatility, which is often calculated at feed condition. These assumptions will lead to an unrealistic oversimplification and thus reducing the accuracy of the model developed.

Hence, a more rigorous distillation model has to be considered to give better predictions of the distribution of the components. Although some works based on the semi-rigorous model have been reported for the design of the DWC (Amminudin et al., 2001; Kim, 2005b; Kim et al., 2004), their proposed models are mainly developed with the purpose to obtain the structural variables, which are subsequently used to initialize the rigorous simulation model in the existing process simulator, such as Aspen HYSYS. Several conditions such as exact matching of the compositions at the connecting trays are not considered in their works.

Therefore, in this work, a new semi-rigorous design procedure is developed based on the stage-by-stage design approach as the foundation of the rigorous model for the DWC, so that the design and optimization of the DWC can be carried out directly without preliminary estimation of structural variables. Moreover, the procedure for the equipment design of the DWC considering the hydraulic design issue is also considered in this work to provide more practical and realistic design solutions. In developing the optimization model for a DWC, it is crucial to address the following questions:

- How to incorporate various models into the mathematical optimization representing the DWC?
- What is the cost function for the DWC?
- What are the constraints and decision variables for the optimization of DWC? How are they related to each other?

1.3. Research Objectives

The main aim of this study is to explore and unify the major phases involved in a complete procedure for the design of a dividing-wall column (DWC). These phases are process design, equipment design, and optimization. In this study, a practical approach based on the fundamental stage-by-stage distillation model will be developed, taking into account the technical and economic aspects, to achieve optimal design of a DWC.

The specific objectives required in order to achieve this main aim are as follows:

- To evaluate the process design options for the conventional distillation column and the complex column arrangements.
- To develop novel algorithms to solve the dividing-wall column (DWC) design based on a stage-by-stage model.
- To propose and outline the procedural steps for the mechanical design of the DWC (tray column) with hydraulic tests.

- To formulate the optimization problem and perform optimization on the DWC based on the proposed new design models.
- To demonstrate the applicability of the new design concept of the DWC in replacing existing conventional natural gas liquid (NGL) fractionation units in an industrial-scale gas plant.

1.4. Novelty, Contributions and Significances

In this dissertation, the novelty of the research study can be viewed in three phases of DWC design:

- Process design phase

  In process design phase, two novel design algorithms for DWC are developed based on stage-by-stage design approach. The first algorithm is proposed with the feature of reduced design parameters, whereas the second algorithm is developed with the feature of improved convergence rate in solving the DWC model.

- Equipment design phase

  A new and more detailed methodology for column sizing of DWC is developed considering tray hydraulics.

- Optimization phase

  For the optimization phase of DWC design, an optimization methodology combining both process design and equipment design which satisfies the hydraulic conditions of the column is established.

The research contributions toward the design and optimization of the DWC are as follows:

- The first main contribution by the novel process design algorithms proposed is to allow rigorous design of DWC to be executed independently without the requirement of applying the short-cut or semi-rigorous models;

conventionally, short-cut or semi-rigorous model is used in conjunction with the rigorous model to obtain more accurate design and study of the column.

- Through the new design algorithm developed based on the Lewis-Matheson (LM) approach (Chapter 6), the degrees of freedom required in the existing rigorous models (rating methods) of DWC design can be reduced. Besides that, the accuracy of feed stage composition matching and speed of convergence at the interlinking stages can also be improved by incorporating the feed stage composition ratio to the existing equations of theta method.

- The third contribution can be achieved via another newly developed stage-by-stage design algorithm which is covered in Chapter 7. In this new algorithm, the tedious and ad-hoc trial-and-error procedures often used to solve the model, which converges at selected locations, e.g., feed and side-stream trays, can be eliminated as the computation is started at the feed and side-stream trays. The convergence rate of the DWC model can be increased through two newly assigned tuning parameters.

- The fourth contribution is to provide a systematic procedure for the equipment design of DWC considering the tray hydraulics (sieve tray) since limited works have been published regarding this matter. Improvement has been made in determining the location of the dividing wall by using the fractional area as the main adjustable variable instead of several parameters (tray specifications) as suggested by Rodr ́guez-Ángeles et al. (2015).

- Another main contribution of the present work is the establishment of an optimization methodology combining both process and equipment designs of DWC will ensure the feasibility of the results obtained.

This research is significant for the following reasons:

- In this research, different design options for the conventional and non-conventional distillation arrangements for the separation of multi-component mixtures will be explored, with a detailed analysis of the DWC. This research gives a better knowledge of the pros and cons of the design methods (process design and equipment design).

- This study proposes new process design algorithms to simplify the existing two-step design procedure and design tasks of the DWC. Reduced degrees of freedom and improved convergence speed of the design algorithms will save the computation time and allow the optimization of the DWC to be carried out at ease. This is important as advances in the theory of design of the DWC will lead to commercial exploitation and its application will become more common in plants in the future.
- This research presents a complete procedure for the design of DWC which consists of three major phases: process design, equipment design and optimization. This complete procedure can give an overview of the methodologies required to perform a practical design of DWC and the relationships among the design phases in the computation of the total annualized cost (TAC) for economic analysis. This is crucial because the lack of a proven and straightforward design methodology has been the major cause for the slow acceptance of the DWC by process industry.
- This research proposes a more practical design and optimization procedure to achieve optimal design of the DWC for industrial applications. By considering the hydraulic conditions, the feasibility and reliability of the design can be achieved and this will increase the implementation of the DWC in process industries.

1.5. Research Scope

The scope of this research project covers the multi-component distillation in a continuous, steady-state process. The type of DWC considered in this work is limited to ternary separation and DWC with middle diving wall – the main focus is on the development of procedures to complete the system design. The development of the new algorithm for the DWC using the single column as the basic model, involves not only the process design model but also considering the hydraulic design (tray column). The model developed is applicable to many types of hydrocarbon systems besides the fractionation units of the gas plant. The types of software used in this study include Aspen HYSYS V7.3, MATLAB version R2014b, and Microsoft Excel.

1.6. Thesis Outline

The thesis has been structured into ten chapters with references and appendix provided at the end of the thesis.

Chapter 1 is the introduction of the research topic. This chapter provides the background of distillation, problem statement, research objectives, research scope and overview of the various chapters in this research work.

Chapter 2 presents the overview of multi-component distillation, which includes conventional arrangements with drawbacks, alternative arrangements for single column case and complex distillation arrangements. This chapter ends with a summary which states the selection of the best configuration, namely DWC, for this research work.

Chapter 3 provides the literature review of the design and optimization methods for the complex distillation arrangements, namely Petlyuk columns and DWCs. Besides that, the review in this chapter also covers the sizing methods for the design of DWC and existing process design methods for the conventional column. This chapter ends with a summary which also states the gaps in the DWC research.

Chapter 4 describes the simulation of the Petlyuk/DWC columns. The step-by-step method of simulating the Petlyuk column using HYSYS for the application of depropanizer/debutanizer system is illustrated. The results of the Petlyuk column design are interpreted for gaining insights into the DWC design.

Chapter 5 gives the development of the single column models for the multi-component distillation, which is later used as fundamental models for the design and optimization of DWC. The models developed in this chapter cover the process design and equipment design with hydraulic check of a conventional column.

Chapter 6 presents a new process design procedure to solve the DWC model using the modified Lewis-Matheson (LM) stage-by-stage procedure as proposed in Chapter 5. The reduction of the degree of freedoms in the design model via the derivation of additional equations and introduction of new convergence criterion is also discussed in the chapter.

Chapter 7 proposes a stage-by-stage modelling procedure using the McCabe-Thiele method and Lewis-Matheson (LM) design approach as the basis. The design method proposed can provide direct solutions by performing the stage-by-stage calculations from the feed and side withdrawal points without the tedious iterations done for composition matching at the interlinking trays.

Chapter 8 shows a methodology for the mechanical design of a DWC, which is developed based on the conventional design procedure of a single column.

Chapter 9 provides a summary of the overall design procedure and discusses the optimization and economic evaluation of the DWC.

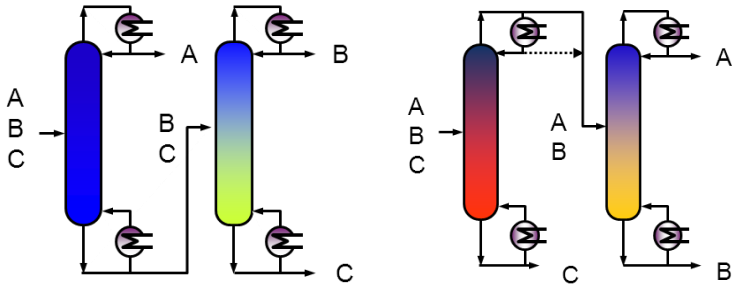
Chapter 10 summarizes the main conclusions from the study along with some recommendations for further works in the future.

CHAPTER 2: OVERVIEW OF MULTI-COMPONENT DISTILLATION

In this chapter, an overview on conventional distillation column for multi-component separation processes is presented. Due to the low thermodynamic efficiency in the conventional distillation column, several improvement options have been proposed in order to overcome the low efficiency, such as via process integration. Several alternative arrangements for a single column case as well as complex distillation arrangements have also been proposed by a number of researchers. The pros and cons of each option are discussed this chapter. The rest of this chapter is arranged as follows. Section 2.1 describes the conventional distillation arrangement with its problems in multi-component separation. Section 2.2 discusses the energy efficient distillation technologies introduced to overcome the problems faced by the conventional distillation. The summary of this chapter is provided in Section 2.3.

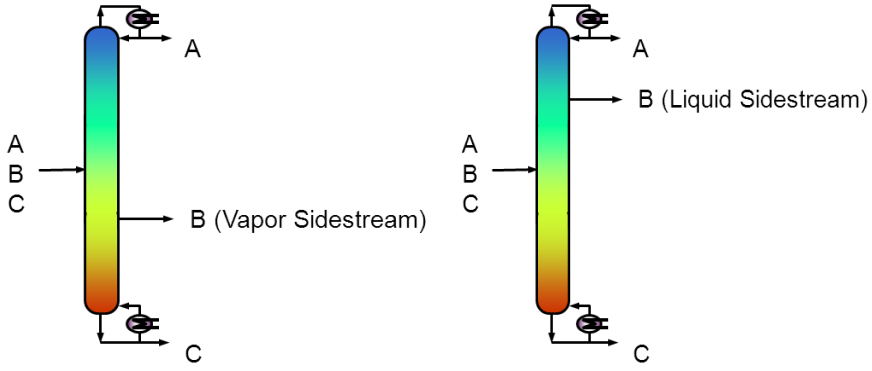
2.1. Conventional Distillation

The separation of multi-component mixtures usually involves a sequence of distillation columns, with at least two distillation columns is applied. In the case of ternary mixtures, two most often used distillation column arrangements are the direct and indirect sequences as shown in Figure 2.1. Although a conventional column with a side draw (Figure 2.2) is also feasible and more cost-effective than the simple direct and indirect arrangements, this side-stream arrangement is only applicable in certain circumstances, which is highly dependent on the feed composition. In order to effectively use side-stream arrangement, it is important that the feed is dominated by a middle product (middle component), where the quantity of either one of the other two (light or heavy) components is minor as well as large relative volatilities. These conditions are required in order to attain high purity requirements of all the product streams (R. Smith, 2005).



(a) (b)

Figure 2.1 Direct (a) and indirect (b) sequence for ternary mixtures separation (Seki & Shamsuzzoha, 2012)



(a) (b)

Figure 2.2 Single column side-stream arrangements with vapo**u**r side-stream (a) and liquid side-stream (b)

As noted previously, in the direct sequence, as shown in Figure 2.1a, the lightest component (highest volatility or lowest boiling point) is taken overhead in each column. For the indirect sequence as shown in Figure 2.1b, the trend is the converse of the direct sequence, in which now the heaviest component (lowest volatility or highest boiling point) is removed first as the bottom product. The lighter components will then undergo further separation in the next column. These conventional column arrangements are favourable in practice as they require simple control and operation systems. However, the remixing effect caused by irreversible split often results in a low energy efficiency in these arrangements (Asprion & Kaibel, 2010).

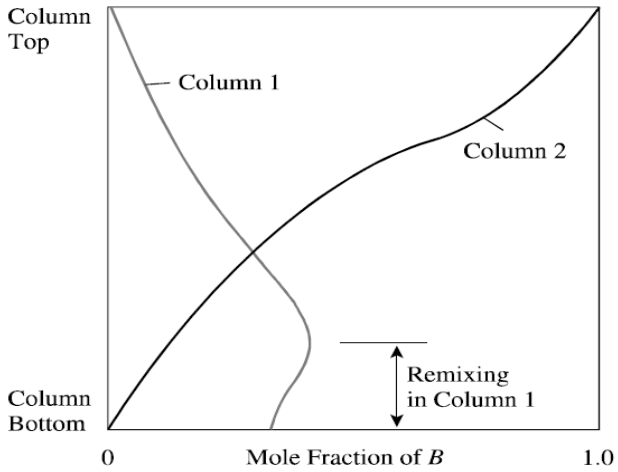


Figure 2.3 Composition profile for the intermediate component (B) in the conventional direct distillation sequence showing remixing effect (R. Smith, 2005)

The remixing effect is a phenomenon that occurs naturally in the conventional distillation sequences. This remixing effect is acknowledged as the main source of irreversibility, which can lead to a low thermal or thermodynamic efficiency leading high energy requirements in the reboilers of the conventional columns. In the case of a conventional direct distillation sequence for ternary separation, the remixing phenomenon can be described through the composition profile of the intermediate component, as illustrated in Figure 2.3.

Note that, the remixing effect occurs in the first column. As seen in Figure 2.3, the composition of the intermediate component B in the first column increases until it reaches a maximum at a certain point below the feed. Then, its composition declines before reaching the bottom of the column. This condition is a consequence of remixing for component B (intermediate) and which results in unnecessary consumption of energy. This is because energy has been supplied to separate component B to a maximum purity. However, since it is not separated at this point, the component is re-mixed with the heavy component (C) which is removed at the bottom of the column. Therefore, in the second column, a supplementary amount of energy is required to re-purify the mixture (Hernández et al., 2006; R. Smith, 2005).

A similar condition is deemed to happen in the indirect sequence. In this case, the difference from the direct sequence is that, the intermediate component (B) in the first column of the indirect sequence increases until it reaches a maximum point above the feed. Then, it starts to decrease before reaching the top of the column due to remixing with the light component A (Hernández et al., 2003; R. Smith, 2005).

Besides the remixing effect, a mixing effect also takes place in a multi-component separation as one of the sources of the thermodynamic inefficiency in the separation process. The mixing effect occurs when a feed stream entering a distillation column has different composition or temperature from that of the feed stage. These mismatches cause the disruption of the composition profile in the column when the feed is mixed with the material within the column. This effect does not occur in the simple column for the binary distillation as the composition and temperature of the feed and the feed stage are similar. Although an exact match is not always possible, the influence of the feed mismatches on the mass transfer at the feed stage may be negligible for a binary mixture. On the other hand, for the multi-component separation, the exact match of the composition or temperature between the feed stream and the feed stage is virtually impossible in most practical situations, except for a very few specific conditions. Hence, the losses occur due to the feed stage mixing effect gives rise to thermodynamic inefficiency, which results in increasing amounts of heating and cooling duties of the column (Dejanović et al., 2010; Halvorsen & Skogestad, 2011; Jobson, 2014; R. Smith, 2005).

2.2. Energy Efficient Distillation

To improve the energy efficiency of a distillation column, several options have been proposed to deal with the mixing and remixing effects in the column. The first option which has been considered is process integration, also known as external heat integration. However, because of the limitation of the external heat integration as discussed in Section 2.2.1, an extensive research on the improvement of the column has been conducted focusing on the distillation operation itself, thus introducing some highly efficient energy saving technologies. The energy saving technologies for single-column and multiple-column cases are discussed in the following sections.

2.2.1. Process integration

Process integration, also known as external heat integration, is one of the methods often used in reducing the energy costs for conventional distillation in chemical industries. The concept of external heat integration was first introduced approximately 70 years ago, with the basic idea of allowing heat exchange between hot process streams and cold process streams (Jana, 2010). This approach has been used to integrate the conventional distillation columns into the overall process through exchanging the heat between the condensers and reboilers of the distillation towers with the cold and the hot streams available from the other parts of the plant (Linnhoff et al., 1983). However, the scope for the integration with the background process is often limited by the heat flows in the background process. Furthermore, operational problems like the occurrence of excessive fouling in the reboiler of one of the distillation columns can also restrict the applicability of an external heat exchange strategy (Muralikrishna et al., 2002). Therefore, if the integration is limited by the above mentioned factors, alternative strategy for improvement must be directed to the distillation operation itself or energy-integrated solutions between the individual columns and non-conventional arrangements to develop highly efficient energy saving technologies (e.g. heat pump assisted distillation) and thermally-coupled distillation columns (Annakou & Mizsey, 1996; Kiss et al., 2012; R. Smith, 2005).

2.2.2. Advanced technologies for single column

Bear in mind that, a conventional distillation column has a relatively low thermodynamic efficiency (Araújo et al., 2007). In order to perform a separation task, the distillation column requires the input of high quality energy in the reboiler while a similar amount of heat at a lower temperature is released in the condenser at the top of the column. Hence, this practice causes inefficient use of energy overall leading to high operating cost of the column involved. To alleviate this issue, several heat pump concepts have been suggested with the purpose to upgrade and reuse the discharged energy in the condenser for evaporation in the reboiler. In the mid-1970s, a heat pump assisted distillation column using mechanical compression, was first proposed in separating low relative volatility mixtures (Jana, 2010). The overview

and selection schemes of the heat pump assisted distillation technologies for new designs and retrofit applications are reported by Kiss (2014), Kiss et al. (2012) and Long and Lee (2014). Among the heat pump designs, heat integrated distillation column (HIDiC) is the most attractive approach using internal heat integration.

The development of various heat pump configurations has motivated several comparative studies for the case of a stand-alone unit. Mészáros and Fonyó (1986) evaluated three types of heat pump assisted distillation configurations, namely vapour compression (VC), mechanical vapour recompression (MVR) and bottom flashing (BF), from the view-point of thermodynamic efficiency. In a later work, Fonyo et al. (1995) compared a stand-alone butane splitter to three mechanically heat pumped alternatives (VC, MVR and BF) and three absorption heat pump alternatives: single stage with parallel and sequential operations, and double stage parallel operation. They found out that the costs of heat pump systems in all cases were lower than that of the conventional distillation. For the retrofitting industrial case study of light hydrocarbons, the heat pump-assisted technologies could help achieve total cost saving of about 15% (Fonyo & Benkő, 1996).

The aforementioned research work in heat pump was further extended to absorption heat transformer (AHT), where Fonyo and Benkö (1998) presented a comparison among mechanical heat pumps, absorption heat pumps and AHT. Based on the economic evaluations for a butane splitter, the AHT appeared to be the worst choice, whereas the heat pump with a sequential operation was the best one. Also, Díez et al. (2009) compared the costs of the conventional distillation with the heat pump-assisted distillation systems by simulating a mixture of i-butane and n-butane distillation process. The study showed that the energy costs of MVR and BF were reduced by 33% and 32% respectively from the conventional distillation, with the reduction of economic potential (a combination of capital and operational costs) of 9% and 10% for MVR and BF respectively. The absorption heat pump approach was not suitable for the system due to its higher energy consumption than the conventional column. Besides that, the distillation with intermediate heating and cooling plus an optimal side stream return were also discussed in detail by Lynd and Grethlein (1986).

In addition to the heat pump system, the application of self-heat recuperation technology (SHRT) in the distillation process is also recommended as an economical way of conserving energy. In heat pumps, only the heat recovery duty to the distillation column is considered. On the contrary, the SHRT proposed by Kansha et al. (2009), involves the circulation of both latent and sensible heat in the distillation process without any heat addition by using a compressor (Long & Lee, 2013b; Long & Lee, 2014; Matsuda et al., 2011). The comparison of conventional distillation with heat pump (MVR), SHRT and modified SHRT was performed by Long and Lee (2013b). The results from the comparison study showed that the modified SHRT with heat exchangers implemented in parallel can achieve the highest annual operating cost and total annual cost (TAC) savings, which were 67.19% and 44.18% respectively compared to the conventional one.

Besides the heat pumps and SHRT, several other advanced distillation technologies have been proposed, such as the cyclic distillation (CyDist) and multiple effect distillation (MED). Some major benefits of these other technologies include savings in primary energy requirements (PER) and total annual costs (TACs) which may be up to 80% under certain conditions. However, the majority of the aforementioned enhancement technologies tend to encounter constraints, especially in terms of intensive capital costs and complexity in operation. Hence, they can only be industrially viable for high capacity separation with close boiling points (Long & Lee, 2013a). Interestingly, the strategies based on feed splitting and preheating (Soave & Feliu, 2002), inter-reboiling, side reboiling, side reboiler or side condenser, changing the feed thermal conditions and operating pressure have been recognized as promising technologies to minimize energy consumption, especially for the retrofit of a single column (Long & Lee, 2014).

2.2.3. Advanced technologies for multiple column

In order to achieve significant reduction in energy and investment costs for multi-component separation, a variety of techniques based on process intensification has become the main trend in both design and retrofit in chemical industries. Process intensification is a process design philosophy of combining multiple conventional processes or units into a single unit with the aim to improve the process flexibility,

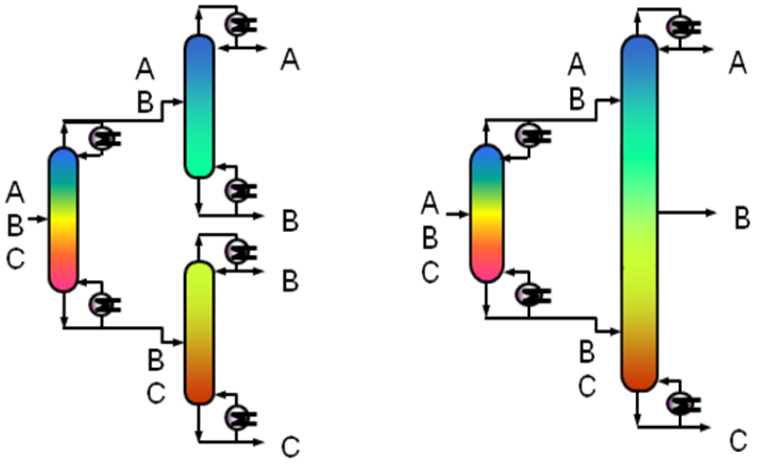
product quality, speed to market and inherent safety, with the added benefit of reduced environmental footprint (Kiss, 2014). Non-conventional distillation arrangements which are also broadly known as complex distillation arrangements have been developed based on the governing principle of process intensification.

The concept governing a non-conventional distillation is not new. These types of columns have already been widely used in the petroleum industry and for cryogenic air separation (Dünnebier & Pantelides, 1999). As mentioned before, the thermodynamic inefficiency in the conventional distillation separation is caused by the remixing and mixing effects which occur in the systems. In order to overcome the thermodynamic inefficiency inherent in the conventional columns, a three columns configuration, known as distributed or sloppy distillation has been proposed.

As shown in Figure 2.4a, in the distributed distillation arrangement, the entire light component (Component A) is separated in the top of the first column and the entire heavy product (Component C) in the bottom of the column. The middle distillate (Component B) is split between both of these streams. Then, further separation is performed by two subsequent columns, where the light component is separated from the middle component in one of the columns; the middle component is separated from the heavy component in another column. Although this arrangement is energy saving, it is inefficient in the use of equipment because three columns are needed instead of two, and six heat exchangers are required instead of four (Dejanović et al., 2010; Seki & Shamsuzzoha, 2012; R. Smith, 2005).

As an improvement to the distributed distillation, prefractionator arrangement (Figure 2.4b) is introduced by simply connecting the second and third columns of the distributed sequence if both of the columns have similar pressure. As a result, this arrangement consists of only two columns, a prefractionator and a main column. The prefractionator has its own condenser (partial) and reboiler, connected to the main column. The main column produces three products with the middle product taken as a liquid side stream.

The distributed and the prefractionator arrangements can provide energy savings by 20% to 30% as compared to conventional arrangements for the same separation duty (R. Smith, 2005). This cost difference is due to the elimination of the remixing effect



(a) (b)

Figure 2.4 Distributed or sloppy distillation (a) and prefractionator arrangement (b) for ternary mixtures separation
(Seki & Shamsuzzoha, 2012)

and the reduction of the mixing loss at the feed trays inherent in the conventional column arrangements. As observed in Figure 2.5, the intermediate component (B) is distributed between the top and bottom of the prefractionator. The prefractionator enables the composition of component B for upper and lower sections in the main column to reach a maximum at the same point, which is then separated as a side stream product. Therefore, it can be seen that there is no remixing effect and thus no excessive use of energy. Also, the distributed component B in the prefractionator can reduce the mixing effect at the feed tray by increasing the freedom to match the feed composition with one of the trays in the column (Jobson, 2014; R. Smith, 2005).

Instead of having a reboiler and a condenser for each column, a thermal coupling scheme is used to provide simultaneous mass and heat transfer between the different tasks in the separation sequence (Long & Lee, 2014). Some of these thermal coupling arrangements include a side stripper, a side rectifier and a fully thermally coupled distillation system (FTCDS) or Petlyuk column. Of the possible thermal coupling arrangements, the side stripper and the side rectifier have been widely used, respectively, in refinery distillation and cryogenic air separation (Amminudin et al., 2001). The Petlyuk column, introduced by Petlyuk et al. (1965) in 1965, is a three-product system with two columns as illustrated in Figure 2.6a. It was developed from

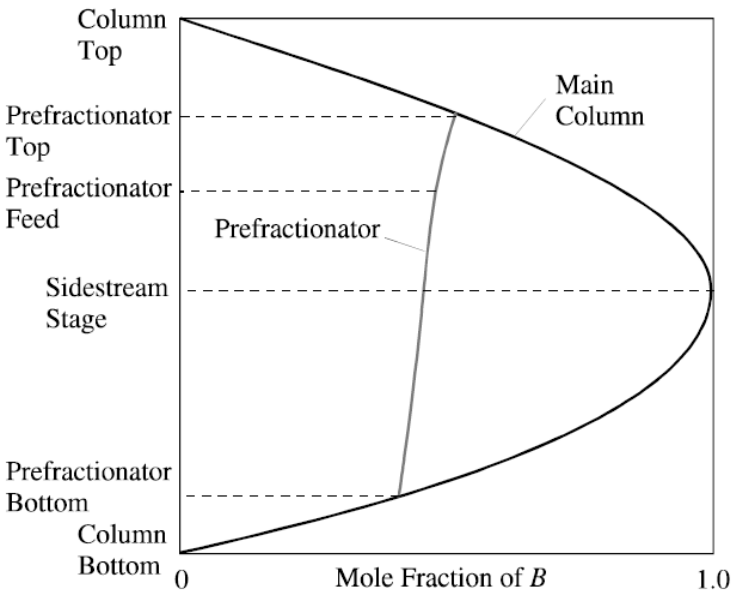
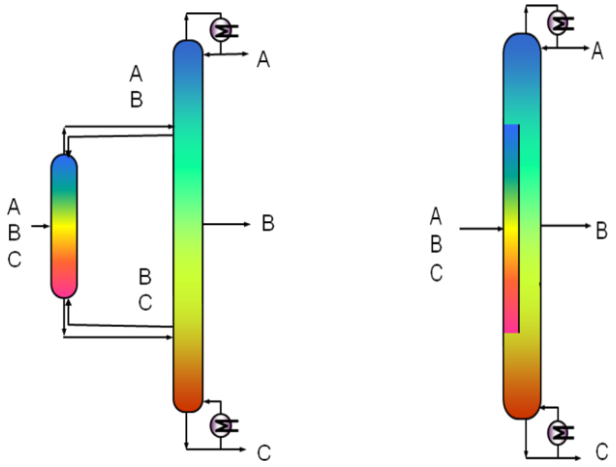


Figure 2.5 Composition profile for the intermediate component (B) in the prefractionator arrangement
(R. Smith, 2005)

the idea of thermal coupling of the prefractionator arrangement through substitution of the prefractionator condenser and reboiler by extra plates. Many studies have confirmed that this column requires typically 30% less energy than a conventional arrangement using simple columns (R. Smith, 2005). Recently, six alternative thermally coupled schemes proposed by Agrawal and Fidkowski (1998a),(1998b, 1999) and the extensions of the ideas presented in those works have shown an interesting potential in terms of their energy efficiency (Jiménez et al., 2003).

A further development into the thermally coupled column can be achieved when a dividing-wall column (DWC) is implemented by integrating two distillation columns into a single column shell as shown in Figure 2.6b. The concept of the DWC was introduced in 1949 by Wright (1949) but it was not commercialized until 1985, when BASF SE started up the first unit for its own use in Ludwigshafen (Dejanović et al., 2010). Since then the DWC has become a widely used column, which grows rapidly in number to more than 100 in 2010 and in size of its applications, such as extractive, azeotropic and reactive separations (Kiss et al., 2012; Yildirim et al., 2011). In addition to energy and capital savings, the DWC also provides a reduction in the plant footprint and is capable of delivering high purity side products. A DWC shown



(a) (b)

Figure 2.6 Fully thermally coupled distillation system (FTCDS) or Petlyuk column (a) and dividing-wall column (b) for ternary mixtures separation

in Figure 2.6b is able to produce three products, with the middle product being a liquid side stream on the opposite side of the dividing wall to the feed. This arrangement is thermodynamically equivalent to the Petlyuk column, but is usually much cheaper due to the need for only a single column shell.

Despite the advantages of the DWC, the application of the DWC is often limited by its complex operation at a single pressure, larger size of equipment, larger temperature span across the column and inherent complexity in its dynamics. Hence, several research studies have been done focusing on the design and control of DWC so that its usage can be further extended to other useful configurations such as split-column, Kaibel column or even multi-partitioned dividing-wall column (Dejanović et al., 2010; Kiss, 2014; Kiss & Bildea, 2011; Yildirim et al., 2011).

2.3. Summary

Several energy efficient technologies have been introduced to deal with the low thermodynamic efficiency in the conventional distillation column. Heat pump and self-heat recuperation technologies have been proposed to improve the thermodynamic efficiency of the column through the application of a compressor.

These options are considered as promising technologies if the distillation process is carried out in a standalone column. In other words, they are not preferable if the distillation process involves a sequence of columns because of intensive capital costs and complexity in operation.

Other strategies such as feed splitting and preheating, inter-reboiling, side reboiling, side reboiler or side condenser, changing the feed thermal conditions and operating pressure are also recommended for the minimization of the energy consumption of a single column. Although these strategies can also improve the thermodynamic efficiencies of the columns in multiple-column case, another better alternative based on process intensification, namely non-conventional or complex distillation is considered.

The remarkable complex distillation arrangements for the multi-component separation are prefractionator arrangement, side-stripper or side rectifier, Petlyuk column and DWC. These arrangements are preferable for the separation of multi-component mixture because it can cut down the number of equipment units required and hence lead to a reduction in the capital cost besides achieving savings in terms of energy. This is different from the strategies as mentioned previously of which additional equipment units are required or existing equipment units are maintained.

Among the complex distillation arrangements, DWC is selected as the best configuration to be studied in this research work because it can provide a reduction in the plant footprint and is capable of delivering high purity side products besides energy and capital savings. Recently, the implementation of DWC in the industry has been growing steadily in numbers. It has been applied in benzene-toluene-xylene fractionation (Exxon Mobil), separation of hydrocarbons from Fischer-Tropsch synthesis unit (Linde AG), separation of benzene from pyrolysis gasoline (Uhde), and so on (Kiss, 2014). However, the key challenge faced by the application of the DWC in the industry is the complexity in its design and operation due to a higher number of degrees of freedom. This gives the motivation for the current study to address the challenge in the design of DWC process. Therefore, the reviews on the design and optimization of the DWC (process and equipment) and its equivalent configuration, which is Petlyuk column, are provided in the following chapter to

reveal the existing works accomplished and identify the main gaps in the design and optimization of DWC.

CHAPTER 3: LITERATURE REVIEW

In this chapter, the literature review corresponding to the complex distillation arrangements, namely the Petlyuk columns and dividing-wall columns (DWCs) is presented. In Section 3.1, the review on various design and optimization methods for the complex distillation, especially Petlyuk column and DWC has been discussed. The related works on the sizing methods for the design of DWC are covered in Section 3.2. This chapter ends with Section 3.3 which provides the summary and highlights of some of the research gaps in the DWC design.

3.1. Design and Optimization of Complex Distillation

Complex distillation or thermally coupled distillation systems (TCDS) offer large potential savings in terms of energy and capital costs. However, their applications in the industries are rather limited because of the complexity of the procedure for designing the systems. Additionally, a lack of the operational experience is another limitation to applying TCDS in practice. The design procedures of the TCDS, especially the DWC design are more complicated than those used for designing the conventional distillation arrangements. One reason for the complexity in designing the DWC is because of its higher number of degrees of freedom than that of the conventional distillation column. For a ternary separation as shown in Figure 3.1, the parameters required for the DWC design are number of stages in six different column sections, reflux ratio, liquid split ratio, vapour split ratio, heat input in the reboiler, and the side product flow rate (Dejanović et al. (2010).

One of the challenging parts in the design and optimization of a DWC is to solve the multivariable system of equations involved by finding the rights values for the aforementioned parameters. Note that, many of these parameters interact with each other and as such they must be optimized simultaneously to achieve reliable and optimal design solution (R. Smith, 2005). It should be pointed out that, the system of equations describing a given DWC consists of three major types of equations: (1) mass-energy balances, (2) vapour-liquid equilibrium (VLE) relations, and (3) a set of

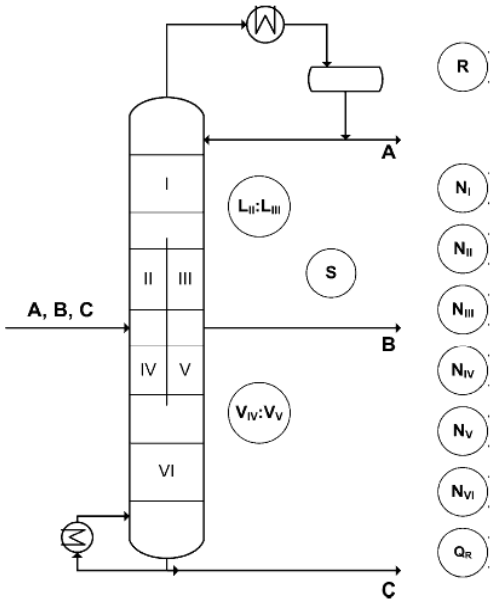


Figure 3.1 Design parameters for DWC with three-component separation

(Dejanović et al., 2010)

correlations representing the physical properties. Interestingly, the search for an efficient method of solving this system of equations remains an open problem in the DWC design.

Similar to the conventional column design, one of the important design outputs of DWC is the number of stages required to achieve certain specified product requirements. Since the number of stages is an integer variable, the column optimization is categorized as a mixed integer non-linear programming problem (MINLP), which cannot be solved using most of the commercially available process simulators. Therefore, external optimization routine is often needed, which is coupled with the commercial process simulator (Dejanović et al., 2010). It is worth mentioning that, several design and optimization procedures for the thermally coupled distillation systems have been reported in the literature. Most of the design methods covered in the following sections are related to the ternary separations.

3.1.1. Short-cut design methods

Generally, most of the previous studies dedicated to developing the procedures for the design and optimization of TCDS are accomplished using the short-cut design

methods. Due to the complexity of the design problems coupled with the requirement to assess rapidly the alternative designs, these short-cut methods have often been utilized to perform the preliminary optimization.

In some earlier studies, the approximate design and optimization of TCDS were often performed based on the minimum vapour flow rates in a ternary system (Fidkowski & Krolikowski, 1986; Nikolaides & Malone, 1988) until the emergence of structural design of fully thermally coupled distillation systems (FTCDS) suggested by Triantafyllou and Smith (1992). The short-cut procedure for the design and optimization of the FTCDS was developed based on the conventional Fenske-Underwood-Gilliland-Kirkbride (FUGK) equations using a three-column model to represent a given FTCDS. The prefractionator section of the FTCDS was assumed to be the same as a conventional column with a partial condenser and a partial reboiler. On the other hand, the main column of the configuration was decomposed into two sections, which were represented by two conventional columns. The top section of the main column was assumed to be equipped with a total reboiler, whereas a total condenser was assumed to be employed in the bottom section of the main column. In this FUGK design method, instead of just considering the minimum vapour flow rate, the optimization procedure took into account both energy and capital costs. The design variables required to be optimized in their work were reflux ratios and the recoveries of the key components in the prefractionator section.

Employing a similar short-cut method (FUGK equations), Muralikrishna et al. (2002) proposed a simpler optimization approach to represent all of the feasible designs of a DWC for the ternary separation. The concept of design space was introduced to give a broad view on the feasible designs available so that some attractive options could be selected to be further explored through rigorous simulation. Decomposing the DWC into three simple columns, the design space of the DWC was developed by applying FUGK equations to the prefractionator column and two downstream columns. The possible designs of the DWC were later presented graphically on a 2-dimensional plot. With these ‘visible’ designs, the optimum design of the DWC was achieved through a search on the plot.

Caballero and Grossmann (2004) presented a novel superstructure for designing sequences of distillation columns for ranges of types from conventional to FTCDS through the application of two-stage decomposition procedure. The first stage of the procedure involved the selection of a sequence of separation tasks. Then, the extraction of the best configuration of actual columns among all the thermodynamically equivalent options was conducted in the second stage. The equations applied in the design model were FUG equations. The formulation of the model as a generalized disjunctive programming problem improved the flexibility of the model as modification of the equations and migration to any other types of model could be done easily.

According to Sotudeh and Shahraki (2007), the use of the Fenske equation for the estimation of the minimum number of stages of a DWC was inadequate. This is because the Fenske equation is based on the assumption of equal compositions of liquid and vapour streams at the top and bottom of the prefractionator, which is not applicable in the case of the DWC. Therefore, they introduced a method for the design of DWC based on the Underwood equations instead. Besides showing the bounded nature of the split of the internal reflux over both sides of the middle wall of the column, they also recommended a method for the selection of the proper value of the split ratio.

Ram ŕez-Corona et al. (2010) presented an optimization procedure for the FTCDS or the DWC using a short-cut design method (FUG) as the basis. The composition of the interconnecting streams was predicted using feed line and operating line equations. Besides the short-cut equations, the optimization model also included thermodynamic relationships, mass and energy balances for each stream of the system. The procedure allowed the system to be modelled as a non-linear programming (NLP) problem. The objective function of the model was to minimize the total annualized cost (TAC), which consisted of operating cost and annualized capital investment.

Lee et al. (2011) proposed a two-step approach for the DWC design. An optimal DWC structure was first determined by applying the classical Fenske-Underwood-Gilliland (FUG) shortcut method to a sloppy configuration. Then, an optimal internal

flow distribution was then found from the corresponding DWC configuration. The authors claimed that the determination of the near-optimal structure design of DWC through the sloppy configuration was sufficient in the preliminary design stage.

Chu et al. (2011) introduced a new short-cut approach which utilized a rational and efficient net flow model to simplify the existing short-cut calculation. The new short-cut model, which was developed through the application of Fenske, Underwood, Gilliland and Kirkbride equations (FUGK), allowed the near-optimal values of important design parameters for three most common types of DWCs to be determined quickly. The procedure started with estimation of the composition for the key components, followed by setting the reflux ratio of the column based on the calculated minimum reflux ratio, calculating the minimum number of trays for each section, setting the split ratios and calculating the inlet reflux ratio, and finally computing the number of trays for each section. If the computed number of trays (main column) did not agree with the Kirkbride equation, the computation was repeated using revised tray numbers. The requirement of the iterative adjustments in the design of the main column makes the procedure to be quite tedious. This method was applied by Cho et al. (2015) in the design of a DWC for the fractionation of biodiesel.

An implementation of the conventional design procedure in the FTCDS design using three-column model can lead to a difficulty caused by the interlinking streams in the column. Because of the interlinking streams, an iterative trial-and-error calculation is needed to find the stage numbers which match the trays' compositions of the prefractionator and main column connected by the interlinking streams. Moreover, Amminudin et al. (2001) revealed that the use of Gilliland correlation to determine the number of trays and Kirkbride equation to find the thermal coupling locations can potentially lead to errors when the initial design result is transferred to rigorous simulation.

To overcome the difficulty, an approximate design procedure to find the structural column information, such as the interlinking locations between the prefractionator and main column of the given FTCDS was proposed by Kim (2002). This method was applied to a feed system consisting s-butanol–i-butanol–n-butanol. In a separate

work, the same method was applied to a benzene-toluene-xylene (BTX) feed system (Kim, 2005a). In the author's works, a stage-by-stage computation starting from the side withdrawal tray for the main column and feed tray for the prefractionator column was suggested. An equilibrium relation was applied for stage-by-stage computation. The number of trays in the system was then taken to be twice of the estimated trays since the computed number of trays was at its minimum. However, this rule is not always true and may not be appropriate for every system.

Halvorsen and Skogestad (2003) demonstrated the application of the minimum vapour flow rate or minimum energy requirement (V-min) diagram method for minimizing the energy requirements of the FTCDS. V-min diagram method is a graphical visualization of minimum energy, which is represented by the normalized vapour flow as a function of the feed distribution. With the assumptions of constant molal overflow, infinite number of stages, and constant relative volatilities, the theoretical minimum boil-up ratio is estimated based on the Underwood's equations. Then, the adjustments of the liquid and vapour splits are required to keep the boil-up in its optimum point. This analytical method was then further extended to computing important operational parameters for an infinite-staged DWC as a function of the feed composition, feed enthalpy, and relative volatilities (Halvorsen & Skogestad, 2004).

Recently, a new design method based on the Kremser approximate group method was provided by Uwitonze, Han, Kim, et al. (2014) to design a FTCDS for the fractionation of ternary component mixtures. In this design approach, the approximate method that relates the compositions of multi-component vapour and liquid streams inside the column section and leaving streams was employed to determine the number of stages. The design procedure has some advantages over the FUG or FUGK based methods in terms of eliminating the iterations encountered in the composition matching on the interlinking trays. Also, it eliminates the requirement to perform the calculation based on the Gilliland correlation for the actual reflux ratio, theoretical stages and computation for the location of feed stage. It is interesting to note that, another design method for the FTCDS which adopts the approximate group method and the Fenske equation was proposed (Uwitonze, Han, & Hwang, 2014). For this method, the Fenske design equation was applied to obtain

the structure of the main column. The application of the approximate group method in the design of the prefractionator section was later extended to the design of the main column section of the FTCDS in which the equations for the estimation of the distribution of non-key components were derived (Uwitonze et al., 2016).

3.1.2. Semi-rigorous design methods

Amminudin et al. (2001) proposed a semi-rigorous design model based on the equilibrium stage composition concept to provide a more accurate design than the standard short-cut design methods. The proposed method started with the specifications of product compositions which then followed by backward calculations to determine the specified design parameters. The design and optimization of the FTCDS were executed after the feasible products were estimated. Although fewer assumptions are employed in this method, certain assumptions, such as constant molar overflow and relative volatility are still required for estimating the product distribution from basic design information. Moreover, the adoption of six design variables in the design method tends to cause a difficulty in the optimization involved.

In another work, Kim et al. (2004) developed a new structural design for the FTCDS using a semi-rigorous model. This proposed method was similar to the method as proposed by Kim (2002). However, instead of using the equilibrium relation, the tray compositions in this new design procedure were computed using the material balances and Peng-Robinson (PR) equilibrium relation. This new design model was then applied to a multi-component system, known as hexane process in this work. In a separate work, the performance of the model was tested on three examples of distillation processes (butanol, BTX and hexane-heptane mixtures) using UNIQUAC activity model and PR equation of state (Kim, 2005b). Although this model is more rigorous than the short-cut design, adjustment is still required when the results of the design are transferred to HYSYS simulation. Moreover, the rule of taking twice of the computed number of stages as the actual number of stages may not be applicable to every system.

3.1.3. Rigorous design methods

In order to give improved predictions of the distribution of components in the column, some studies have been reported on the optimal design of a FTCDS or a DWC based on a rigorous, stage-by-stage distillation model, i.e., by using the deterministic (conventional) optimization approach. For an example, Dünnebier and Pantelides (1999) described a rigorous design technique based on the detailed column superstructures coupled with mathematical optimization to determine the design and the operational characteristic of the individual columns of TCDS. The detailed tray models which included mass and energy balances and equilibrium relation equations were employed for the design and optimization of the column. Because of these equations, the assumptions, namely constant relative volatility and constant molar overflow were removed from the design procedure. However, the authors claimed that this method would increase the computational complexity and lead to further difficulties in solving the mathematical problems involved, i.e., very hard to achieve global optimality when dealing with non-ideal systems.

Yeomans and Grossmann (2000) proposed improvement on the rigorous design of the complex distillation columns by introducing a generalized disjunctive programs (GDPs). The optimization models used for the separation of ideal and azeotropic mixtures were derived based on the superstructures established using a state-task network (STN) representation. The problem was solved with the modified logic-based outer approximation algorithm in order to determine the structural parameters of the columns. The size of the NLP sub-problems was reduced in this method. Nevertheless, the optimization of the superstructures is still non-trivial because of the non-linearities and non-convexities inherent in the problem.

To increase the robustness of the design, Barttfeld et al. (2004) established a decomposition method to synthesize the complex column configurations in which the superstructure was modelled using tray-by-tray GDP. The superstructure was developed based on the reversible distillation sequence model (RDSM). Also, rigorous MESH equations were applied to each column section of a given superstructure. Because of these highly non-linear and non-convex equations and large size of formulation, solving the tray-by-tray models often encountered

convergence problems. Therefore, an iterative decomposition strategy which decomposed the discrete decisions in the problem into two hierarchical levels was suggested. The first level of the solution involved the derivation of a configuration through the selection of column sections, whereas in the second level of the solution, the feed location and the number of trays corresponding to the selected sections were optimized. Various superstructure representations and methods for solving the problems for the complex configurations were also discussed by Grossmann et al. (2005). In addition, the design and optimization of the TCDSs using a new mixed integer linear programming (MILP) approach, maintaining the rigorous characteristic of the mixed integer non-linear programming (MINLP) models, were also demonstrated in the work of Caballero and Grossmann (2014).

Premkumar and Rangaiah (2009) studied the use of a commercial process simulator in the design and optimization of a DWC. In their work, a step-by-step procedure for designing the DWC via Aspen HYSYS was described. The rigorous simulation of the DWC was performed based on the equivalent FTCDS. Meanwhile, the optimization of DWC or FTCDS was carried out by varying one variable at a time while keeping others constant. The design variables which consisted of feed and side tray location, dividing wall section, internal vapour and liquid flow to the prefractionator were adjusted systematically and sequentially. However, this method is time-consuming, tedious and costly as a lot of work is required in adjusting the parameters which interact with each other.

Statistical method has also been suggested recently as a more practical and simpler way for the optimization of the DWC design. One of the statistical approaches applied to the design of the DWC is the one based on the factorial design methodology. This methodology has been widely used in the experimental investigation to obtain the information on the studied factors and their interactions from minimal experimental data (Long & Lee, 2012a). The application of this method was discussed in the works of Long and Lee (2012a) and Long and Lee (2012d). In their works, the factorial design was employed to solve the complex multivariate problems and optimize the interacting factors to obtain the best design through minimizing the total annualized cost (TAC). Although this method can only

provide relative values, it is still useful for the design of the experiments or simulation in laboratory and industrial settings.

Response surface methodology (RSM) is another statistical approach used for the optimization of DWC. RSM is a general technique for exploring the relationships between the independent input variables and one or more response variables based on the least-square fitting to experimental data. Several studies have demonstrated the use of this method to optimize the operational parameters and to evaluate the effects of interactions among these parameters on the energy efficiency of DWC (Long & Lee, 2012b, 2013a; Vikas Kumar Sangal et al., 2013; Vikas K. Sangal et al., 2012, 2014). This method can reduce significantly the number of simulation runs required for the optimization of DWC. Despite being relatively simple when compared with a rigorous method, the results of the optimization obtained often agreed well with the rigorous simulation results.

Another optimization approach based on the stochastic search method has also been proposed to find the optimal design of DWC/FTCDS without the requirement of massive simulations and hence avoiding a convergence problem. The commonly used stochastic approach for this purpose is genetic algorithm (GA). The application of GA was demonstrated in the works of Bravo-Bravo et al. (2010), Gómez-Castro et al. (2008), Gutiérrez-Antonio and Briones-Ramírez (2009), and Vazquez–Castillo et al. (2009). They suggested the use of simulation tools in conjunction with an external optimization routine based on a multi-objective GA to find the optimum column design. A systematic optimization method based on a combination of radial basis function neural network (RBF-NN) and GA was also developed by Ge et al. (2014) for determining the optimal design of DWC.

The GA starts by generating a random population. Then, it is evolved repetitively through a combination of genetic operations, which are random selection of many individual solutions, crossover and mutation (Gutiérrez-Antonio & Briones-Ramírez, 2009). This method is attractive in the DWC design because it does not require explicit information on the mathematical models and the knowledge of initial feasible points. GA uses several points simultaneously for the search of the optimal solution. Moreover, GA also offers several multi-objective techniques in its

application (Gómez-Castro et al., 2008; Gutiérrez-Antonio & Briones-Ramírez, 2009).

3.1.4. Section summary

The design and optimization methods for the Petlyuk column and DWC are summarized in Table 3.1. Based on the above analysis, it cannot be denied that many studies, focusing on the short-cut design method, have been carried out. Several short-cut design models have been proposed as they are preferable in industry, especially when applied to column optimization because of their robustness, computationally easy to converge and quicker to solve characteristics. Although these methods can simplify the complex problem, the application of the short-cut design models has limitation. The limitation arises from the use of assumptions, such as approximation as ternary mixtures of multi-components, sharp separations, saturated liquid feed, constant molar overflow and constant relative volatility. These assumptions are often adopted in the short-cut design approach to simplify the complex problem, but at the expense of causing the design to be less realistic than what is often required in the real situation. Therefore, these short-cut methods are usually used in the preliminary design phase to provide the design and operational variables required for the initialization of the rigorous simulation.

Moreover, most of the short-cut methods proposed apply FUGK equations in their design model. The use of the Fenske equation for the estimation of the minimum number of stages of a DWC is insufficient as the assumption of equal compositions of liquid and vapour streams at the top and bottom of the prefractionator is inappropriate. Also, the use of Gilliland correlation to determine the number of trays and Kirkbride equation to find the thermal coupling locations can potentially lead to errors when the initial design result is transferred to rigorous simulation (Amminudin et al., 2001). Therefore, a stage-by-stage computation using equilibrium relation has been proposed (Kim, 2002). This method has its limitation because it applies the rule of taking twice of the computed number of stages as the actual number of stages. This rule is not always correct and may not be applicable to every system.

Therefore, semi-rigorous and rigorous methods have been proposed to improve the accuracy of the designs. However, these methods have drawbacks. The method

proposed by Amminudin et al. (2001), developed using 3-column model required six parameters for the design of the column. Such a large number of design parameters used may cause difficulty in solving the optimization problem. On the other hand, the method proposed by Kim (2005b) required numerous tuning when the results are transferred to HYSYS simulation. Also, the model applies the rule of taking twice of the computed number of stages as the actual number of stages in the design which is not always true for every system. In addition, the semi-rigorous methods suggested are mainly with the intention to provide the operational and structural variables for the rigorous simulation. Hence, their works did not consider exact composition matching at the feed and interconnecting streams.

For the rigorous methods, they are generally complicated to use in the design and can lead to convergence difficulties when solving the system of equations representing the DWC. Moreover, several rigorous methods suggested, including those used in the process simulators are developed based on the rating methods. Therefore, these methods are not directly applicable to the design problem and as such iterative steps are needed when they are used in the design of a new column. In other words, with an initial estimate of the operational and structural variables, which can be approximated using short-cut methods, the calculations are repeated with updated estimates until a satisfactory design solution is achieved. To overcome this difficulty, a two-step design is often applied: (1) initialize the design model using short-cut method, followed by (2) rigorous design of the model.

Besides that, the use of rating methods in the design of DWC also involves a higher number of degrees of freedom. These variables are reflux ratio, number of stages of the column, locations of the feed, side withdrawal and interlinking trays, and flow profiles. The existence of the large number of variables will increase the computational complexity when the rating methods are used for solving the optimization problems. For this reason, several optimization approaches have been proposed: (1) tuning method, (2) factorial design method, (3) RSM, (4) GA and (5) GA and RBF-NN.

Table 3.1 Summary of design and optimization methods for the Petlyuk column and DWC

Reference	Configuration	Model	Design Method	Description / Details
Triantafyllou and Smith (1992)	Petlyuk Column	Three-column model	Short-cut (FUGK equations)	A short-cut design method was proposed and applied in the separation of close boiling mixtures of C4's. The developed optimization method, considering both operating and capital costs, was developed to optimize the reflux ratios and the recoveries of the key components in the pre-fractionator.
Dünnebier and Pantelides (1999)	Petlyuk Column / DWC	Superstructure	Rigorous	A rigorous design technique based on the detailed column superstructures coupled with mathematical optimization was proposed to determine the design and the operational characteristic of the individual columns of thermally coupled distillation systems (TCDS). The feed systems applied in this work were multi-component hydrocarbon mixtures.
Yeomans and Grossmann (2000)	TCDS	Superstructure	Rigorous	Optimal design of complex distillation columns using rigorous tray-by-tray, generalized disjunctive programming (GDP) models was proposed. The GDP models derived were solved with a logic-based outer approximation algorithm.
Amminudin et al. (2001)	Petlyuk Column	Three-column model	Semi-rigorous (equilibrium stage composition concept)	A design procedure, which was developed based on equilibrium stage composition concept, enabled the design parameters to be optimized simultaneously and these optimized parameters could be used for rigorous simulation. The feed system used in the case study was a 9-component light hydrocarbon mixture.

Table 3.1 *(continued)*

Reference	Configuration	Model	Design Method	Description / Details
Muralikrishna et al. (2002)	DWC	Three-column model	Short-cut (FUGK equations)	A short-cut approach was proposed to represent the feasible designs of a DWC graphically (2-dimensional plot). The proposed procedure was used for separating an equi-molar ternary feed mixture of benzene-toluene-xylene (BTX).
Kim (2002); Kim (2005a)	Petlyuk Column	Two-column model	Short-cut (equilibrium relation)	A structural design procedure for the design of fully thermally coupled distillation column was suggested. The twice of the number of stages obtained from the stage-by-stage computation was taken to be the actual number of stages of the column. This method was applied to ternary systems of s-butanol–i-butanol–n-butanol and benzene-toluene-xylene (BTX).
Halvorsen and Skogestad (2003)	Petlyuk Column	Two-column model	Short-cut (V_{min} diagram)	A minimum vapour flow, or so called V_{min} diagram method was proposed to determine the minimum energy consumption. The method was developed based on Underwood's equations with the assumptions of constant molar flows, infinite number of stages, and constant relative volatilities.
Barttfeld et al. (2004)	TCDS	Superstructure (Reversible Distillation Sequence Model)	Rigorous	A decomposition method for synthesizing complex column configurations was proposed by using tray-by-tray GDP models to model the superstructure. Each column section of the superstructure was modelled using rigorous MESH equations.

Table 3.1 *(continued)*

Reference	Configuration	Model	Design Method	Description / Details
Caballero and Grossmann (2004)	TCDS	Superstructure	Short-cut (FUG equations)	A two-stage decomposition procedure was proposed for designing sequences of distillation columns that ranged from conventional to fully thermally coupled systems. Using the FUG approximations, the model was formulated as a generalized disjunctive programming problem.
Kim et al. (2004); Kim (2005b)	Petlyuk Column	Two-column model	Semi-rigorous	A structural design procedure for the design of fully thermally coupled distillation column using the material balances was suggested. The twice of the number of stages obtained from the stage-by-stage computation was taken to be the actual number of stages of the column. This method was applied to feed systems of butanol, benzene-toluene-xylene (BTX), hexane-heptane mixtures, and multi-component mixtures for hexane process.
Sotudeh and Shahraki (2007)	DWC	Three-column model	Short-cut (Underwood's equations)	A method for the design of DWC was proposed based on Underwood equations only because the authors claimed that the use of the Fenske equation in estimating the minimum number of stages was inappropriate in DWC design. This method was tested using an equi-molar ternary feed mixture of benzene-toluene-xylene (BTX).

Table 3.1 *(continued)*

Reference	Configuration	Model	Design Method	Description / Details
Premkumar and Rangaiah (2009)	DWC	Two-column model	Rigorous (Simulation tool / tuning method)	A commercial process simulator (HYSYS) was used in the design and optimization of a DWC. Developing the DWC model based on the equivalent Petlyuk column in simulation environment, the optimization of DWC was carried out by varying one variable at a time while keeping others constant.
Gómez-Castro et al. (2008); Gutiérrez-Antonio and Briones-Ramírez (2009); Vazquez–Castillo et al. (2009)	Petlyuk Column / DWC	N/A	Rigorous (Simulation tool / genetic algorithm)	The use of simulation tools in conjunction with an external optimization routine based on a multi-objective genetic algorithm (GA) was proposed to find the optimum column design.
Ramírez-Corona et al. (2010)	Petlyuk Column / DWC	Three-column model	Short-cut (FUGK equations)	An optimization model, which consisted of FUG equations thermodynamic relationships, mass and energy balances for each stream of the system, was suggested to achieve minimum total annual cost. The composition of the interconnecting streams was estimated using feed and operating line equations.
Lee et al. (2011)	DWC	Three-column model	Short-cut (FUG equations)	A two-step approach for the DWC design was proposed: determination of optimal DWC structure through sloppy configuration; determination of optimal internal flows through DWC configuration.

Table 3.1 *(continued)*

Reference	Configuration	Model	Design Method	Description / Details
Chu et al. (2011)	DWC	Five-section model	Short-cut (FUGK equations)	A component net flow model was proposed to determine the near-optimal values of important design parameters for three most common types of DWCs.
Long and Lee (2012a); Long and Lee (2012d)	DWC	Two-column model	Rigorous (Simulation tool/ factorial design)	A practical method of designing and optimizing DWCs was developed based on factorial design to achieve optimal design with respect to the total annualized cost.
Long and Lee (2012b); Long and Lee (2013a); Vikas K. Sangal et al. (2012); Vikas Kumar Sangal et al. (2013); Vikas K. Sangal et al. (2014)	DWC	Two-column model	Rigorous (Simulation tool/ response surface method)	A response surface method was proposed to optimize the operational parameters and to evaluate the effects of interactions among these parameters on the energy efficiency of DWC.
Uwitonze, Han, and Hwang (2014)	Petlyuk Column	Six-section model	Short-cut (Fenske equation and approximate group methods)	A structural design procedure for the Petlyuk column was developed using approximate group method and Fenske equation. The approximate group method was used for the design of the prefractionator, whereas the Fenske equation was applied to the design of the main column. The method was then tested using different hydrocarbon feed mixtures.

Table 3.1 *(continued)*

Reference	Configuration	Model	Design Method	Description / Details
Uwitonze, Han, Kim, et al. (2014)	Petlyuk Column	Six-section model	Short-cut (approximate group methods)	A novel design method was proposed to determine the structural design of Petlyuk column. The number of stages in each section was determined based on the flow rates and product specifications. The feed systems used for analysis were benzene-toluene-xylene (BTX), ethanol-n-propanol-n-butanol, and ethane-propane-i-butane.
Caballero and Grossmann (2014)	TCDS	Superstructure	Rigorous	A new mixed integer linear programming (MILP) was proposed for the design and optimization of the TCDSs. The rigorous characteristic of the existing mixed integer non-linear programming problem (MINLP) was maintained in the MILP model.
Ge et al. (2014)	DWC	N/A	Rigorous (Simulation tool / neural network and genetic algorithm)	A systematic optimization method based on a combination of radial basis function neural network (RBF-NN) and GA was developed for determining the optimal design of DWC.
Uwitonze et al. (2016)	Petlyuk Column	Six-section model	Short-cut (approximate group methods)	A structural design method considering the distribution of non-key components was presented. The proposed method was then applied to three multi-component feed systems. Besides that, the authors also performed the controllability analysis of Petlyuk column.

3.2. Equipment Design of Dividing-Wall Column (DWC)

The sizing of the DWC is essential to perform the calculation of capital cost, which is then used for then column optimization. Similar to the conventional column, the DWC can be classified into tray (plate) and packed (random or structured) column. The methods to be applied for the sizing of the column with its internals are dependent on types of internals used. The development in terms of equipment or mechanical design is mostly accomplished by private industry. Therefore, most of the details regarding this matter are not discussed in the open literature. Therefore, limited published works are available on the sizing of the DWC. In this chapter, only a few methods related to sizing are discussed.

Shah (2002) suggested to use the existing sizing procedure available in Aspen Plus for the design of complex columns. Also, Rangaiah et al. (2009) carried out the design of a 3-product DWC using a commercial process simulator by viewing the separated sections of the DWC as parallel cylindrical columns. The separated columns were later sized by utilizing the same procedure as the conventional columns.

For packed columns, Olujic et al. (2004) introduced the Delft-model which could improve the accuracy in predicting the mass transfer efficiency and pressure drop without any adjustable, packing specific parameter. Rix and Olujic (2008) developed a pressure drop model for liquid collectors and distributors to predict the pressure drop caused by packed column internals. This method enabled the possibility of adjusting the pressure drop of the liquid redistribution through the column sections when applied in the design of a packed DWC. Olujić et al. (2012) gave a detailed methodology for the sizing of a packed, 4-product DWC. According to the researchers, the pressure drop equalization is a determining factor to ensuring the required vapour splits among parallel sections.

For the design of tray DWC, Dejanović et al. (2010) suggested that the best way was to perform the hydraulic design of a DWC by considering it as a combination of several sieve tray columns. The method was applied according to the procedure provided by Stichlmair (1998). Recently, Rodr ́guez-Ángeles et al. (2015) presented a methodology for the mechanical design of DWC with sieve trays for a hydrocarbon

mixture system. The method was developed based on the traditional design methodology for conventional column proposed by Kister (1992). In their work, the top and bottom sections of the main column were designed using the same procedure as applied to the conventional column. The best location of the dividing wall in the column was optimized with the objective of minimizing the total diameter.

3.3. Design Methods for Conventional Column

In general, the methods used for the design and optimization of the conventional column in multi-component separation can be categorized into short-cut and rigorous methods. Short-cut methods are favourable in industry, especially for the separation of the hydrocarbon mixture, due to its robustness, ease to converge computationally and simple to solve features. The importance of these features is obvious when the methods are utilized in column optimization. However, short-cut models are only suitable for rough design due to their limiting assumptions: constant molar overflow within each column section and constant relative volatilities throughout the column. These assumptions are often invalid for multi-component and non-ideal mixtures, which will lead to a large inaccuracy in the design. Therefore, they are usually used as initial estimates of column conditions for rigorous models (Gadalla et al., 2003).

Although rigorous models are hard to converge computationally when the initial estimates are poor, they can give more accurate results and predictions of component distributions than the short-cut models. The rigorous models for distillation are classified into two types as: (1) equilibrium-stage models and (2) rate-based models. The former assumes that the full vapour liquid equilibrium (VLE) on each stage is known, or the stage efficiency based on existing industry is known. Rate-based models are more realistic than the equilibrium-stage models as they do not assume any phase equilibrium, but they have a difficulty in predicting the interfacial area and mass transfer coefficients. Consequently, this becomes one of the reasons why they are not widely applied in the industry.

In recent years, the equilibrium-stage models have become more favourable to solving multi-component distillation problems due to the availability of large digital

computers. Please note that the methods available in obtaining solutions to rigorous models can be classified into design and rating methods (Perry & Green, 1997). In the design method, the distributions of the components between the distillate and bottom are required to determine the number of stages. Conversely, the rating method requires the specification on the number of stages and feed stage location in order to determine the distributions of components in the top and bottom product streams.

The rigorous design method applied to the multi-component problems was first proposed by Lewis and Matheson (1932). This method involves stage-by-stage calculations from both (rectifying and stripping) sections of the given column and attempts to match the compositions at the feed stage by using the approximate distillate compositions. The product compositions are then revised through correcting the discrepancy between the feed stages' compositions obtained from both sections. Bonner (1956) presented a modified version of the Lewis-Matheson (LM) method to suit for the computer applications. The detailed application of this method was discussed by B. D. Smith (1963). This method is not commonly implemented in modern computer algorithms because of two major drawbacks: difficulties in convergence at the feed stage and providing an initial estimation of the component distributions at the top and bottom products.

Other than the design methods, several rating methods have also been proposed to determine the performance of existing or specified columns. These methods include Thiele-Geddes (TG), bubble-point (BP), sum-rates (SR), simultaneous-correction (SC), and inside-out (IO) methods (C. D. Holland, 1981; Khoury, 2005; Perry & Green, 1997; B. D. Smith, 1963). With the exception of TG method, which solves the equilibrium-stage equations one at a time, all the other methods mentioned use the tridiagonal matrix algorithm to solve the system of equations simultaneously. Similar to the LM method, the TG method faces the convergence problem at the feed stage. To overcome this problem, theta method has been recommended and the details of the method are described by C. D. Holland (1981). Besides that, the convergence problem at the feed stage can also be eliminated by introducing the tridiagonal matrix algorithm as applied in the other rating methods. However, these

methods are not frequently used for the process optimization of column as they are complex and difficult to solve – requiring huge computational effort.

3.4. Summary

In Section 3.1, the works on the design and optimization methods for the complex distillation arrangement are reviewed. Based on the analysis, it can be concluded that a lot of research studies have been carried out on the design and optimization of the DWC/FTCDS. However, most of the design and optimization of TCDS are carried out based on the short-cut design methods, especially FUGK methods. Although the short-cut methods are quick and easy to use in determining the operational and structural parameters of the DWC, the solution obtained from the methods may not be reliable and may suffer from serious deviations from the real condition due to the several assumptions used, especially the constant relative volatility assumption.

Therefore, semi-rigorous and rigorous methods have been proposed to improve the accuracy of the designs. However, these methods have drawbacks. For the method proposed by Amminudin et al. (2001), the complexity may arise when it is used in solving the optimization problems. The limitations of the method suggested by Kim (2005b) are the requirement of numerous tunings when the results are transferred to HYSYS simulation and the used of rule indicating that actual number of stages is taken twice of the computed number of stages. Moreover, exact composition matchings at the feed, side withdrawal and interlinking trays are not considered as these semi-rigorous methods are developed with the main purpose to provide the operational and structural variables for the rigorous simulation.

The rigorous methods proposed in previous works are usually complicated to use and may lead to convergence problems when they are used in the design. As the rigorous methods suggested are developed based on rating methods, several initial variables have to be assumed at the beginning of the computation procedure. Therefore, a two-step design is required when the rigorous design is carried out. Moreover, the existence of higher number of degrees of freedom will also add to the complexity in solving the optimization problems. Several optimization approaches have been

proposed to tackle this issue. Besides process design method, the works related to the equipment design, especially on the column sizing of DWC are also reviewed and provided in Section 3.2.

Based on the reviews of the literature presented in Sections 3.1 and 3.2, the research challenges and gaps identified are summarized as follows.

- Complexity in the design and optimization of DWC due to higher degrees of freedom (rigorous rating methods).
- Short-cut or semi-rigorous methods have to be applied in conjunction with the rigorous methods for more accurate design and study.
- Limited works have been published on the equipment design of DWC considering the tray hydraulics.
- Optimization methodology combining both process and equipment design of DWC (including the tray design) is rarely reported in existing literature.

Thus, based on the above analysis, the motivation of this thesis is to develop a new algorithm for the design and optimization of a DWC based on the rigorous design method. From the methods reviewed in Section 3.3, Lewis-Matheson (LM) method is chosen as the basis in developing the design model because it is more rigorous than the short-cut methods and requires less number of assumptions to initiate the calculations of the model equations when compared with the rating methods (rigorous). For the column sizing of the DWC, a detailed methodology on the column sizing with hydraulic trays (sieve) will be proposed in this thesis by modifying the procedure as proposed by Kister (1992) and Rodr ǵuez-Ángeles et al. (2015), i.e. using the fractional area is the main adjustable variables instead of the tray layout specifications at the dividing wall section.

CHAPTER 4: PROCESS SIMULATION OF DIVIDING-WALL COLUMN (DWC) USING HYSYS

This chapter describes the simulation of the Petlyuk column and dividing-wall column (DWC) separation processes. The step-by-step method of simulating the Petlyuk column using Aspen HYSYS V7.3 is illustrated based on the application to ternary separation, i.e., depropanizer/debutanizer system. The results of the Petlyuk column are adopted for the DWC design. This chapter is structured as follows. Section 4.1 gives an overview of the steps involved in the simulation of a DWC. The design specifications required for simulation are provided in Section 4.2. Section 4.3 outlines the steps required to carry out the short-cut simulation using a three-column model, whereas Section 4.4 provides the steps required to perform the rigorous simulation using Petlyuk column (two-column model). The summary of the chapter is given in Section 4.5.

4.1. Introduction to Process Simulation

This chapter provides a step-by-step simulation procedure for the design of a DWC distillation using Aspen HYSYS V7.3. The ternary system mixture is used as an example for the simulation of depropanizer and debutanizer in one single DWC. For the preliminary design, one starts with the identification of suitable inputs required for the DWC system, which are often the feed conditions, product specifications and operating conditions. Then, a static or steady-state simulation is developed using a short-cut method where the DWC is approximated by three-column model, which is used to obtain initial estimates of variables required for rigorous simulation. Finally, a rigorous simulation is performed to get more accurate and realistic results (Premkumar & Rangaiah, 2009; Rangaiah et al., 2009). The detailed of the preliminary design is discussed in the following sections.

4.2. Design Specifications

In this work, the inputs required for the initial design of DWC are obtained from the fractionation section of a gas plant in Malaysia (Ching et al., 2016). The depropanizer/debutanizer system is first developed and simulated in Aspen HYSYS V7.3. Aspen HYSYS is chosen as the simulator in this study because it is the most commonly used process simulator in the industry for the steady state modelling purpose. The in-built property or fluid package helps in obtaining accurate predictions of the thermodynamic, physical and transport properties of hydrocarbon, non-hydrocarbon, petrochemical and chemical fluids. Furthermore, it has flexibility in modelling a wide range of operations comparable to realistic situations. The Peng-Robinson (PR) property package is used as the equation of state to predict the vapour-liquid equilibrium (VLE) of the developed models. This property package can support the widest range of operating conditions. Therefore, it is adequate to predict the equilibrium of light hydrocarbon mixtures (Aspen Technology, 2011).

Figure 4.1 shows the HYSYS flow diagram of the conventional NGL fractionation trains, which comprise a depropanizer and a debutanizer columns. The feedstock to the depropanizer unit is the bottom product of a deethanizer (Stream C6) and the condensate treatment unit (Stream C6-1) in the natural gas plant. In the present study, the feed streams from the deethanizer and the condensate treatment, respectively contain 897.1 kmol/h and 284.4 kmol/h of a mixture of light hydrocarbons, ranging from propane to decane. In the depropanizer, the propane is separated as distillate (Stream C7), whereas the remaining product is fed to the debutanizer via Streams C8 and C9. Then, i-butane and n-butane are separated in debutanizer as top product (Stream C10). The feed conditions of the mixture, the product specifications, and the column specifications of the depropanizer and debutanizer units are presented in Table 4.1 and Table 4.2.

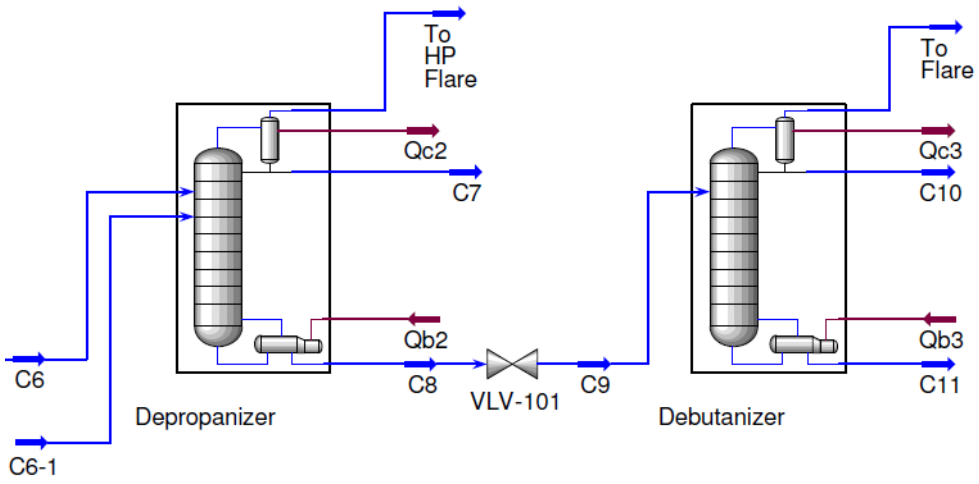


Figure 4.1 HYSYS flow diagram for the depropanizer/debutanizer system for conventional distillation process

Table 4.1 Feed conditions of the depropanizer

Component	Mole Fraction	
	Feed 1 (C6)	Feed 2 (C6-1)
Ethane (C_2)	0.0091	0.0050
Propane (C_3)	0.5907	0.1508
i-Butane (iC_4)	0.1624	0.0943
n-Butane (nC_4)	0.1202	0.0948
i-Pentane (iC_5)	0.0518	0.0843
n-Pentane (nC_5)	0.0269	0.0555
n-Hexane (nC_6)	0.0190	0.0949
n-Heptane (nC_7)	0.0111	0.1280
n-Octane (nC_8)	0.0069	0.1804
n-Nonane (nC_9)	0.0019	0.1113
n-Decane (nC_{10})	0.0000	0.0008
Total Molar Flow (kmol/h)	897.1	284.4
Temperature (^oC)	70.18	155.00
Pressure (bar)	16.00	16.10

Table 4.2 Column specifications, product specifications, and energy performance of existing columns sequence

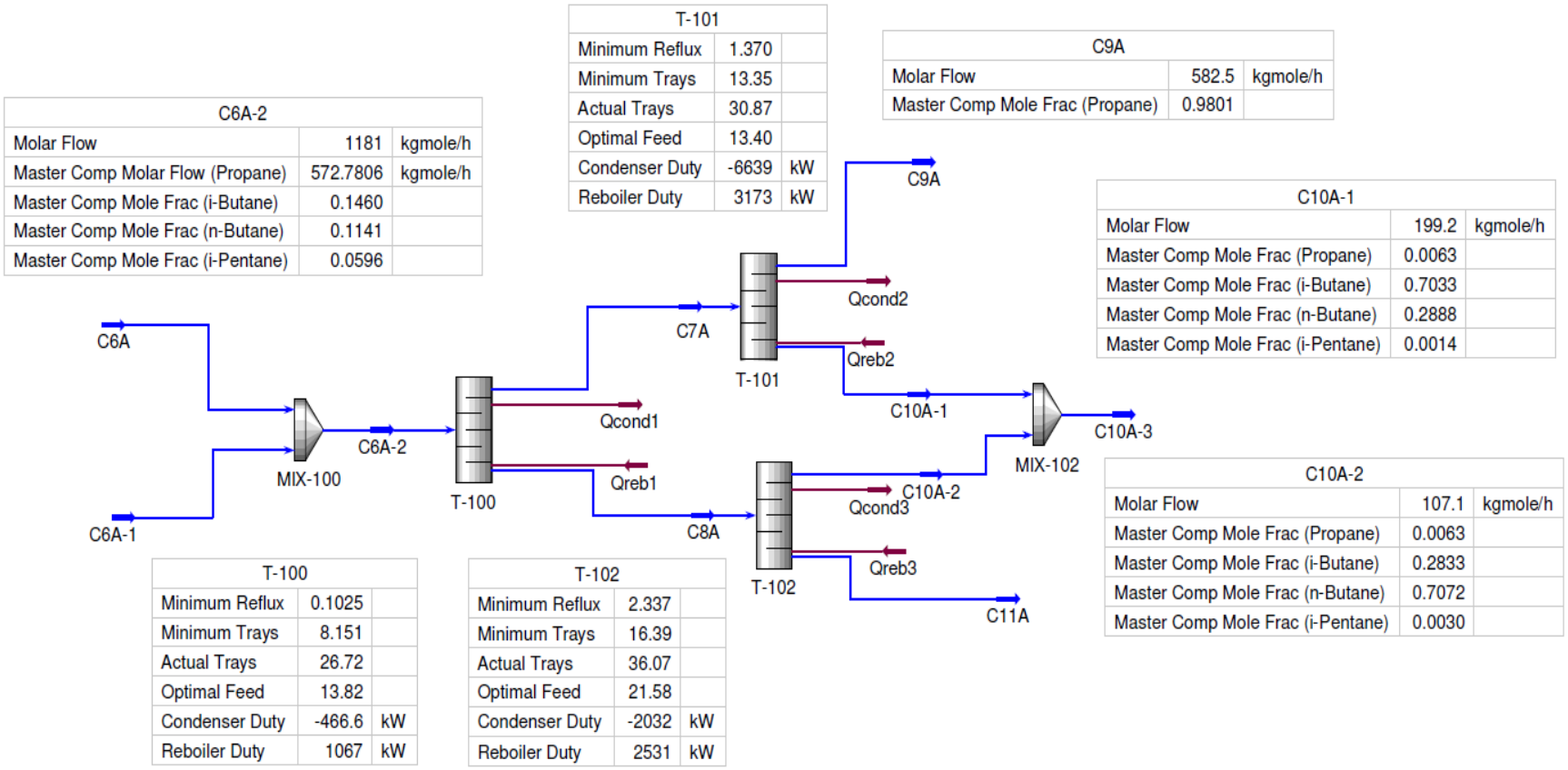
Specifications	Depropanizer	Debutanizer
Number of trays	53	53
Feed tray location (Feed 1 and 2)	26	26
Reflux ratio	2.20	1.50
Purity of C_3 (Mole fraction)	0.98	-
Purity of C_4 (Mole fraction)	-	0.985
Pressure of top product stream (bar)	14.91	5.11
Pressure of bottom product stream (bar)	16.20	5.81
Condenser Duty (kW)	7243	4109
Reboiler Duty (kW)	5762	2920

4.3. Short-Cut Simulation using Three-Column Model

To initiate the design of DWC for the combined depropanizer and debutanizer system, the short-cut column in Aspen HYSYS is used as the initial estimates of the design variables, such as number of stages and feed stage for rigorous simulation. As recommended by Amminudin et al. (2001), the DWC column is decomposed into three short-cut columns as shown in Figure 4.2. In this model, the column T-100 is used to represent the prefractionator section of the DWC, whereas the rectifying section of the column T-101 and stripping section of the column T-102 are correspondingly used to represent the top and the bottom sections of the conventional column. The stripping section of column T-101 and the rectifying section of column T-102 are equivalent to the dividing-wall section (split-tray zone) of the DWC.

The overhead product in the prefractionator section has to be in vapour phase so that it can better represent the material stream, thermally linked to the main section (columns T-101 and T-102). On the other hand, the overhead products for the other two short-cut columns have to be in liquid phase as they represent the individual final product streams. The feed of the column is defined as the feed conditions provided in Table 4.1. By adopting a PR property package, the steps for the short-cut simulation of a DWC through three-column model are stated as below.

Step 1: Define and provide input parameters for the feed stream.



C6A-2		
Molar Flow	1181	kgmole/h
Master Comp Molar Flow (Propane)	572.7806	kgmole/h
Master Comp Mole Frac (i-Butane)	0.1460	
Master Comp Mole Frac (n-Butane)	0.1141	
Master Comp Mole Frac (i-Pentane)	0.0596	

T-101		
Minimum Reflux	1.370	
Minimum Trays	13.35	
Actual Trays	30.87	
Optimal Feed	13.40	
Condenser Duty	-6639	kW
Reboiler Duty	3173	kW

C9A		
Molar Flow	582.5	kgmole/h
Master Comp Mole Frac (Propane)	0.9801	

C10A-1		
Molar Flow	199.2	kgmole/h
Master Comp Mole Frac (Propane)	0.0063	
Master Comp Mole Frac (i-Butane)	0.7033	
Master Comp Mole Frac (n-Butane)	0.2888	
Master Comp Mole Frac (i-Pentane)	0.0014	

C10A-2		
Molar Flow	107.1	kgmole/h
Master Comp Mole Frac (Propane)	0.0063	
Master Comp Mole Frac (i-Butane)	0.2833	
Master Comp Mole Frac (n-Butane)	0.7072	
Master Comp Mole Frac (i-Pentane)	0.0030	

T-100		
Minimum Reflux	0.1025	
Minimum Trays	8.151	
Actual Trays	26.72	
Optimal Feed	13.82	
Condenser Duty	-466.6	kW
Reboiler Duty	1067	kW

T-102		
Minimum Reflux	2.337	
Minimum Trays	16.39	
Actual Trays	36.07	
Optimal Feed	21.58	
Condenser Duty	-2032	kW
Reboiler Duty	2531	kW

Figure 4.2 HYSYS flow diagram of the three-column short-cut columns for simulating a Petlyuk column or DWC

The feed streams, which are defined as Streams C6A and C6A-1 in Figure 4.2, are mixed and fed to column T-100. The feed conditions required to converge the feed streams are components, flow rate, pressure and temperature as given in Table 4.1.

Step 2: Solve for column T-100.

In column T-100, the light key components (mainly propane) will be separated as distillate while the heavy key components (C5+) will be separated as bottom product. The intermediate components, which are i-butane and n-butane, will be distributed between the top and bottom products. By taking the propane as the light key component and i-pentane as the heavy key component since they are dominants in their corresponding flows, the mole fraction of the light key in the bottoms and the heavy key in the tops are estimated as 0.006 and 0.0005, respectively. Taking into consideration of balancing the investment cost and operating cost, the DWC is designed at the lowest possible pressure to minimize the investment cost and energy consumption (Long & Lee, 2012d). Therefore, the condenser pressure and the reboiler pressure are specified as 8 bar and 9 bar, respectively. The external reflux ratio is calculated as 1.2 times the minimum reflux ratio (Turton et al., 2009).

Step 3: Solve for column T-101.

In column T-101, the top product stream from column T-100, which is rich in light key components and intermediate components, will be separated. The light key component and the heavy key component specified in this column are propane and i-butane, respectively. The light key in the bottoms (propane) is specified as 0.0063 while the heavy key in the tops (i-butane) is specified as 0.0035 as per the purity requirements provided in Table 4.2. The condenser pressure, reboiler pressure and external reflux ratio are specified similar to that of column T-100.

Step 4: Solve for column T-102.

The bottom product stream of column T-100 is fed to column T-102 which consists of product rich in intermediate components and heavy key components. In this column, n-butane is identified as the light key component, whereas i-pentane is the heavy key component. Taking into account of the purity requirement shown in Table 4.2, the light key in the bottoms and the heavy key in the tops are specified as 0.0050

and 0.0030, respectively. Then, the condenser pressure, reboiler pressure and external reflux ratio are specified similar to that of column T-100. This is to complete the short-cut simulation of column T-102.

Step 5: Solve for the three-column model.

Finally, the specifications of the light key in the bottoms (Stream C7A) and heavy key in the distillate (Stream C8A) of column T-100, which are estimated earlier in Step 2, are varied by trial and error until one has achieved nearly equal compositions of the two side streams, especially for the middle key (butane). The results of the short-cut simulation with the estimated design parameters are displayed in Figure 4.2. The final values obtained for the light and heavy key components of column T-100 are 0.0017 and 0.0004, respectively. In this three-column model approach, the middle product is represented by the addition of two streams: bottom product of column T-101 (Stream C10A-1) and top product of column T-102 (Stream C10A-2). These estimated structural and operational parameters are retrieved for initialization of the rigorous simulation.

4.4. Rigorous Simulation of DWC

Upon completion of the short-cut simulation, the rigorous simulation of the DWC is performed in Aspen HYSYS based on the configuration of Petlyuk column (two-column model) to achieve more accurate results in terms of reflux ratio, condenser duty, reboiler duty, composition distribution and flow rates of interlinking streams and product streams. The DWC is represented by Petlyuk column in Aspen HYSYS simulation because the basic model for the DWC is not provided in Aspen HYSYS's library. Note that, the Petlyuk column is chosen because this configuration is thermodynamically equivalent to actual DWC, assuming negligible heat transfer across the dividing wall (Schultz et al., 2002).

The adoption of several assumptions in short-cut simulation, such as constant relative volatility, constant liquid or vapour molar flows on all stages and single feed, have been reported to lead to inaccuracies or invalid column specifications (Amminudin et al., 2001; Rangaiah et al., 2009). Therefore, it is important that the rigorous

simulation is performed. Please note that, a rigorous simulation can be carried out using equations based on the equilibrium stage model or rate based model, which involves fewer assumptions and hence more realistic than the model used in the short-cut method (Premkumar & Rangaiah, 2009). In this study, the rigorous simulation used is based on the equilibrium-stage model. The types of equations used to represent each stage in this model are material balances, equilibrium relationships, summation equations and heat or enthalpy balances (MESH).

The rigorous simulation starts with the selection of the components and fluid package. In this study, the PR property package is adopted. The steps for the rigorous simulation of a DWC through Petlyuk column (Figure 4.3) are stated as follows.

Step 1: Define and provide input parameters for the feed stream.

As illustrated in Figure 4.3, the feed streams are defined as Streams C6A-5 and C6A-1-4. The feed conditions, which are components, flow rate, pressure and temperature as given in Table 4.1, are provided to the feed streams in Aspen HYSYS.

Step 2: Define and provide input parameters for the input streams to the main column.

As seen in Figure 4.3, the input streams are defined as Stream Main_Vap Internal for the top interlinking stream and Stream Main_Liq Internal for the bottom interlinking

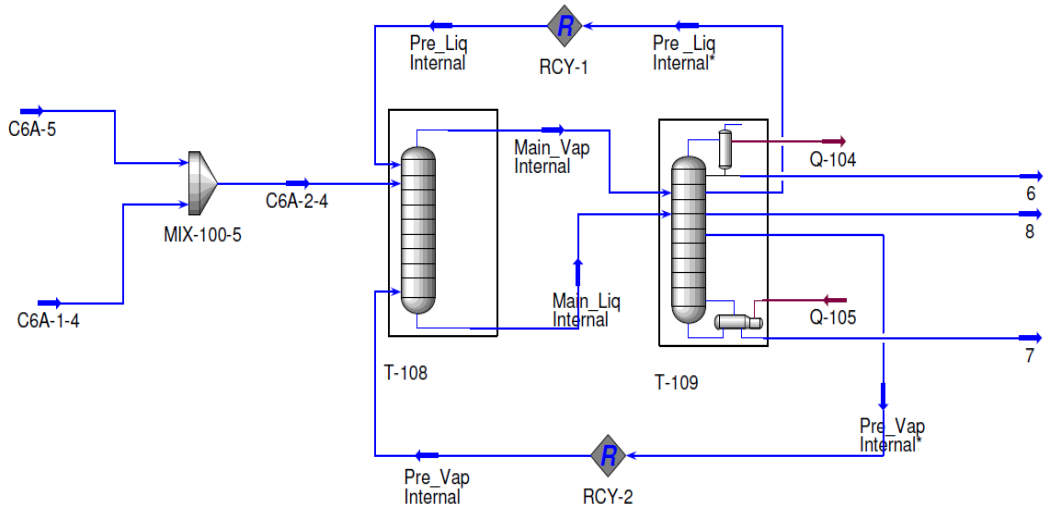


Figure 4.3 HYSYS model for rigorous simulation of a DWC through Petlyuk column

stream. The specifications for both of the streams are obtained from the short-cut simulation. These streams are equivalent to Streams C7A (top interlinking) and C8A (bottom interlinking) in the short-cut simulation.

Step 3: Create the model for main section of the Petlyuk column.

The main section of the Petlyuk column is created in Aspen HYSYS using a distillation column unit. The main section is named as column T-109 in Figure 4.3. The main column (T-109) in the rigorous design is represented by columns T-101 and T-102 in the short-cut simulation. Hence, the number of stages is calculated as the sum of number of trays of columns T-101 and T-102, which are 31 and 37 respectively, with extra two stages. The extra stages are due to additional condenser and reboiler in the short-cut simulation when compared with the rigorous design. It is noted that the additional condenser and reboiler will eliminate each other when columns T-101 and T-102 are combined as one single column in rigorous configuration. Here, the total number of stages calculated is 70 (= 31 + 37 + 2).

Step 4: Attach the input streams to the main column.

The defined input streams (Stream Main_Vap Internal and Stream Main_Liq Internal) are connected to the main column (T-109) using the data (stage locations) obtained from the short-cut simulation. The feed stages of Main_Vap Internal and Main_Liq Internal in the rigorous simulation are taken with respect to their corresponding streams (Streams C7A and C8A) in the short-cut simulation. Their corresponding feed stages obtained are 14 and 54 (= 31 + 22 + 1). Additionally, one stage is required because of the tray numbering in the short-cut simulation.

Step 5: Define the output streams for the main column.

From Figure 4.3, it can be seen that, besides the input streams, the main column is attached to five output streams: Pre_Liq Internal*, Pre_Vap Internal*, top product stream 6, side stream 8 and bottom product stream 7. Streams Pre_Liq Internal* and Pre_Vap Internal* are the connecting streams attached to the top and bottom of the prefractionator, respectively. The energy streams for the column are defined as Q-104 for the condenser and Q-105 for the reboiler.

Step 6: Solve for the main section of the Petlyuk column.

Column T-109 is simulated by employing the data from the short-cut simulation, which are the column specifications and the stage locations for side stream 8, Pre_Liq Internal* and Pre_Vap Internal*. Stream Pre_Liq Internal* leaving the column has the same stage location as Stream Main_Vap Internal entering the column. Also, the stage locations for Streams Main_Liq Internal and Pre_Vap Internal* are the same. The side stream 8 is drawn from the column at stage 31, which is the last stage of column T-101. The specifications selected for the column to converge for this work are reflux ratio, side stream product flow rate, flow rate for Stream Pre_Vap Internal*, and purities of distillate and side stream product.

Step 7: Create the model for prefractionator section of the Petlyuk column.

The prefractionator section of the column is created using an absorber column because it does not have a reboiler and condenser. It is named as column T-108 in Figure 4.3.

Step 8: Define and provide specifications for the interlinking streams (input) of the prefractionator column.

The top and bottom interlinking streams for the prefractionator, which are respectively defined as Pre_Liq Internal and Pre_Vap Internal in Figure 4.3, are specified using the data of the converged streams, Streams Pre_Liq Internal* and Pre_Vap Internal*.

Step 9: Solve for the prefractionator section of the Petlyuk column.

The feed streams, Streams Pre_Liq Internal and Pre_Vap Internal are connected to the prefractionator column (T-108) as shown in Figure 4.3. The location of the feed stage is 14, which is obtained from the short-cut simulation.

Step 10: Solve for the Petlyuk column.

Finally, to complete the simulation, output streams from the main column, Streams Pre_Liq Internal* and Pre_Vap Internal* are connected to the prefractionator column via Streams Pre_Liq Internal and Pre_Vap Internal, respectively using recycle unit

operation in Aspen HYSYS. Manual adjustment of tuning parameters, which are the column specifications as mentioned in Step 6, are required until the convergence of the rigorous simulation is achieved.

4.5. Summary

The simulation design of DWC using the configuration of FTCDS in Aspen HYSYS is presented. Through the identification of the required inputs, a static or steady-state simulation is developed using the short-cut, three-column model for the estimation of the variables required for rigorous simulation. From the rigorous simulation, the parameters for the DWC design are obtained and summarized in Table 4.3.

The design procedure of DWC/FTCDS using Aspen HYSYS is found to be a tedious process. This is because it always requires the transfer of the data from the short-cut columns to the rigorous model which often leads to slow or poor convergence due to the recycle streams. Some trial and error iterations have to be performed to obtain the design results. Therefore, new design procedures will be proposed in the following sections. The results generated via Aspen HYSYS using the design procedure as discussed in this chapter are used as the basis to validate the proposed new model and method.

Table 4.3 Summary of the DWC Design based on rigorous simulation

Parameters	**Prefractionator Section**	**Main Column**
Number of Trays	29	70
Feed Stage	14	-
Feed stage of Main_Vap Internal	-	14
Feed stage of Main_Liq Internal	-	54
Stage location of side stream 8	-	31

CHAPTER 5: FUNDAMENTAL MODELS FOR DISTILLATION

In this chapter, an improved Lewis-Matheson (LM) stage-by-stage procedure is proposed by incorporating the Fenske equation to enhance the estimation of the non-key component distributions, and thus avoiding infeasible solutions to the stage-by-stage system of equations of mass and energy balances. A modified theta method is also included in the design procedure to satisfy the feed stage matching criteria. Instead of only using the theta method for the feed plate matching as in most of the existing calculation methods, a ratio of the liquid compositions is also introduced as the convergence criterion to increase the accuracy of the matching. The output from the process design is then used in equipment and tray hydraulic designs. The equipment design discussed in this chapter includes column and its internals, reboiler, and condenser. The hydraulic test is also performed to ensure the feasibility of the determined column size. The effectiveness of the proposed design procedure is demonstrated using an industrial-scale natural gas liquids (NGLs) depropanizer fractionation unit. The rest of this chapter is structured as follows. In Section 5.1, an improved process design procedure is proposed and its details are discussed in the same section. In Section 5.2, the equipment design for the distillation unit is discussed. The case study to demonstrate the application of the design model is provided in Section 5.3 and followed by a summary in Section 5.4.

5.1. Process Modelling of a Distillation Column

In this study, the multi-component distillation column (hydrocarbon system) is modelled using a modified rigorous model, which is developed based on the proposed modified LM stage-by-stage design procedure at steady state and ideal stage conditions. Figure 5.1 presents a typical distillation column with N stages (including a partial reboiler): a column with one feed, a liquid distillate stream (D) and a liquid bottom product stream (B) with no side product stream. In the column, the vapour and liquid, contacting each other, is assumed to reach equilibrium on each

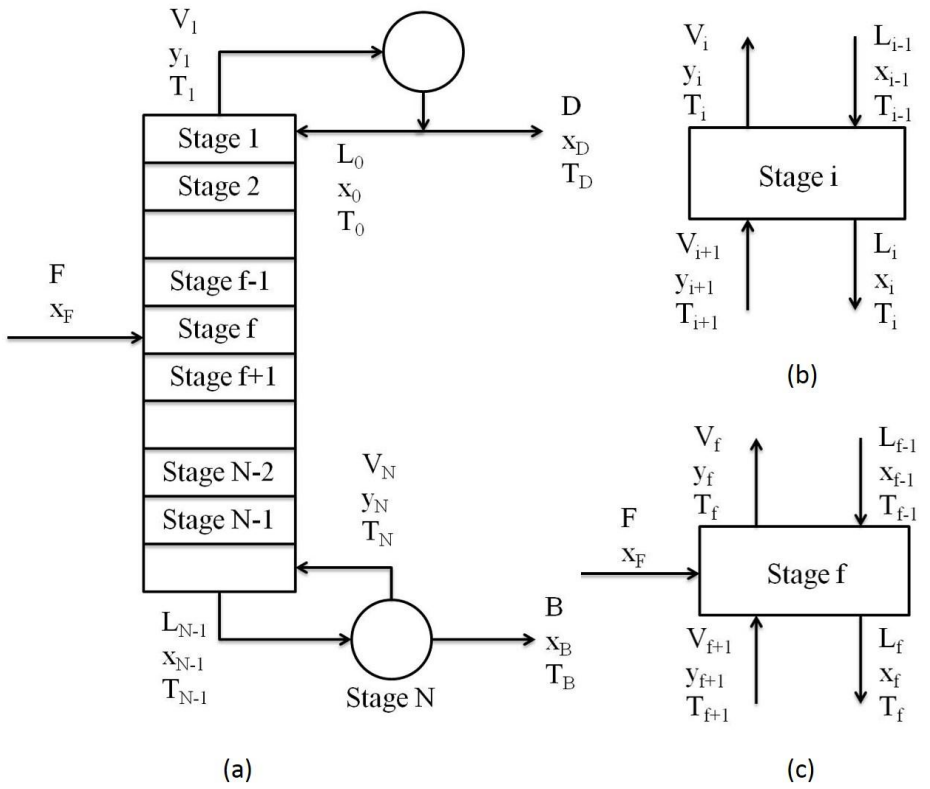


Figure 5.1 Distillation column models: (a) Overall column model; (b) Stage model; (c) Feed stage model

tray. The counter-current flow of the vapour and liquid in the column carries the light (volatile) components to the top while the heavy components to the bottom. A condenser at the top and a reboiler at the bottom of the column are to provide the condensing liquid and boil-up vapour, respectively.

5.1.1. Basic assumptions and equations

The types of condenser and reboiler used in the distillation design are assumed to be a total condenser and a partial reboiler. As illustrated in Figure 5.1, the trays are numbered from the top to the bottom of the column. The feed (F) enters the column at feed stage *f* as saturated liquid. At this feed stage, the liquid compositions calculated from the top and bottom sections are matched by correcting the initial estimate on the distillate composition. The pressure drops in the condenser and across a column tray are taken as 14 kPa and 0.7 kPa (per tray), respectively (Seader et al., 2011).

The basic equations for each component, known as MESH (Mass-Equilibrium-Summation-Heat) equations, are used to construct the distillation models for the reboiler, condenser, and each stage. Denoting *i* as the tray index numbering from stage 1 (top) to the reboiler and *j* as the component, the balance equations for the column are described below.

Overall material balances are as follows.

The mass balance in the condenser:

$$L_0 + D - V_1 = 0 \tag{5.1}$$

The mass balance in a i^{th} tray in the sections where *i = 1, 2,...f-1* and *i = f+1, f+2,...N-1*:

$$L_i + V_i - L_{i-1} - V_{i+1} = 0 \tag{5.2}$$

Meanwhile, the mass balance in the feed stage (*i = f*) is:

$$L_i + V_i - L_{i-1} - V_{i+1} - F = 0 \tag{5.3}$$

and in the reboiler (i = N):

$$B + V_N - L_{N-1} = 0 \tag{5.4}$$

Component material balances are given as follows.

For the condenser:

$$(L_0 + D)x_0^j - V_1 y_1^j = 0 \tag{5.5}$$

In the column sections where *i = 1, 2,...f-1* and *i = f+1, f+2,...N-1*:

$$L_i x_i^j + V_i y_i^j - L_{i-1} x_{i-1}^j - V_{i+1} y_{i+1}^j = 0 \tag{5.6}$$

In the feed stage (*i = f*):

$$L_i x_i^j + V_i y_i^j - L_{i-1} x_{i-1}^j - V_{i+1} y_{i+1}^j - F x_F^j = 0 \tag{5.7}$$

For the reboiler:

$$Bx_B^j + V_N y_N^j - L_{N-1} x_{N-1}^j = 0 \tag{5.8}$$

Note that, the equilibrium relation, which assumes that the streams leaving the stage are in equilibrium with each other, is expressed as:

$$y_i^j - K_i^j(T_i, P, x_i)x_i^j = 0 \tag{5.9}$$

The summation equation, as shown in (5.10), is provided to ensure the correct specifications on the mole fractions.

$$\sum_{j=1}^{C} y_i^j - \sum_{j=1}^{C} x_i^j = 0 \tag{5.10}$$

Heat (enthalpy) balances are described as follows.

The enthalpy balance in the condenser ($i = 0$) is:

$$(L_0 + D)H_{L0} - V_1 H_{V1} + Q_{cond} = 0 \tag{5.11}$$

For the column sections where $i = 1, 2,...f-1$ and $i = f+1, f+2,...N-1$:

$$L_i H_{Li} + V_i H_{Vi} - L_{i-1} H_{Li-1} - V_{i+1} H_{Vi+1} = 0 \tag{5.12}$$

In the feed stage ($i = f$) the enthalpy balance is:

$$L_i H_{Li} + V_i H_{Vi} - L_{i-1} H_{Li-1} - V_{i+1} H_{Vi+1} - F H_F = 0 \tag{5.13}$$

In the reboiler ($i = N$):

$$BH_B + V_N H_{VN} - L_{N-1} H_{LN-1} - Q_{reb} = 0 \tag{5.14}$$

The notations used in the mass-energy balance equations: L and V denote the liquid and vapour flows respectively, D and B the top and bottom product flow, x and y the component fractions in liquid and vapour phase, H_L and H_V the enthalpies for the liquid and vapour phases, Q_{cond} and Q_{reb} the condenser and reboiler duties, and K denotes the equilibrium constant calculated based on the Peng-Robinson (PR) vapour-liquid equilibrium (VLE) equations, which are widely used for light hydrocarbon mixtures (Aspen Technology, 2011). The models for PR and enthalpies of the liquid and vapour can be found in Appendix A.

5.1.2. Process design procedure

Figure 5.2 illustrates the steps involved in the proposed modified LM design method. The details on the step-by-step procedures are described as follows.

Step 1: To initiate the stage-by-stage calculation, the feed composition and flow rate, reflux ratio (*R*), flow rate of distillate (*D*) or bottom product (*B*), and fractional recovery of the light key (LK) or heavy key (HK) component in the distillate or bottoms have to be specified.

Step 2: With these initial estimates on the distillate and bottom component flow rates, the dew point and bubble point calculations are performed respectively on the top and bottom products.

Step 3: The distributions of the components calculated for each stage using the standard LM model are very sensitive to the initial guess values of the distillate component flow rates. Hence, good initial guess values of the flow rates for non-key components are required for achieving a rapid convergence of the column calculations. To overcome this limitation, the Fenske equations as given in (5.15) and (5.16) are incorporated into the standard LM model to revise the estimated product distributions of the non-key components.

$$d_j = \frac{f_j (d_r / b_r)(\alpha_{j,r})_m^{N_{\min}}}{1 + f_j (d_r / b_r)(\alpha_{j,r})_m^{N_{\min}}} \tag{5.15}$$

$$b_j = f_j - d_j \tag{5.16}$$

where d_j, b_j and f_j are the flow rates of the components in the distillate, bottom product and feed, respectively; d_r and b_r are the corresponding reference (LK or HK) components' flow rates in the distillate and bottom steams, and $(\alpha_{j,r})_m^{Nmin}$ is the geometric-mean relative volatilities with N_{min} is the minimum number of stages determined using (5.17).

$$N_{\min} = \log\{[x_{LK} / x_{HK}]_d [x_{HK} / x_{LK}]_b\} / \log \alpha_{LK,HK} \tag{5.17}$$

where $\alpha_{LK,HK}$ is the average relative volatility of the light key with respect to the heavy key, whereas $[x_{LK} / x_{HK}]_d$ and $[x_{HK} / x_{LK}]_b$ are the ratios of the compositions for the corresponding distillate and bottom products.

Step 4: With the revised product distributions, stage-by-stage calculations are performed in both of the rectifying and stripping sections to determine their respective number of stages. In the rectifying section, the top-down calculations are carried out; the bottom-up calculations are executed in the stripping section until the feed stages' liquid compositions converge to the feed compositions.

Step 5: Then, the bottom-up calculations in the stripping section are revised to meet the feed stage pressure drop.

Step 6: Another restriction of the standard LM design method is the slow convergence problem at the feed stage. The theta method, as proposed by C. D. Holland (1981) in Thiele-Geddes (TG) calculation for correcting the compositions of the distillate and bottom products, is used in the classic LM model to satisfy the feed plate matching condition. The plate matching condition indicates that the liquid composition leaving the feed stage calculated from the rectifying section (x^{j}_{fT}) must equal to the composition obtained from the stripping section (x^{j}_{fB}) for all components. To achieve a better matching at the feed stage of the liquid compositions obtained from both sections, the original equations from the theta method are modified by introducing a ratio of the liquid compositions at the feed stage, γ^{j}. The proposed equations that serve to correct the distillate component flows or compositions are described as follows:

$$\gamma^{j} = x^{j}_{fT} / x^{j}_{fB} \tag{5.18}$$

$$g(\theta) = \sum_{j=1}^{C} \frac{F x^{j}_{F}}{1 + \theta \gamma^{j} \left(b^{j} / d^{j} \right)_{cal}} - D = 0 \tag{5.19}$$

$$d^{j} = \frac{F x^{j}_{F}}{1 + \theta \gamma^{j} \left(b^{j} / d^{j} \right)_{cal}} \tag{5.20}$$

$$x^{j}_{D} = d^{j} / \sum_{j=1}^{C} d^{j} \tag{5.21}$$

where θ is the positive root which makes $g(\theta) = 0$. The convergence has been achieved if the $g(\theta)$ obtained is within the prescribed tolerance. Otherwise, the calculations are repeated by revising the distillate component flows using new γ^j and θ. It should be noted that, the resulting column design based on the modified LM method can be further compared and validated using other techniques, e.g., using Aspen HYSYS.

5.2. Equipment and Tray Hydraulic Designs

Once the process design is established, the design of the major equipment for the distillation system begins. Generally, a conventional distillation unit consists of a vertical shell, column internals such as trays or packings, a condenser, and a reboiler. The equipment and plate hydraulic designs do not only provide preliminary estimates of the equipment size and tray features, but also to ensure that flooding condition, weeping point, pressure drop, entrainment, and other constraints are all within reasonable ranges.

Over the last decades, there have been many hardware design methodologies and procedures proposed for the distillation unit (Biegler et al., 1997; Kister, 1992; Perry & Green, 1997; Sinnott, 2005). However, there is a lack of work demonstrating the application of these methodologies in the capital cost calculation for the economic analysis of the distillation system. Most of the works only provide simple estimation of the column diameter without taking into consideration of the hydraulic conditions. Therefore, a heuristic for the mechanical design with tray hydraulic calculations is presented in this section to ensure the feasibility of the determined column size and tray features. The heuristic is developed based on the adaptation of the methodology proposed by Kister (1992). This methodology has been known as one of the most favourable methodologies applied for the mechanical design of a conventional distillation column. Some modifications have been made to the procedure for the ease of computation in Matlab programme. The detailed procedure for the design is discussed in the following sections.

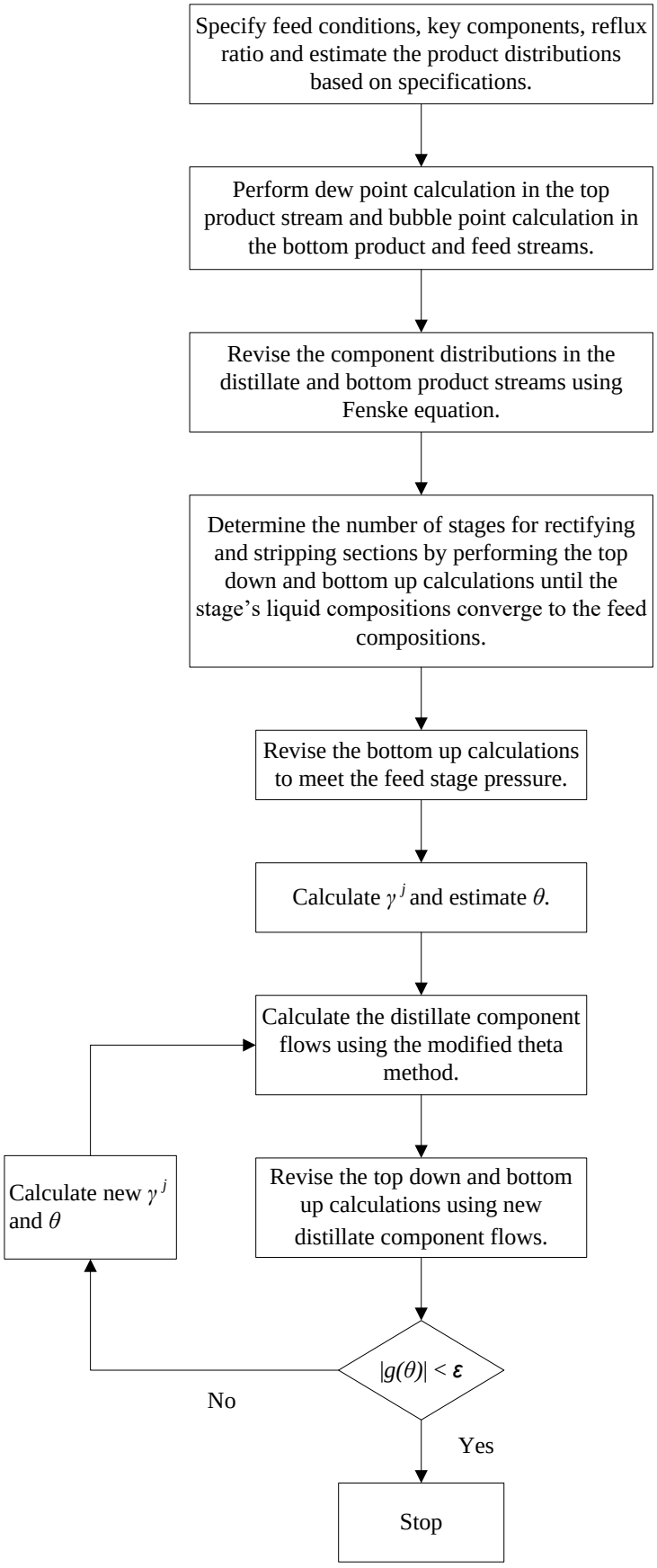


Figure 5.2 Flow chart for proposed modified LM model

5.2.1. Column and tray hydraulic designs

The types of the column internals widely used in the industry today can be classified as two: trays and packing. In a tray column, the gaseous mixture and the liquid are brought into contact through a series of trays; while the gaseous mixture and the liquid in a packed tower are contacted counter-currently in continuous manner. The factors for the selection of the column type depends upon the operating pressure, liquid and vapour loads, characteristic of the process (fouling, corrosive, and foaming), and design reliability (Chuang & Nandakumar, 2000).

Tray column is usually more preferable than the packed column when handling wide range of liquid and vapour rates, fouling liquids, and substantial temperature change during operation and high operating pressure. On the other hand, packed column is more suitable for foaming and pressure sensitive system, and able to handle toxic and flammable liquids because of the low liquid holdup. In this work, the tray column is chosen for the mechanical design as the columns involved in the NGLs fractionation unit, e.g. deethanizer and depropanizer, are high pressure system, where pressure drop is not a significant consideration. Moreover, the tray column is also more economic than the packed column for large diameter column (size larger than 2 feet) (Perry & Green, 1997).

The mode of flow for the tray column may be categorized as cross-flow and counter-current (dual flow) plates (Perry & Green, 1997). The cross-flow plate, as illustrated in Figure 5.3a, allows the liquid to move from tray to tray in the column through downcomers and a weir is employed on each plate to control the liquid level on the trays. The vapour flow path in the column is perpendicular to the liquid flow path. Conversely, the liquid and vapour for the counter-current plate (Figure 5.3b) pass through the openings in the plates without the downcomers. The cross-flow plate is a more widely used plate contactor than the counter-current plate due to the wider operating range and better heat-mass transfer efficiency. For the cross-flow plate, three basic types of the plates are sieve plate, valve plate and bubble cap plate. Among them, sieve and valve plates are most frequently encountered in modern distillation practice. In this study, sieve tray is chosen for the column design because

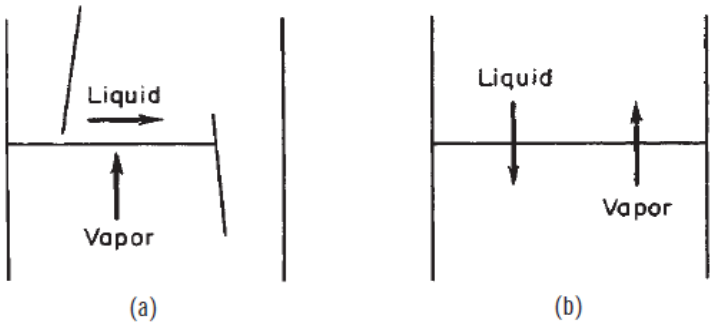


Figure 5.3 Mode of flow for tray column: (a) Cross-flow plate; (b) Counter-current plate

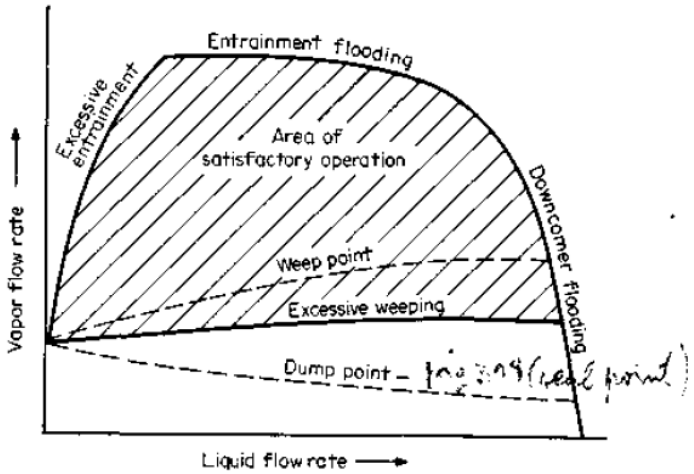


Figure 5.4 Sieve tray performance diagram

of its well established design procedure, low capital and maintenance cost, high capacity, and ease of cleaning although it has smaller turndown ratio (Kister, 1992).

The main objective of the column sizing is to determine the column diameter and height, which are later used in the capital cost calculation (Chuang & Nandakumar, 2000). The column diameter is depending on the liquid and vapour loads obtained from the process design, whereas the column height is relying on the number of equilibrium stages required for the separation process. To achieve minimum cost of the column, it is crucial to ensure the minimization of the column volume. Moreover, the hydraulic check on the column is also incorporated in the costing procedure to ensure the feasibility of the column size. To ensure satisfactory operation, a sieve tray should operate in the shaded area which is bound by the tray stability limits as shown in Figure 5.4. From the figure, it can be seen that the upper capacity is set by

the condition of flooding, while the lower limit is determined by the weeping condition (Kister, 1992).

The procedure for the column and its internal design is illustrated in Figure 5.5. The descriptions on the step-by-step procedures are presented as follows.

Step 1: The first step of the procedure is to obtain the data required for the mechanical design. The information required include liquid and vapour flow rates which are gained from the process design discussed in Section 5.1. Besides that, the physical properties of the mixture, such as molecular weight, density, viscosity, and surface tension, are also required. The selection of the methods in the calculations of the required physical properties in this work have to be appropriate to the hydrocarbon system since the scope of this study is limited to NGLs fractionation unit. The molecular weight of the mixture is computed via Kay's rule using the data from Perry and Green (1997); the Hankinson method has been employed for calculating the density of the liquid phase; the PR equations are employed to calculate the density of the gas phase; the viscosity of the liquid mixture is determined through a mixing rule developed by Kendall and Monroe based on the components' viscosities calculated utilizing the procedure as outlined in the API Technical Data Book (Fitzgerald & Daubert, 1997); the surface tension of the mixture is computed using the approach originally proposed by Macleod (1923) and further developed by Sugden (1924).

Step 2: Since the vapour and liquid loads and the physical properties change throughout the column, the column is designed by first diving it into two sections: rectifying section and stripping section. For each section, the stages selected for hydraulic calculations are the stages with maximum and minimum throughput (vapour and liquid loads). All of the hydraulic calculations are carried out based on the maximum throughput of the stages for each section except for the weeping condition. This is due to the reason that the operational issues often occur on the stage with highest flow rate. The weeping check on the stages is performed based on the minimum throughput at turndown state. The main purpose of considering the design at turndown state is to define the limit at which the efficiency starts to decrease due to weeping.

Step 3: After the data required has been computed, the preliminary specifications of the tray which are essential for the initial estimation of column diameter are proposed. For accessibility purpose, the initial tray spacing suggested is 600 mm (24 in). Assuming mildly fouling service, the hole diameter of 12.7 mm (0.5 in) is commonly used to initiate the calculation. Other parameters proposed are clear liquid height at the transition from the froth to spray regime of 63.5 mm (2.5 in), flooding factor of 0.8, and foaming factor of 0.9 (Kister, 1992; Turton et al., 2009). Using these assumed values, the preliminary determination of tray area for each section is performed via the application of the Kister and Haas (1987). This correlation is chosen for the prediction of the flooding velocity in the initial step because it is the least conservative approach which can prevent oversized issue as the over-sizing of the column can cause higher capital cost. After the estimation of the downcomer area, the column diameters for each section are computed.

Step 4: According to Kister (1992), if the diameter difference between the rectifying and stripping section is less than 20 percent, it is likely to be economical to use uniform column diameter. Therefore, the larger of the two computed diameters will be selected as the preliminary column diameter. The selected diameter is then round to the next smallest half foot (0.1524 m).

Step 5: Once the diameter of the column is computed, the first parameter to be set is the number of tray passes. The flow path arrangements used in the tray column can be divided into single-pass, and multi-pass as shown in Figure 5.6. When the liquid flow rate exceeds 13 gpm per inch of outlet weir, the multi-pass trays will be considered. In this work, the number of passes up to four, excluding three-pass trays, are considered because less symmetrical characteristic of odd number of passes will cause difficulty in achieving adequate liquid distribution. The design for the multi-pass trays is based on the manufacturer (Koch-Glitsch, 1993).

Step 6: After that, a trial tray layout is specified based on the guidelines provided by Kister (1990). The parameters to be specified or revised at this section are tray spacing, hole size, fractional hole area, weir height (50.8 mm or 2 in), downcomer clearance (38.1 mm or 1.5 in), and plate thickness. The turndown required is also set at a typical range of 60 to 70 percent of full load flow rates.

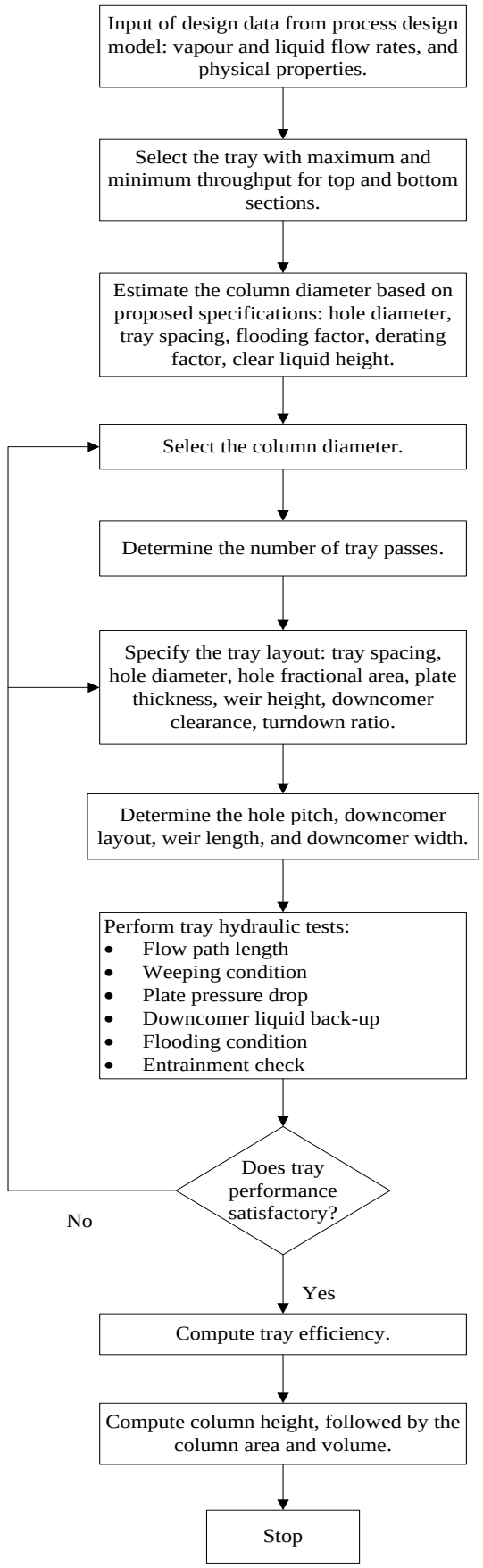


Figure 5.5 Procedure for column sizing with hydraulic test (sieve tray)

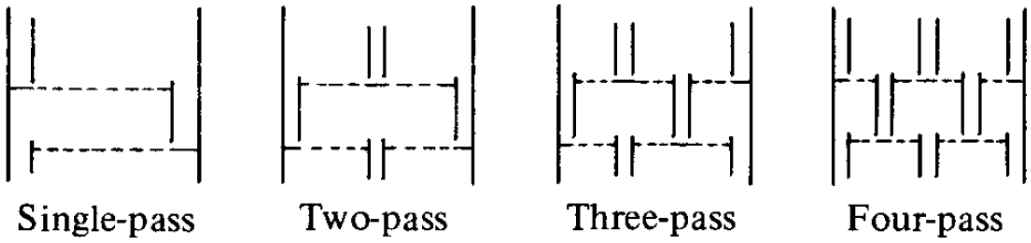


Figure 5.6 Flow path arrangements for tray column: (a) Single-pass; (b) Two-pass; (c) Three-pass; (d) Four-pass

Step 7: Utilizing these specified values, the hole pitch (equilateral triangular arrangement), downcomer layout, weir length and downcomer width are determined.

Step 8: Then, the performance or hydraulic tests are made to ensure the feasibility of the design. The first check is done on the liquid flow path length. According to the guideline provided by Kister (1990), the flow path length has to be larger than 0.4064 to 0.4572 m (16 to 18 in). If the minimum path length is exceeded, the diameter of the column can be increased (go to Step 4). The second check is performed on the weeping at turndown condition using the weeping velocity method as proposed by Sinnott (2005) or pressure balance method as suggested by Wankat (2012). If the weeping condition is excessive, the hole diameter and fractional hole area can be reduced or the turndown percent can be increased (go to Step 6). The design range for the hole diameter is 5 to 19 mm (3/16 to 3/4 in) and the fractional hole area is 5 to 10 percent for pressurized operation.

The next hydraulic check is performed on the tray pressure drop using Fair's pressure drop correlation (Perry & Green, 1997; Sinnott, 2005). The pressure drop at the range of 0.0055 to 0.0083 bar (0.08 to 0.12 psi) per tray is recommended for stable operation. This range is closed to the pressure drop per tray of 0.007 bar used earlier in the process design in Section 5.1. Thus, there is no requirement to revise the pressure drop per tray in the earlier section. If the pressure drop calculated is outside the desired range, the adjustment can be made to the fractional hole area if dry pressure drop dominates or the weir height if wet pressure drop dominates (go to Step 6). Alternatively, the column diameter can be altered (go to Step 4).

Then, the downcomer liquid back-up is checked to ensure the aerated liquid must not exceed the sum of the tray spacing and weir height. If this is excessive, the tray spacing or diameter will be increased (go to Steps 4 or 6). This procedure is later followed by flooding and entrainment tests. The flooding is computed based on the procedures of Kister and Haas, Fair, and Smith as proposed by Kister (1992). The flooding percent calculated must fall below 100% for the tray to be operable. The liquid entrainment, which is calculated using the Fair's entrainment correlation, must be lower than 1%. Otherwise, the column diameter or the tray spacing can be increased to prevent flooding (go to Steps 4 or 6).

Step 9: The main output from the above column sizing and hydraulic tests are the column diameter and tray spacing. To proceed with the calculation of the column height, the column efficiency has to be determined first due to the initial assumption of equilibrium state at each stage used in the process design. This assumption may not be practical because the vapour phase and liquid phase compositions for the streams leaving a stage are not in equilibrium with each other in real condition. Therefore, the actual number of stages of a column must be obtained by considering stage efficiency. Several methods have been proposed to estimate the tray efficiency (Kister, 1992; Seader et al., 2011; Sinnott, 2005). Among these methods, the O'Connell correlation, which is one of the best empirical methods available for tray efficiency prediction and highly recommended by Kister (1992) and most literature sources, is applied in this study. Moreover, since the NGLs fractionation unit is the focus of this work, it is reasonable and reliable to utilize this correlation as it is developed based on the test data from hydrocarbon or hydrocarbon related components.

Step 10: The total height of column is calculated by taking into account of tray stack, extra feed space, disengagement space (top and bottom) and skirt height. The tray stack of the column is estimated using the obtained tray spacing and actual number of stages, whereas the disengagement space (top and bottom) and the skirt height are taken as 3 m and 1.5 m respectively. The extra feed space is assumed to be 1.5 m (Biegler et al., 1997). Last of all, the column area and volume are computed for capital cost estimation.

5.2.2. Condenser and reboiler designs

For the reboiler and condenser, the areas are calculated as:

$$A = \frac{Q}{U\Delta T_M} \tag{5.22}$$

where $Q =$ Heat transfer per unit time, W

$U =$ Overall heat transfer coefficient, W/m^{2o}C

$$\Delta T_M = \frac{\left(T_{hot,out} - T_{cold,in}\right) - \left(T_{hot,in} - T_{cold,out}\right)}{\ln\left(\frac{T_{hot,out} - T_{cold,in}}{T_{hot,in} - T_{cold,out}}\right)}, \ ^{o}\text{C}$$

The overall heat transfer coefficients for the reboiler and condenser are 1140 W/m^{2o}C and 850 W/m^{2o}C, respectively (Turton et al., 2009).

5.3. Case Study

The new design procedure from Section 5.1 and Section 5.2 is demonstrated in a case study to ensure the feasibility of the procedure. To validate the process design model (Section 5.1), the results from the proposed model will be compared with the rigorous simulation results in Aspen HYSYS. An industrial-scale natural gas liquids (NGLs) fractionation unit, i.e., a depropanizer column is chosen as the case study by considering a 5-component hydrocarbon mixture (Long & Lee, 2012c). The proposed design procedure is developed and solved using Matlab (Appendix B.1 and B.2).

5.3.1. Input parameters for the process design

In the depropanizer, the propane is removed from the mixture as the distillate, whereas the remaining hydrocarbons end as the bottom product. The minimum purity of the propane at the top product stream is 0.9027 and its amount at the bottom product stream is set to be less than 0.02. The steam supplied to the reboiler is assumed to be low pressure steam at a pressure of 5 barg and a temperature of 160^{o}C.

Table 5.1 Feed and products conditions of the depropanizer

Components	Mole Fraction
Ethane (C_2)	0.0418
Propane (C_3)	0.4990
i-Butane (iC_4)	0.1222
n-Butane (nC_4)	0.2610
i-Pentane (iC_5)	0.0759
Total Molar Flow (kmol/h)	3769
Feed Pressure (bar)	17.75
Feed liquid fraction, q_F	1
Pressure of top product stream (bar)	17.50
Minimum purity of C_3 at top stream (Mole fraction)	0.9027
Minimum purity of C_{4+} at bottom stream (Mole fraction)	0.9800

For the condenser, the cooling water is supplied from cooling tower at a temperature of 30^{o}C. The distillate pressure chosen has to ensure that the dew point of the distillate to be substantially above that of the cooling water temperature. In this case, the distillate pressure of 17.5 bar is taken.

The feed mixture at 31.47 bar pressure as given in the work of Long and Lee (2012c) will be flashed to the column feed stage pressure of 17.75 bar before supplied to the column. The feed stage pressure is estimated from the average of dew point calculation of top product stream and bubble point of the bottom product stream. Assuming saturated liquid feed, the feed temperature of 68^{o}C is obtained. The required feed and products conditions of the depropanizer for the computation are presented in Table 5.1. From the components provided in the table, the propane is defined as the light key and the i-butane is defined as the heavy key.

5.3.2. Verification of the process design model

The equipment and hydraulic tray sizing are highly depending on the output of the process design model. Therefore, it is crucial to validate the proposed process design model to ensure the viability of the overall design. For the validation purpose, the rigorous process design is carried out based on the modified LM design procedure as

given in Figure 5.2, with estimated initial values for product distributions and reflux ratio (R). By using the rigorous model, the minimum R value required to achieve the convergence is 2.05. Therefore, the R specified for the process design must be larger than this value. Due to the nonlinear characteristic of the light key purity as shown in Figure 5.7, the reflux ratio of 2.2 is chosen in this case study to meet the minimum purity requirement at the top product stream.

Then, using the same specified parameters and the variables obtained from the proposed design model as given in Table 5.2, the rigorous simulation is performed using Aspen HYSYS. The process design modelled in the Aspen HYSYS is known as the "actual" or benchmark design. The results obtained from the proposed model are compared with those obtained from Aspen HYSYS. The results of the comparison are presented in Table 5.3. From the table, it can be observed that the results from the rigorous simulation, which include the condenser duty, reboiler duty, compositions, total molar flow, and temperature for top and bottom products, agree well with the results computed using the proposed model.

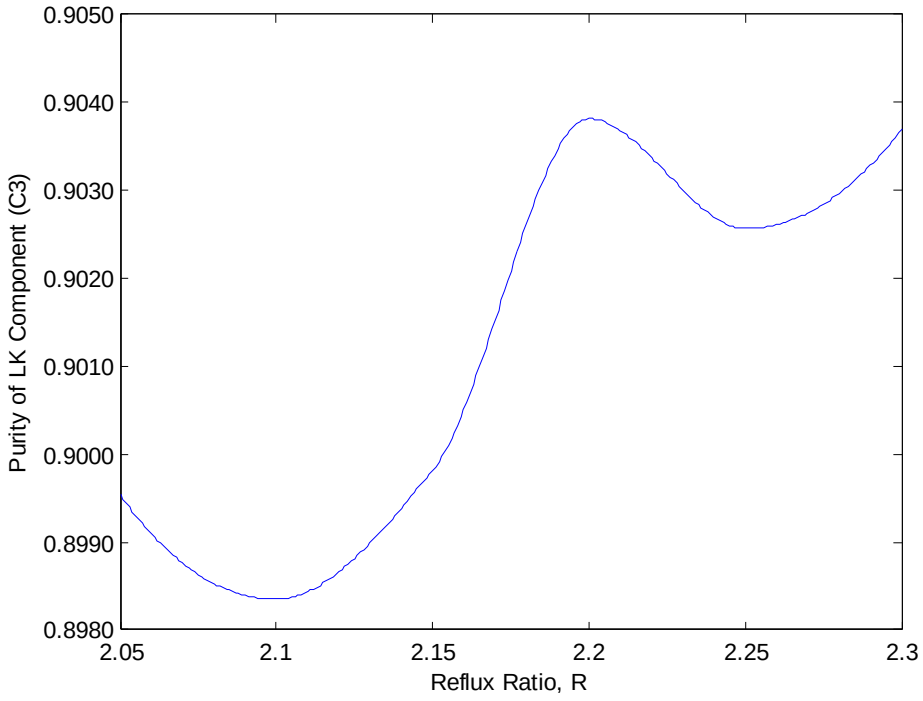


Figure 5.7 Purity of the light key component (C_3) at distillate for increasing reflux ratio

Table 5.2 Variables obtained from the proposed design model for Aspen HYSYS simulation

Parameters	Value
Purity of C_3 at top stream (Mole fraction)	0.9038
Number of stages, NT	25
Feed stage location, Nf	12
Pressure at first stage (bar)	17.64
Pressure at final stage (bar)	17.79

Table 5.3 Comparison of the results between the proposed design model and Aspen HYSYS simulation

Components	Proposed Model (Mole Fraction)		HYSYS Simulation (Mole Fraction)	
	Top Product	Bottom Product	Top Product	Bottom Product
Ethane (C_2)	0.0768	2.29E-8	0.0764	0.0000
Propane (C_3)	0.9038	0.0152	0.9038	0.0109
i-Butane (iC_4)	0.0161	0.2491	0.0166	0.2497
n-Butane (nC_4)	0.0033	0.5691	0.0032	0.5719
i-Pentane (iC_5)	9.29E-7	0.1667	0.0000	0.1675
Total Molar Flow (kmol/h)	2052	1717	2060	1709
Temperature (^oC)	49.60	108.97	44.69	108.7
Condenser Duty, Qcond (MW)	22.14		23.58	
Reboiler Duty, Qreb (MW)	24.43		25.32	

The validation of the internal condition of the column can also be performed via comparison in terms of temperature and compositions profile. Figure 5.8 illustrates the temperature profile for the HYSYS Simulation and the proposed model; while the liquid compositions profile is given in the Figure 5.9. As seen from the figures, the profiles obtained from HYSYS simulation shows a strong agreement with the profiles from the proposed model. This means that the proposed method works well for the distillation process design. The effectiveness of the modified theta method in increasing the accuracy of feed stage composition matching is shown in Table 5.4. From the table, it is noticed that up to 53 % of relative differences of the feed stage

compositions computed from the rectifying and stripping sections can be achieved using the original theta method. These relative differences are reduced to around 0.01% when the modified theta method is applied.

Table 5.4 Comparison between feed stage compositions obtained using original theta method and modified theta method

Components	Theta Method			Modified Theta Method		
	x_{fT}* (Mole Fraction)	x_{fB}** (Mole Fraction)	Relative error (%)	x_{fT}* (Mole Fraction)	x_{fB}** (Mole Fraction)	Relative error (%)
Ethane (C_2)	0.011297	0.005327	52.8426	0.011398	0.011397	0.0039
Propane (C_3)	0.500521	0.530027	5.8951	0.513497	0.513472	0.0050
i-Butane (iC_4)	0.156293	0.162509	3.9775	0.167111	0.167112	0.0034
n-Butane (nC_4)	0.269025	0.253083	5.9258	0.258259	0.258275	0.0062
i-Pentane (iC_5)	0.062865	0.049053	21.9705	0.049733	0.049737	0.0087

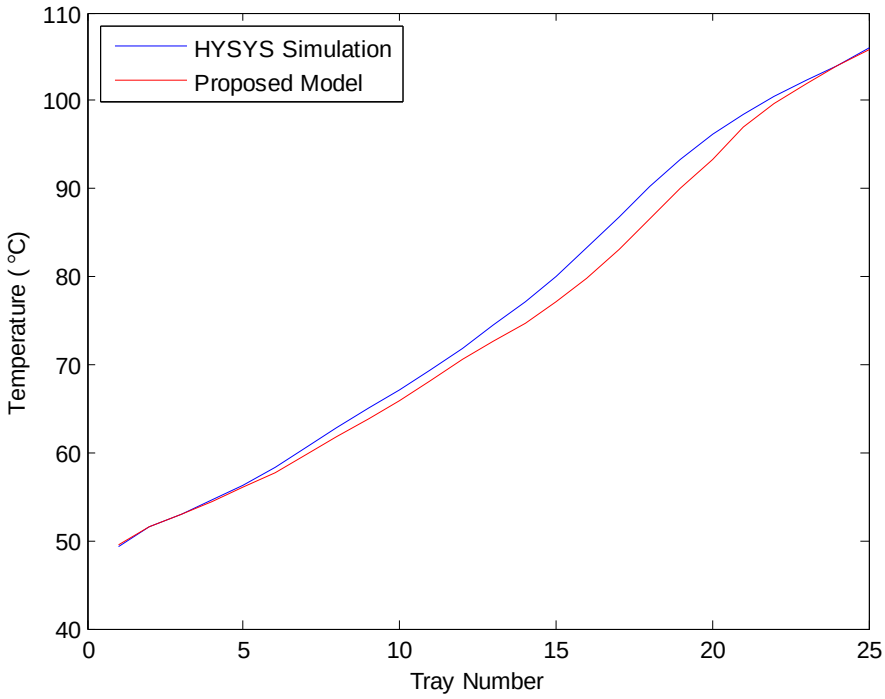
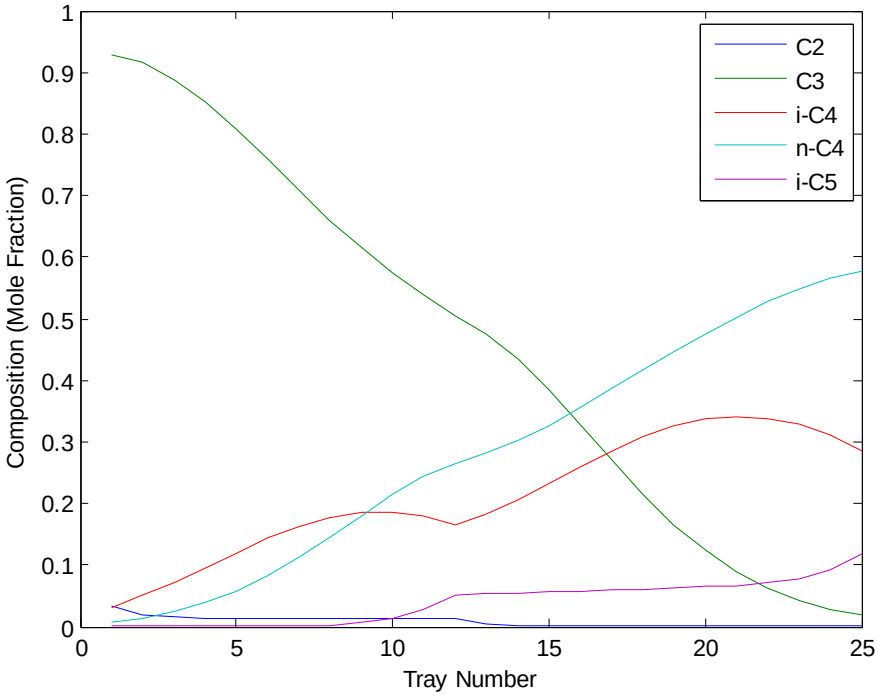
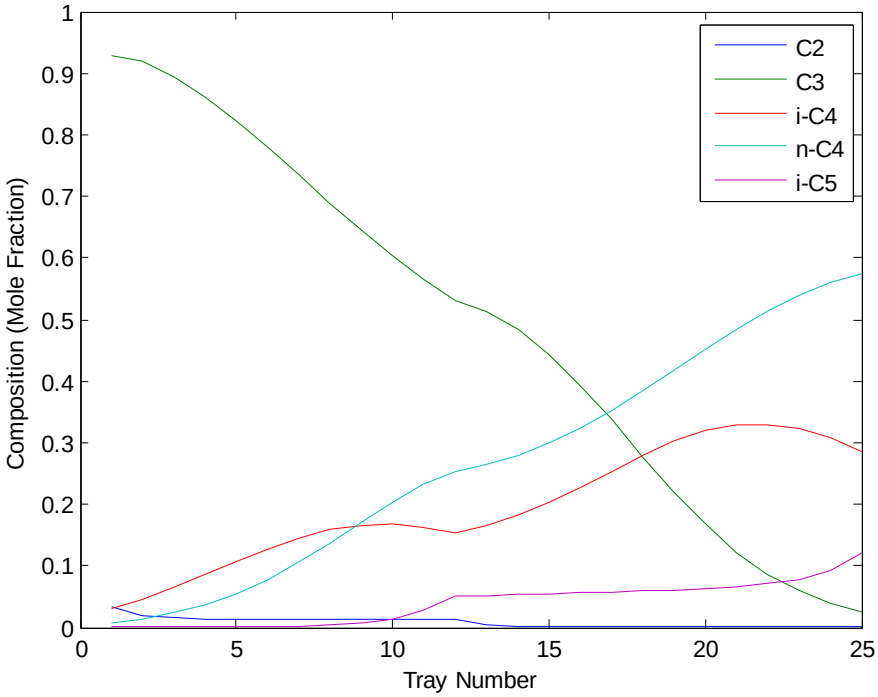


Figure 5.8 Comparison of temperature profile between the proposed design model and Aspen HYSYS simulation



(a)



(b)

Figure 5.9 Liquid compositions profile for column: (a) HYSYS Simulation; (b) Proposed Model

5.3.3. Application of the equipment design procedure

The validated proposed model will be used as a basic model for overall design, of which the sizing of the column system is included. To initialize the mechanical design of the column, the trays selected for the analysis have to be first determined. These trays are chosen based on the C-factor due the difference of trays with maximum and minimum vapour loads in each column section (Kister, 1992). The selected trays for the hydraulic calculations and their corresponding flow rates are given in Table 5.5.

As mentioned in Section 5.2, the hydraulic design of the column is carried out by performing the hydraulic tests until it meets the operable design criteria using the given initial design. All the tests are performed in Matlab and the results of the final design are presented in Table 5.6. After that, the overall efficiency of the column is computed. The overall efficiency obtained is 67.81%. This value is acceptable because it falls within the range of 60 to 90% as given by Turton et al. (2009).

Also, the height calculated, using the actual number of trays estimated based on overall efficiency, tray spacing for top and bottom sections, extra feed space, disengagement space (top and bottom) and skirt height, is 26.32 m. The results of the equipment design for the column, reboiler, and condenser are summarized in Table

Table 5.5 Selected trays with respective liquid and vapour loads for the hydraulic calculations

Parameters	Top Section		Bottom Section	
	Maximum	Minimum	Maximum	Minimum
Stage Number	1	11	22	12
Vapour Mass Flow (kg/h)	284,290	280,790	390,910	280,210
Vapour Volumetric Flow (m^3/h)	7,217	6,886	8,282	6,866
Liquid Mass Flow (kg/h)	192,970	191,360	491,980	393,520
Liquid Volumetric Flow (m^3/h)	423	416	1,085	851

Table 5.6 Final design of the tray overcoming the hydraulic test

Parameters	Top Section	Bottom Section
Diameter, DT (m)	4.57	4.57
Column area, AT (m^2)	16.42	16.42
Active area, AA (m^2)	12.48	10.67
Tray spacing, S (mm)	457.2	660.4
Type of tray	Sieve	Sieve
Number of passes	2	4
Hole diameter, dH (mm)	5	5
Plate thickness, tp (mm)	3.43	3.43
Downcomer type	Straight	Straight
Downcomer area, AD (m^2)	1.97	2.87
Average downcomer width, wdc (m)	0.46	0.36
Average weir length, Lwav (m)	7.45	15.25
Outlet weir height, hw (mm)	50.8	50.8
Downcomer clearance, hcl (mm)	38.1	38.1
Flow path length, FPL (m)	1.57	0.68

Table 5.7 Summary of equipment design for the depropanizer

Parameters	Value
Actual total number of stage, NTact	37
Actual feed stage location, Nfact	18
Column area, AT (m^2)	16.42
Column volume, VT (m^3)	432.10
Condenser area, Acond (m^2)	1444.00
Reboiler area, Areb (m^2)	407.32

5.7. The parameters listed in the table are essential for the estimation of the capital cost. For the condenser, since the calculated area exceeds the maximum area of a typical condenser, thus, the costing of two condensers may be applied.

5.4. Summary

A rigorous stage-by-stage modelling together with the model solution procedure based on the Lewis-Matheson (LM) design approach for the multi-component

separation (NGLs fractionation unit) has been proposed in this chapter. The model solution procedure can be effectively programmed in the Matlab environment, incorporating the equipment sizing and efficiency calculation procedure. It is worth mentioning that, the use of Matlab in the distillation column design provides a huge flexibility in terms of the software capability in a rigorous modelling. In overall, the design procedure in this chapter is divided into two major steps: process design; and equipment sizing with hydraulic test.

The proposed rigorous design model has given improved prediction of the component distributions in the column than the short-cut models. This is because the rigorous model is able to eliminate the unrealistic assumptions in multi-component distillation of the constant molar overflow and constant relative volatilities in the short-cut design methods. The convergence problem in the conventional LM model, caused by poor initial guess values of the distribution of the non-key components in the distillate stream has been overcome by incorporating the Fenske equation into the model solution procedure. To enhance the convergence of calculations of the column at the feed stage for both rectifying and stripping sections, a modified theta method has also been recommended as part of the model solution procedure. Instead of using only the theta value, the feed stage liquid composition ratio has been incorporated into the procedure so as to give higher accuracy of the composition matching at the feed stage, improve the speed of convergence and avoid the deviation of theta value when solving the equations using fzero function in Matlab.

The output parameters from the process design procedure are then applied in the column sizing with hydraulic test, condenser, and reboiler designs. The heuristic for the column sizing is developed based on the adaptation of the methodology proposed by Kister (1992). The overall design procedure is developed in such a way that it can be utilized in the optimization as the parameters for the computation of capital cost and operating cost can be obtained directly from the design. This model solution procedure, which is programmed and implemented in Matlab environment, has been successfully used in the design of the industrial-scale depropanizer column.

CHAPTER 6: MODELLING OF DIVIDING-WALL COLUMN: IMPROVED LEWIS-MATHESON METHOD

The design procedure of a dividing wall column (DWC) is more complex than that of the conventional column due to the large number of degrees of freedom involved. All of these degrees of freedom have to be initialized before the design computation can be performed. A new design procedure for the DWC is proposed in this chapter. The new design procedure is developed based on the modified Lewis-Matheson (LM) stage-by-stage method, which has been successfully applied to the design of a conventional column in Chapter 5. The degrees of freedom of the design are reduced via the derivation of some equations to relate the variables which interact with each other in the design. A different convergence criterion at the feed and interlinking trays is also suggested for simplifying the computation. The feasibility of the proposed design procedure is demonstrated by using an example from the fractionation units of an industrial-scale gas plant. The rest of this chapter is arranged as follows. The basic concept of the proposed design model is described in Section 6.1. The basic assumptions and model equations involved are given in Section 6.2. The details of the proposed design procedure are discussed in Section 6.3. In Section 6.4, the application of the proposed design model in a case study is provided. Lastly, a summary of the chapter is given in Section 6.5.

6.1. Basic Concept of Design Model

A new design procedure is provided in this chapter for the process design of a dividing-wall column (DWC). The design methodology is developed based on the Lewis-Matheson (LM) stage-by-stage design method. As presented in Chapter 5, to improve the convergence at the feed plate (matching point location), a modified version of the LM stage-by-stage design procedure has been introduced and applied successfully to a multi-component distillation column. Therefore, instead of using the conventional LM method, the detailed procedure as outlined in Figure 5.2

(Chapter 5) is used as the basis for the development of an algorithm for solving the DWC design.

Figure 6.1 presents an overall model for a DWC. From the figure, it can be seen that the column is divided into six sections. Section 1_1 and Section 1_2 are the rectifying section and the stripping section, respectively, at the feed side of the dividing wall (prefractionator section). Section 3_1 is the upper part of the side withdrawal section of the dividing wall, whereas Section 3_2 is the lower part of the side withdrawal section of the dividing wall. Section 2 corresponds to a rectifying section and Section 4 is a stripping section of the column. The column is provided with one feed, a liquid distillate stream (D), a liquid side stream (S) and a liquid bottom product stream (B). In the column, the counter-current flows of the vapour and liquid in the column carry the light (volatile) components to the top, middle key components to the side stream and the heavy components to the bottom. A condenser at the top (Section 2) and a reboiler at the bottom (Section 4) of column are provided to condense the vapour and boil-up the liquid, respectively.

6.2. Basic Assumptions and Model Equations

The assumptions made to establish a design procedure for the DWC are as follows:

- Constant molar overflow (CMO)
- Steady state condition
- Vapour and liquid are equilibrium on each stage
- DWC with middle dividing wall
- Same number of trays on both sides of the dividing wall
- Ideal mixing in each tray
- Partial condenser
- Total reboiler
- Feed and side streams are saturated liquids

By referring to Figure 6.1, the overall component material balance and the product compositions summation equations for DWC are given below:

$$Fz_F{}^j = Dx_D{}^j + Sx_S{}^j + Bx_B{}^j \tag{6.1}$$

$$Sx_S{}^j = S_1x_{S1}{}^j + S_2x_{S2}{}^j \tag{6.2}$$

$$S = S_1 + S_2 \tag{6.3}$$

$$\sum_{j=1}^{C} x_D{}^j = 1 \tag{6.4}$$

$$\sum_{j=1}^{C} x_S{}^j = 1 \tag{6.5}$$

$$\sum_{j=1}^{C} x_B{}^j = 1 \tag{6.6}$$

where *F*, *D*, *S* and *B* denote the feed, distillate, side withdrawal and bottom product flow rates, respectively; $z_F{}^j$ is the feed composition in mole percentage; $x_D{}^j$, $x_S{}^j$ and $x_B{}^j$ are the mole percentages of components into the corresponding product streams (*D*, *S*, and *B*). For equations (6.2), S_1 and x_1 are the flow rate and composition of the product stream for the upper section of Section 3, whereas S_2 and x_2 are the product stream's flow rate with its composition for the lower part of Section 3.

The stage model equations involved in solving the DWC are similar to those which are presented in Section 5.1.1 of Chapter 5. With the exceptional of the enthalpy balance equations due to the assumption of the constant molar overflow, the stage model equations of Section 5.1.1 are applied. It is noted that the vapour and liquid flow rates are constant across the trays for each defined sections. The feed stage model as illustrated in Figure 5.1 is applied to the prefractionator section of the column. For the top and bottom interlinking trays and side withdrawal tray, different stage models are utilized as can be seen in Figure 6.1.

According to Amminudin et al. (2001),The conditions which have to be met in the design procedure developed must satisfy the overall mass balance, the product recovery or purity, and equal composition of the middle key components in the side stream product for Streams S_1 and S_2 (Figure 6.1) The pressure drops in the condenser and across a column tray are taken as 14 kPa and 0.7 kPa (per tray), respectively (Seader et al., 2011).

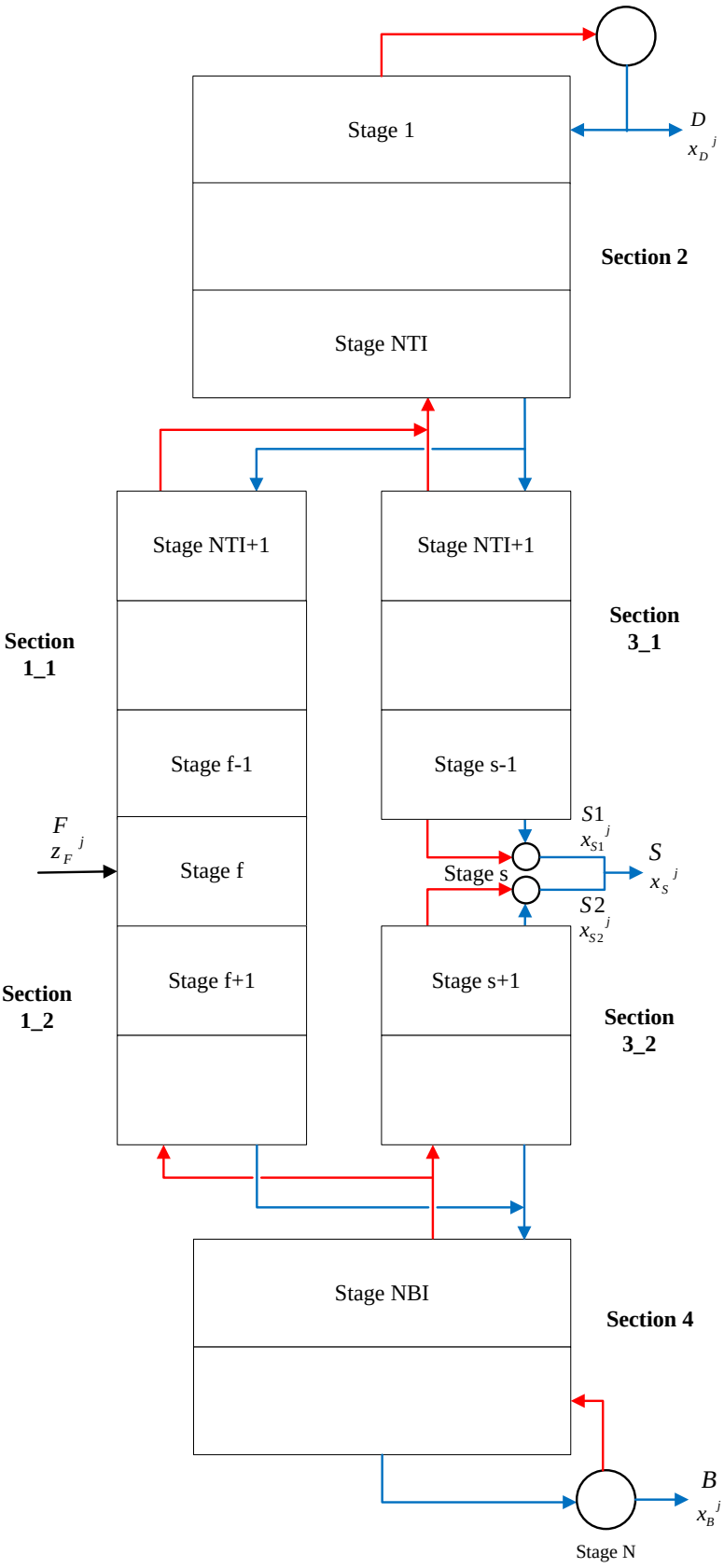


Figure 6.1 Schematic diagram of a dividing wall column (DWC)

6.3. Process design procedure

The steps involved in applying the proposed modified LM design method are presented in Figure 6.2 and described in the following sections.

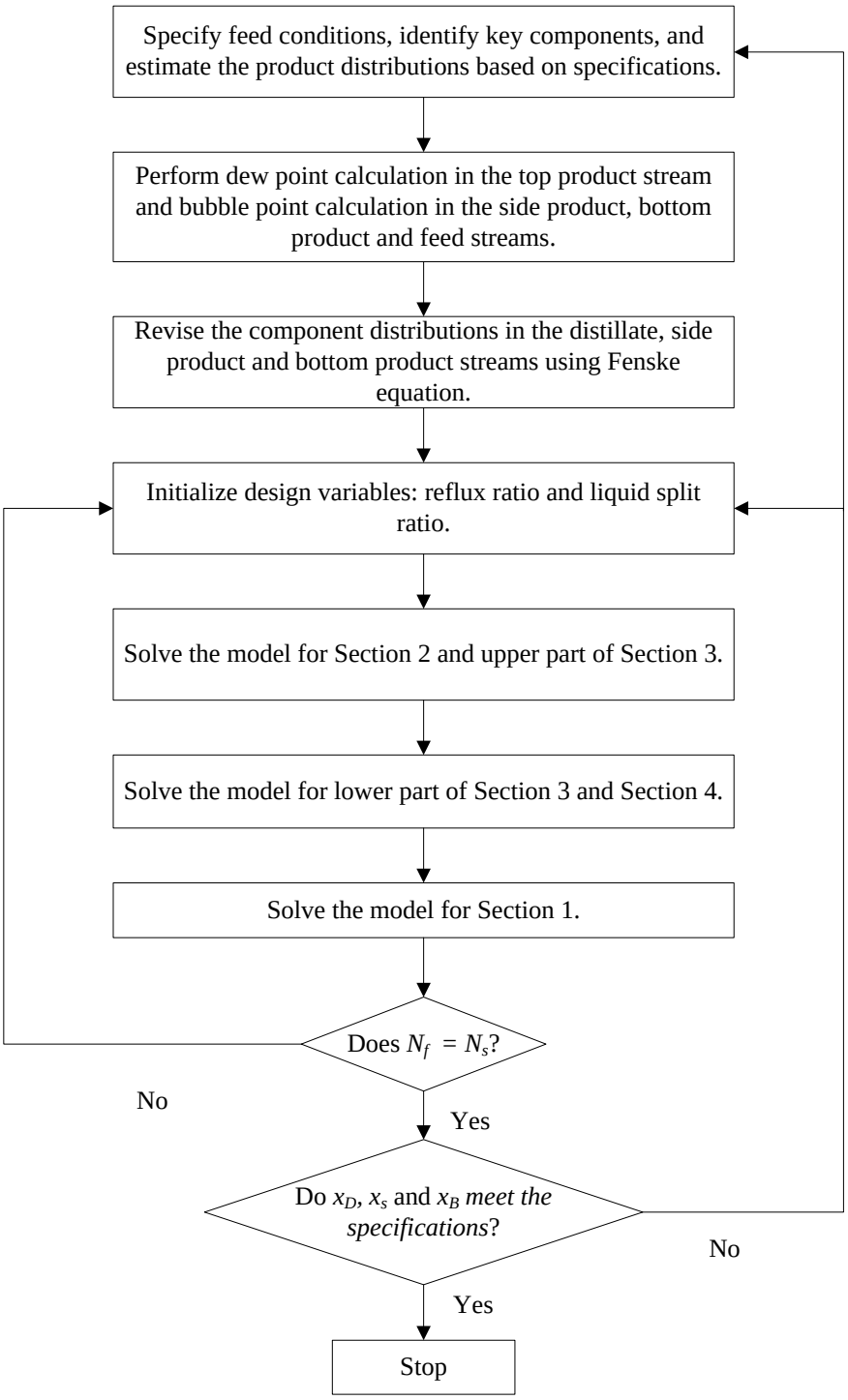


Figure 6.2 Flow chart for the DWC design via the proposed modified LM model

6.3.1. Input parameters

The input or known parameters required for the procedure are the feed conditions and the product distributions. The feed conditions include composition, flow rate, thermal feed quality (q), and pressure or temperature. The thermal quality in this work is equal to 1 due to the assumption of saturated liquid feed. The product distributions here are the compositions and flow rates of the distillate, side stream or bottom products, which two out of the three streams have to be specified based on the recovery or purity. Besides that, the key components, which are light key (LK), middle key (MK), and heavy key (HK) components, have also to be identified in the early step of the procedure.

6.3.2. Feasible product distributions

With the initial estimates on the product distributions, the dew-point calculation is performed on the distillate stream, whereas the bubble-point calculation is performed on the feed stream, side stream and bottom product stream of the column to obtain the relative volatilities required in the product estimation (composition).

According to Amminudin et al. (2001), the feasible product distributions can be estimated using either Fenske equation or Underwood equation. The Fenske equation is applied to obtain the distributions at total reflux, whereas the later is utilized in the case of minimum reflux. For the ease of computation, Fenske equation is selected for the product distributions estimation in this work to overcome the limit of the standard LM model which is very sensitive to the initial guess values of the distillate component flow rates.

A simple 3-column model as shown in Figure 6.3 can be used to estimate the product distributions. The first column (C1) as given in the figure represents Sections 1_1 and 1_2 in the DWC, whereas Sections 2 and 3_1 correspond to column C2. The third column, C3 from the figure represents Sections 3_2 and 4 in the DWC. Then, the Fenske equation, equations (5.15) to (5.17), is applied separately to the three columns to revise the estimated product distributions for streams D1, B1, D, S1, S2 and B.

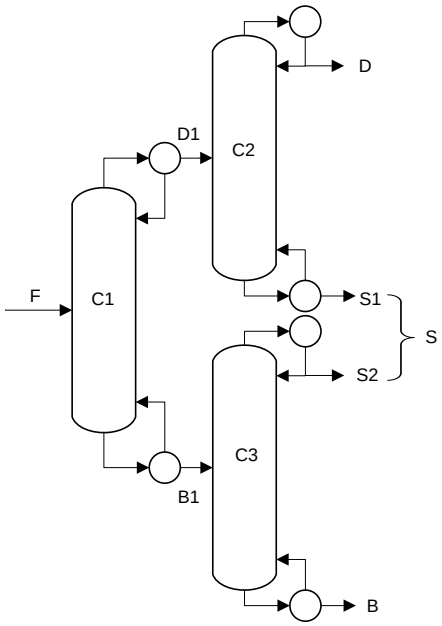


Figure 6.3 A 3-column model for feasible product estimation

6.3.3. Design parameters

The three design parameters required for the DWC design procedure are reflux ratio (R), liquid split ratio (SL) and vapour split ratio (SV). Because of the constant molar overflow assumption, the liquid split ratio and the vapour split ratio are dependent variables in this 3-column model. Due to this condition, the design parameters identified in this work reduce to only reflux ratio and liquid split ratio.

The values for the design parameters have to be assumed to initiate the calculations. It is important to note that, the initial values specified must fall within certain upper and lower limits. Therefore, the determination of the limits is crucial for the column to be operable. The lower limit for the reflux ratio is determined by first considering the minimum reflux ratio (R_{min}), which is determined by using the Underwood equation.

The Underwood equation applied to a conventional single column is given below:

$$R_{\min} + 1 = \sum_{j=1}^{C} \frac{\alpha_j x_{D,j}}{\alpha_j - \Phi} \tag{6.7}$$

where α_j is the relative volatilities of the components with respect to the heavy key, $x_{D,j}$ is the composition of component j in the distillate at minimum reflux and Φ is the root of the equation:

$$\sum_{j=1}^{C} \frac{\alpha_j z_j}{\alpha_j - \Phi} = 1 - q \tag{6.8}$$

where z_j is the composition of component j in the feed and q is the thermal quality of the feed, which is equal 1 (saturated liquid feed) in this work.

Before applying the Underwood equation, Shiras method (Kister, 1992) can be used to determine the number of Φ required by solving the Underwood equation. The equation is given as

$$D_R = \frac{Dx_{D,j}}{Fz_j} = \frac{\alpha_j - 1}{\alpha_{LK} - 1} \frac{Dx_{D,LK}}{Fz_{LK}} + \frac{\alpha_{LK} - \alpha_j}{\alpha_{LK} - 1} \frac{Dx_{D,HK}}{Fz_{HK}} \tag{6.9}$$

where α_{LK} is the relative volatility of the components with respect to the heavy key, $x_{D,LK}$ and $x_{D,HK}$ are the compositions of light key and heavy key components in the distillate, respectively, and z_{LK} and z_{HK} are the compositions of light key and heavy key components in the feed.

The Underwood equation is applied to each column as shown in Figure 6.3. The parameters calculated are defined as $R_{min,c1}$, $L_{min,c1}$ and $V_{min,c1}$ for column 1, $R_{min,c2}$, $L_{min,c2}$ and $V_{min,c2}$ for column 2 and $R_{min,c3}$, $L_{min,c3}$ and $V_{min,c3}$ for column 3. The overall minimum reflux ratio for the DWC can be calculated using the transformation model of Petlyuk from prefractionator arrangement as described in the work by Amminudin et al. (2001). Therefore, the overall minimum reflux ratio for DWC is formulated as

$$R_{\min} = \frac{L_{\min 1,c1} + L_{\min 2,c2}}{D} \tag{6.10}$$

The SL_{min} and SL_{max} can also be estimated by using the equations formulated as follows:

$$SL_{\min} = \frac{L_{\min,c1}}{RD} \tag{6.11}$$

$$SL_{\max} = 1 - \frac{L_{\min,c2}}{RD} \tag{6.12}$$

6.3.4. Solution of DWC model

Prior to the solution of the DWC model, some additional equations have to be included as a result of the transformation of prefractionator arrangement to DWC (Petlyuk column equivalent) as covered by Amminudin et al. (2001). Since the reflux ratio (R) here stands for the overall reflux ratio for the DWC, an equation has to be derived to relate the reflux ratio at Section 3_1 to the overall reflux ratio. The equation is

$$R_{3\_1} = R(1 - SL) \tag{6.13}$$

To satisfy the equalization of the vapour flow conditions between Sections 3_1 and 3_2, the equation derived for the calculation of the reflux ratio at Section 3_2 is

$$R_{3\_2} = \frac{V_{3\_1} - S2}{S2} \tag{6.14}$$

With all the known parameters and design parameters, the stage-by-stage calculations are carried out on the DWC model. The solution of the DWC model as illustrated in Figure 6.1 starts with solving Sections 2 and 3_1 and followed by Sections 3_2 and 4, and finally, Section 1.

Section 1, also known as prefractionator is comprised of two sections coupled around the feed plate. In this section, the separation is achieved between light and heavy components so that as much light components will go to the top and heavy components will go to the bottom of the section. Sections 2 and 3_1 are equivalent to a column section that separates the components which are sent from the top of the prefractionator (Section 1_1). In this column, the light components are separated from the intermediate components and the heavy components which exist in minor quantities. On the contrary, Sections 3_2 and 4 constitute a column section which separates the components fed from the bottom of the prefractionator (Section 1_2). The intermediate components are separated from the heavy components and light components in minor quantities.

Figure 6.4 illustrates the detailed procedure for solving the model for Sections 2 and 3_1. Initially, the top down stage-by-stage calculations are performed on Section 2 until the vapour compositions of the stage converge to the vapour compositions which are fed from Section 1_1. The vapour compositions which are coming from Section 1_1 are assumed to be equal to the compositions of Stream D1 (Section 6.3.2). For Section 3_2, the bottom-up calculations are executed until the stages' liquid compositions converge to the liquid compositions of the top interlinking tray. The top interlinking tray is defined as the last tray calculated in Section 2. Then, the bottom-up calculations of Section 3_2 are revised to meet the top interlinking stage pressure drop. For plate matching purpose, the same procedure as described in Section 5.1.2 is applied. The modified theta equations, from equations (5.18) to (5.21), are used to correct the component flows or compositions.

The same procedure is repeated for solving the model of Sections 3_2 and 4. The procedure for solving the sections is shown in Figure 6.5. After that, the vapour and liquid compositions for the interlinking trays obtained from both of the procedures will be used in the computation of Section 1. The stage-by-stage calculations for Section 1 are performed on both of the rectifying and stripping sections without the condenser and reboiler. The top-down and bottom-up calculations are executed at the respective sections until the stages' liquid compositions converge to the feed compositions. Then, the bottom-up calculations at the stripping section are revised with corrected pressure drop.

The criteria for the solution of the feed and interlinking trays proposed here is different from the works proposed by others (Amminudin et al., 2001; Kim, 2005b; Kim et al., 2004). Instead of calculating the composition difference between every tray for rectifying and stripping sections to find the minimum distance, the reference points as estimated using the 3-model column are utilized. The composition difference is computed between the trays in rectifying section and the corresponding reference point. After the minimum composition difference is achieved, the final tray of rectifying section is now used as the reference point for the computation of the stripping section. This method will reduce the tedious iterations encountered in finding the feed or interlinking stages.

Next, the number of trays at Section 1 (N_f), and Section 3 (N_s) are calculated and checked if they achieve same number of trays. If the number of trays obtained does not match, the computation is repeated with updated liquid split ratio till the convergence is reached. It is then followed by checking the final product compositions if they meet the specifications. If no, the computation is repeated by varying the reflux ratio or product distributions estimated.

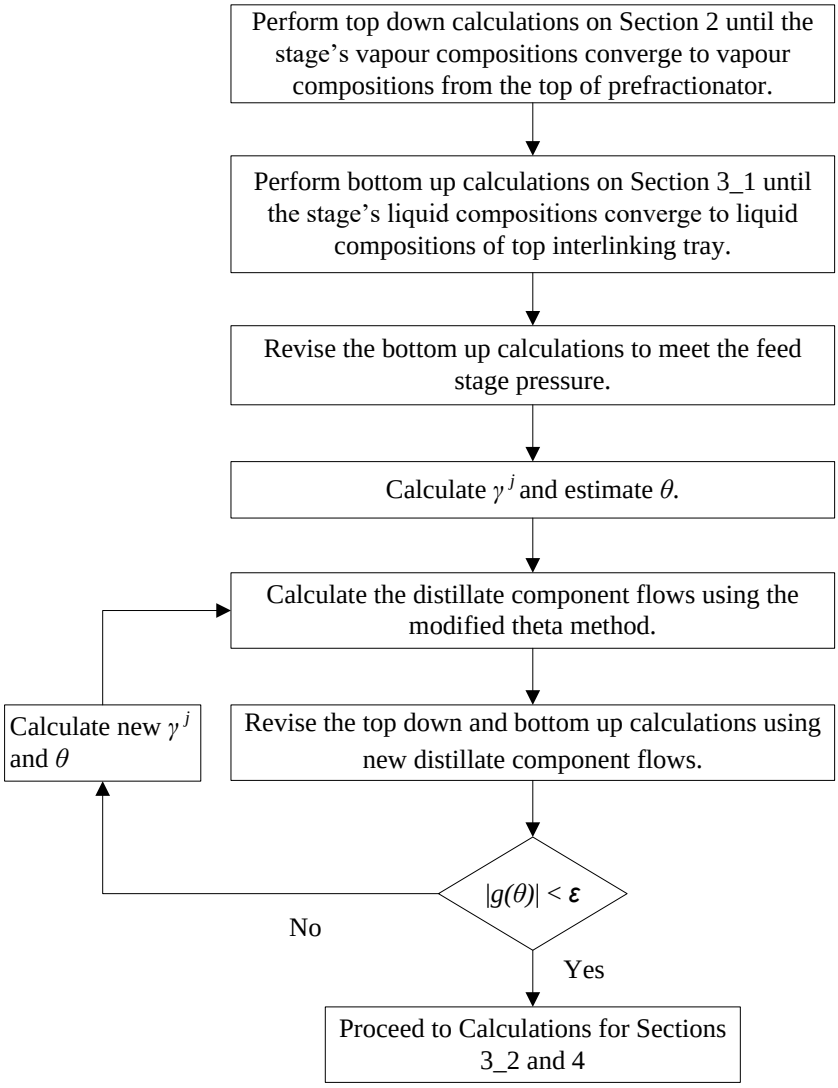


Figure 6.4 The procedure for solving the model of Sections 2 and 3_1

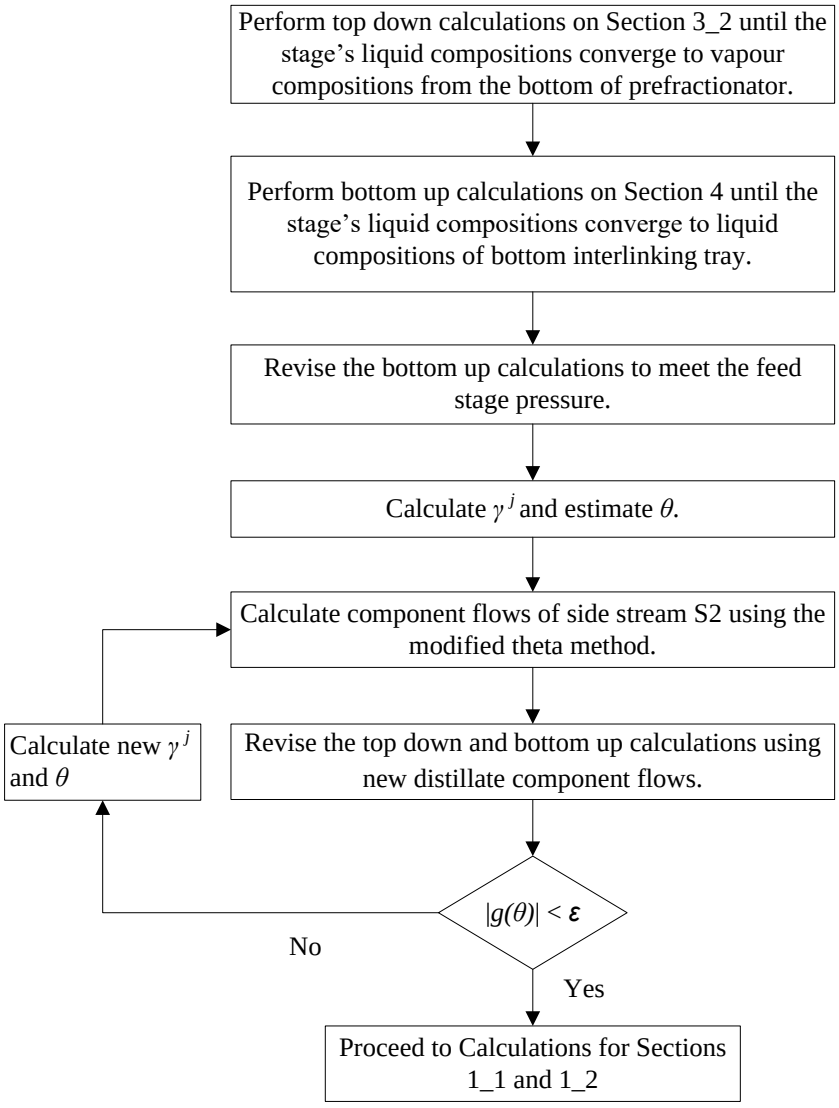


Figure 6.5 The procedure for solving the model of Sections 3_2 and 4

6.4. Case Study

The new design procedure proposed in this chapter is demonstrated on a case study to ensure the feasibility of the model in the design of a DWC. The multi-component feed system selected for this case study consists of 5-component hydrocarbon mixture for the industrial-scale natural gas liquids (NGLs) fractionation units (Long & Lee, 2012c). The proposed design procedure is used to design a new DWC to replace the conventional depropanizer and debutanizer columns in the fractionation train. The proposed design procedure is developed and solved using Matlab

(Appendix B.3). Peng-Robinson (PR) equation of state is used in the model to predict the vapor-liquid equilibrium (VLE) of the developed DWC stage-by-stage model.

6.4.1. Feed condition and product specification

The feed stream considered is a light hydrocarbon mixture, which is made up of five components. The feed components with their respective compositions are shown in Table 6.1. The feed mixture at 31.47 bar of pressure as given in the work of Long and Lee (2012c) will be flashed to the column feed stage pressure of 17.75 bar before supplied to the column. The feed stage pressure is estimated from the average of dew point calculation of top product stream and bubble point of the bottom product stream. Assuming saturated liquid feed, the feed temperature of 68^{o}C is obtained.

The steam supplied to the reboiler is assumed to be a low pressure steam at 5 barg and a temperature of 160^{o}C. For the condenser, the cooling water is supplied from cooling tower at a temperature of 30^{o}C. The distillate pressure chosen has to ensure that the dew point of the distillate to be above that of the cooling water temperature. In this case, the distillate pressure of 17.5 bars is taken.

Table 6.1 Feed condition and product specifications

Components	Mole Fraction
Ethane (C_2)	0.0418
Propane (C_3)	0.4990
i-Butane (iC_4)	0.1222
n-Butane (nC_4)	0.2610
i-Pentane (iC_5)	0.0759
Total Molar Flow (kmol/h)	3769
Feed Pressure (bar)	17.75
Feed liquid fraction, q_F	1
Pressure of top product stream (bar)	17.50
Minimum purity of C_3 at top stream (Mole fraction)	0.9100
Minimum purity of C_4 at side stream (Mole fraction)	0.9700
Minimum purity of iC_5 at botton stream (Mole fraction)	0.9800

Table 6.2 Feasible product distributions estimated from the Fenske Equation

Components	Compositions (Mole Fraction)				
	Top Interlinking (D1)	Bottom Interlinking (B1)	Top Product (D)	Middle Product (S)	Bottom Product (B)
Ethane (C_2)	0.0597	6.84E-06	0.0774	5.35E-06	3.01E-21
Propane (C_3)	0.7049	0.0185	0.9105	0.0203	1.12E-10
i-Butane (iC_4)	0.1132	0.1433	0.0113	0.3023	0.0001
n-Butane (nC_4)	0.1210	0.5876	0.0007	0.6750	0.0174
i-Pentane (iC_5)	1.14E-03	0.2505	3.19E-09	0.0023	0.9825

The DWC is expected to carry out ternary separation where propane will be removed from the mixture as the distillate, and i-butane and n-butane will be withdrawn as the side stream product and i-pentane will end as the bottom product. The objective of the separation is to achieve the products with their corresponding minimum purities: 90% of propane at the top product stream, 97% of i-butane and n-butane in the intermediate product stream and 98% of i-pentane in the bottom product. Therefore, in this study, the propane is defined as the light key component (LK), i-butane and n-butane as the middle key components (MK) and i-pentane as the heavy key component (HK). The feed and products conditions required for the DWC design are summarized in Table 6.1.

6.4.2. Feasible product estimation

The feasible product distributions for streams D1, B1, D, S1, S2 and B in Figure 6.3 are estimated using the Fenske Equation. The results of the estimation are presented in Table 6.2.

6.4.3. Initialization of design parameters

The design parameters which have to be assumed before the start of the calculations are reflux ratio of the DWC (R) and liquid split ratio (SL). To guess the initial value of the reflux ratio, equations (6.10) is first applied and the minimum reflux ratio (R_{min}) obtained is 2.79.

It is found out that setting R_{min} as the lower bound for the reflux ratio is too low for the convergence of the proposed model. Therefore, the real minimum R value is found by gradually increasing the reflux ratio from R_{min} using the proposed model until the convergence is achieved. The minimum R value found is 3.48 which is 1.25 times larger than R_{min}. The reflux ratio chosen for this case study is 4.

From equations (6.11) and (6.12), it can be clearly seen that the minimum and maximum values for liquid split ratio are dependent on the reflux ratio. Therefore, the values can only be calculated if the reflux ratio is provided. Since the reflux ratio of 4 is used in this work, the minimum value for liquid split ratio is 0.2799, whereas its maximum value is 0.583. The main function of the liquid split ratio in the design procedure is to obtain the same number of trays in Sections 1 and 3. Therefore, the liquid split ratio must be adjusted within the specified range to satisfy the objective.

6.4.4. Results from DWC design

The final product distributions and energy performance obtained from the computation are presented in Table 6.3. The results obtained from the proposed model are then validated using Aspen HYSYS. From the table, overall, it can be observed that the results from the rigorous simulation, which include the condenser duty, reboiler duty, compositions, total molar flow, and temperature for top and bottom products, agree well with the results computed using the proposed process design model. For the purities of the product, up to 16.5% difference is obtained, whereas the difference for the other variables falls within 15%.

Upon comparing the compositions of the final products with the estimated product distributions calculated using Fenske equation, it is found that there are only slight changes to the compositions. The structural variables obtained from the proposed design model are presented in Table 6.4. The total number of stages for the DWC, excluding reboiler, is 55. There are 30 stages computed for Section 1 and Section 3 at liquid split ratio of 0.315. The vapour split ratio calculated is 0.5122. With numbering the stages from the top of the column, the top interlinking tray is located at tray 13, whereas the bottom interlinking tray is located at tray 43. The feed location at Section 1 is 34 and the side product in Section 3 is withdrawn at tray 24.

Table 6.3 Final results for the product distributions and energy performance

Components	Proposed Model (Mole Fraction)			HYSYS Simulation (Mole Fraction)		
	Top Product	Side Product	Bottom Product	Top Product	Side Product	Bottom Product
Ethane (C_2)	0.0775	5.35E-06	1.35E-14	0.0776	3.62E-07	6.64E-15
Propane (C_3)	0.9145	0.0168	1.09E-07	0.9160	0.0152	1.58E-07
i-Butane (iC_4)	0.0076	0.3067	0.0004	0.0063	0.3674	0.0011
n-Butane (nC_4)	0.0003	0.6739	0.0167	0.0002	0.6026	0.0169
i-Pentane (iC_5)	8.58E-10	0.0026	0.9829	8.95E-13	0.0148	0.9819
Total Molar Flow (kmol/h)	2030.07	1451.62	287.31	2030.00	1452.00	287.00
Temperature (^oC)	48.65	101.38	147.23	43.79	102.3	146.3
Condenser Duty (MW)		34.13			39.14	
Reboiler Duty (MW)		36.81			41.07	

Table 6.4 The structural variables obtained from the proposed design mode

Parameters	Value
Total number of stages, NT	55
Top interlinking stage location, NTI	13
Bottom interlinking stage location, NBI	43
Feed stage location, Nf	34
Side withdrawal stage location, Ns	24

The temperature profile and composition profile of the middle key components generated from the proposed design model are summarized in Figure 6.6 and Figure 6.7, correspondingly. The prefractionator denotes Section 1 of the DWC, whereas main column corresponds to the Sections 2, 3 and 4 of the DWC. The middle key components here are represented by the summation of compositions for both i-butane and n-butane. From both of the figures, the locations of the top and bottom interlinking trays can be clearly seen through identifying the interception points of the curves for prefractionator and main sections. The top and bottom interlinking trays shown are at the tray 13 and 43 respectively. It can be also noticed from the

composition profile that the side liquid product is withdrawn from the tray that gives maximum middle key composition, which is on 24th tray.

From the figures, it can be observed that the middle key composition and temperature profiles generated for both of the sections are quite smooth overall. The modified theta method proposed is proven to work well in matching the plates at the top and bottom interlinking trays. This is shown by good matching at the intersections of the two curves. From Figure 6.7, it is noticed that there is a slight unsmooth (fluctuation) of the curve at the side withdrawal point. This condition is due to the compositional mismatches between the plates at the side streams (S1 and S2). Since the mismatch occurred is at minimum, it is then will not be considered as a major concern in this work.

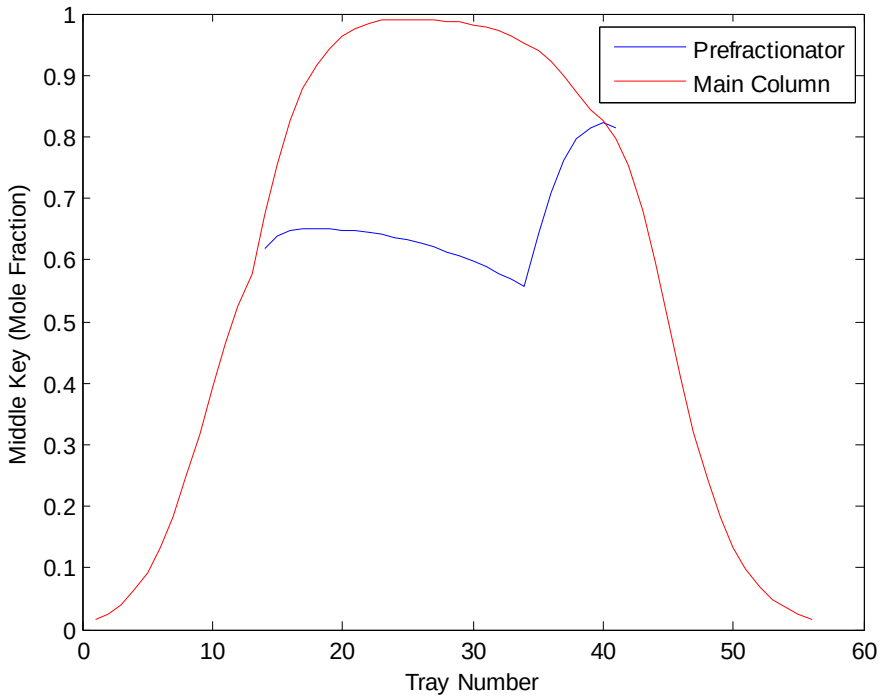


Figure 6.6 Composition profile of middle key components for prefractionator and main sections of the DWC

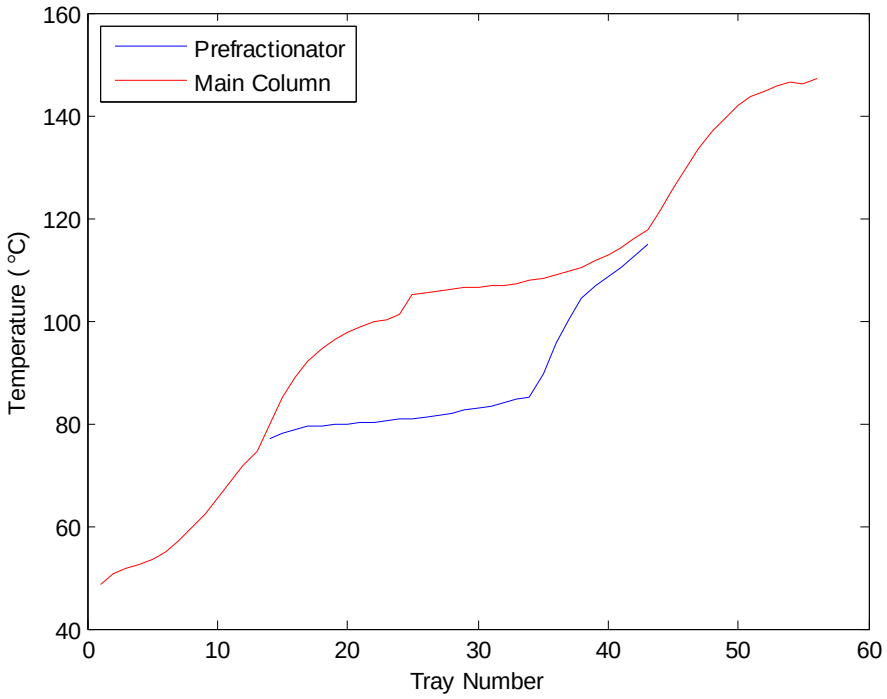


Figure 6.7 Temperature profile for prefractionator and main sections of the DWC

6.5. Summary

This chapter provides a new design method which can be applied to the design of a dividing-wall column (DWC). The stage-by-stage model is developed based on the Lewis-Matheson (LM) design approach. The modified version of the LM model has been proposed for the design of a conventional column in the previous chapter and this model has been successfully applied to a multi-component separation system. Therefore, in this chapter, this model is used as the basis for the design of the DWC. The model solution procedure developed can be effectively programmed in the Matlab environment.

The design model proposed in this work is considered as a semi-rigorous in nature. It is however, can be applied to design the DWC rigorously by removing the constant molar overflow assumption. The design procedure starts with the estimation of the product distributions using Fenske equation. Only two design variables are required to initialize the calculation: reflux ratio and liquid split ratio. The liquid split ratio is

used in the design procedure to ensure that equal number of stages at both sides of the dividing wall is accomplished.

The solution of the model for each section is performed by incorporating modified theta equation for the plate matching at the interlinking stages (top and bottom). To reduce the design variables as in the work of Amminudin et al. (2001), the equations to relate sections in the main column (Sections 2, 3 and 4) are formulated. A different convergence criterion is introduced in this work to reduce the tedious iterations encountered in finding the minimum distance for rectifying and stripping sections. Instead of computing the composition differences between every tray for rectifying and stripping sections, the reference points as estimated using the 3-column model are utilized.

This model solution procedure (implemented in Matlab environment) has been successfully used in the design of a DWC to replace the industrial-scale fractionation units (depropanizer and debutanizer) of a gas plant. The results show that the proposed procedure converges with satisfactory solutions to structural variables, energy performance and temperature, and middle key composition profiles.

CHAPTER 7: MODELLING OF DIVIDING-WALL COLUMN: FAST CONVERGENCE OF STAGE-BY-STAGE DESIGN

In this chapter, a semi-rigorous stage-by-stage modelling procedure is proposed using the McCabe-Thiele method and Lewis-Matheson (LM) design approach as the basis. The design method proposed in this chapter can provide direct solutions by performing the stage-by-stage calculations from the feed and side withdrawal points without the need to undergo tedious iterations for composition matching at the feed, side withdrawal and interlinking trays. Moreover, the stage-by-stage model is solved for the whole DWC without approximation as a multiple-column model, i.e, the use of 3-column model as in the previous chapters is not needed. The feasibility of the proposed design procedure is demonstrated based on a ternary hydrocarbon feed system and the results are validated using Aspen HYSYS V7.3. The rest of this chapter is structured as follows. In Section 7.1, the overall concept of the proposed model is provided. The assumptions and the model equations of the model are presented in Section 7.2. The estimation of the interception points prior to the stage-by-stage calculation is given in Section 7.3. The details of the proposed design procedure are discussed in Section 7.4. A case study is provided in Section 7.5 and the summary of the chapter is given in Section 7.6.

7.1. Overall Concept of Proposed Model

Generally, the thermodynamically equivalent configurations for modeling a DWC can be divided into five: pre-fractionator, post-fractionator, 4-column setup, pump-around model and 3-column setup (Dejanović et al., 2010; Staak et al., 2014). Among the configurations, the pre-fractionator setup is the most frequently used setup for the design and optimization studies of DWC. Recently, the 4-column setup, which was initially presented by S. T. Holland et al. (2010) as total mole net flow model and later evolved into a component net flow model by Chu et al. (2011), has started to gain preference in representing DWC model due to its robustness to

parameter changes and optimization of the various parameters. Therefore, in this work, the 4-column setup is applied in developing the design model for the DWC.

Figure 7.1 shows the schematic diagram of a dividing wall column (DWC). As illustrated in the figure, the DWC is divided into four regions:

- Region 1: feed stream side of the dividing wall (split-tray)
- Region 2: side stream side of the dividing wall (split-tray)
- Region 3: top column above the top split-tray section
- Region 4: bottom column below the bottom split-tray section.

Referring to Figure 7.1, the DWC consists of one feed stream with three output streams: distillate, side withdrawal and bottom products. The light key (LK) components from the feed stream will mostly go to the distillate stream, whereas the middle (MK) and heavy key (HK) components will mostly go to side withdrawal and bottom product streams, respectively. A sharp split assumption is not suitable to be applied to Region 1 due to the requirement of infinite number of trays. Therefore, the composition of the flow at the top split-tray section (interlinking section among Regions 1, 2 and 3) is made up of mostly LK and MK components with little HK components. Likewise, at the bottom split-tray section (interlinking section among Regions 1, 2 and 4), the composition of the flow comprises mostly MK and HK components with little LK components.

The design of the DWC often starts with the estimation of operational variables or structural variables. The operational variables are reflux ratio, liquid split ratio and vapour split ratio or liquid and vapour flow rates, whereas the structural variables are number of stages at the related regions, feed stage and side withdrawal stage locations. As covered in Chapter 3 (Literature Review), the design methods usually begin with the estimation of operational variables. On the other hand, the rating methods normally begin with the approximation of the structural variables. Since the method suggested in this work is based on the design method, taking the method proposed by Lewis and Matheson (1932) as reference, the operational variables have to be guessed in the initial step before proceeding to the structural design.

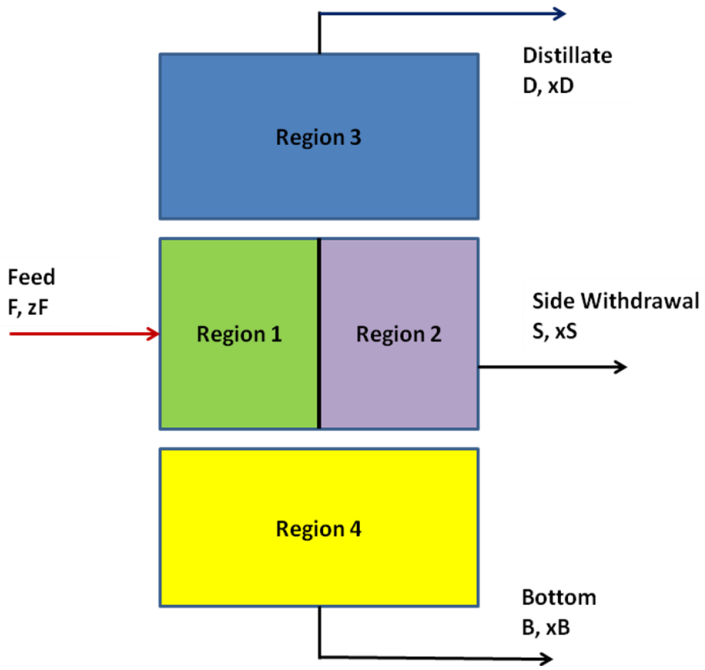


Figure 7.1 Schematic diagram of a dividing wall column (DWC)

The basic concept of the design proposed can be explained by using the McCabe-Thiele diagram. Figure 7.2 presents the diagram for the light key component. From the figure, it can be seen that there are six operating lines which stand for the rectifying or stripping sections for the four regions of the DWC:

- OP1 is the rectifying line for region 3
- OP2 and OP4 are the rectifying and striping lines for Region 1
- OP3 and OP5 are the rectifying and striping lines for Region 2
- OP6 is the stripping line for Region 4.

Considering an ideal case, the six operating line will intersect at six important locations in the column, which are located at the feed ($\phi_f^{\,j}$), side withdrawal ($\phi_s^{\,j}$), top split-tray ($\phi_{st}^{\,j}$) and bottom split-tray ($\phi_{sb}^{\,j}$) sections, and top ($\phi_T^{\,j}$) and bottom ($\phi_B^{\,j}$) in the column.

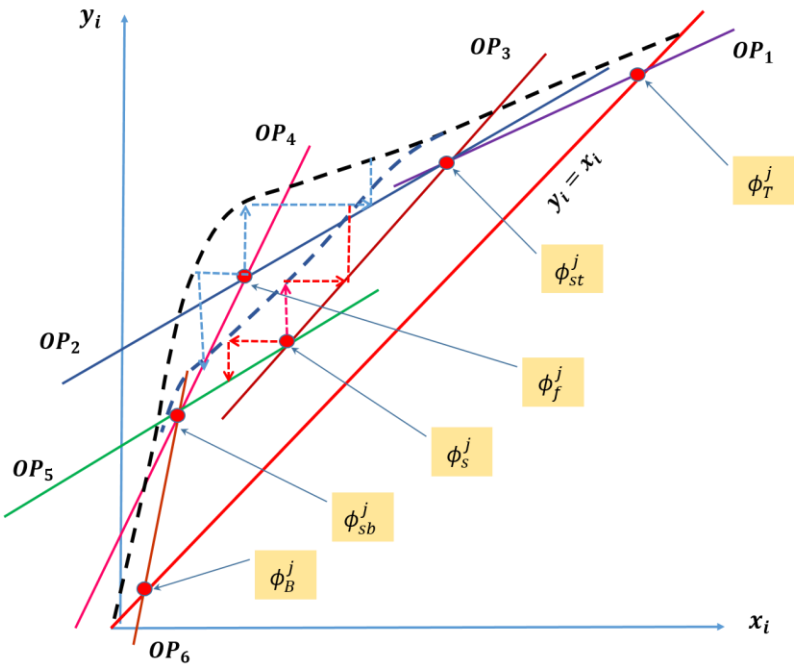


Figure 7.2 McCabe-Thiele diagram for the light key component in DWC

The design method initiates with the determination of the composition at the feed and side withdrawal locations. Then, the operating lines are setup in such a way that the interception points obtained have to fall within the equilibrium curves and the output products have to meet the required specifications. The slopes for the operating lines depend on the reflux ratio, liquid split ratio and vapour split ratio. Therefore, the parameters can be altered for the intersection points to fall within requirement. With the estimated points, the stage-by-stage calculations are performed from the feed and side withdrawal trays in an upward direction to the top (bubble point calculation) and a downward direction to the bottom (dew point calculation). The detailed procedures regarding the proposed work are discussed in the sections below.

7.2. Stage-by-Stage Model Assumptions and Equations

To establish a design procedure for the DWC, several assumptions have been made as follows:

- Constant molar overflow (CMO)
- Steady state condition

- DWC with middle dividing wall
- Same number of trays on both sides of the dividing wall
- Ideal mixing in each tray
- Partial condenser
- Total reboiler
- Feed and side streams are saturated liquids
- Liquid composition in the feed tray is similar to the composition of the feed
- Liquid composition in the side withdrawal tray is similar to the composition of the side stream.

Based on the modelling setup given in Figure 7.1, the overall component material balance and the product composition summation equations for the DWC are as follows:

$$Fz_F{}^j = Dx_D{}^j + Sx_S{}^j + Bx_B{}^j \tag{7.1}$$

$$\sum_{j=1}^{C} x_D{}^j = 1 \tag{7.2}$$

$$\sum_{j=1}^{C} x_S{}^j = 1 \tag{7.3}$$

$$\sum_{j=1}^{C} x_B{}^j = 1 \tag{7.4}$$

where F, D, S and B denote feed, distillate, side withdrawal and bottom product flow rates, respectively; $z_F{}^j$ is the feed composition in mole percentage; $x_D{}^j$, $x_S{}^j$ and $x_B{}^j$ are the mole percentages of components into the corresponding product streams (D, S, and B). The known parameters for the above equations are feed flow rate and its compositions. Other unknown parameters required in order to solve the above equations are top, side and bottom product specifications.

The equations related to the reflux ratio, vapour and liquid split ratios and column internal flow rates are given as below:

$$L_f = \alpha RD \tag{7.5}$$

$$\bar{L}_f = \alpha RD + F \tag{7.6}$$

$$L_s = (1-\alpha)RD \tag{7.7}$$

$$\bar{L}_s = (1-\alpha)RD - S \tag{7.8}$$

$$L = L_f + L_s \tag{7.9}$$

$$\bar{L} = \bar{L}_f + \bar{L}_s \tag{7.10}$$

$$V = \bar{V} = RD + F - S - B \tag{7.11}$$

$$\bar{V}_f = \beta \bar{V} \tag{7.12}$$

$$\bar{V}_s = (1-\beta)\bar{V} \tag{7.13}$$

where R is the reflux ratio; α is the liquid split ratio for Region 1; β is the vapour split ratio for Region 1; L_f and $\bar{L}_f$ are the liquid flow rates above and below feed tray; L_s and $\bar{L}_s$ are the liquid flow rates above and below side withdrawal tray; L and $\bar{L}$ are the liquid flow rates for Region 3 and 4; V and $\bar{V}$ are the vapour flow rates for Region 3 and 4; $\bar{V}_f$ and $\bar{V}_s$ are the vapour flow rates for Region 1 and 2, respectively. The material or component balance equations for Regions 1 to 4 are discussed in the following subsections.

7.2.1. Region 1

Region 1 of the DWC deals with the feed side section of the dividing wall. Consider the number of split-trays above and below the feed tray as follows:

N_{fT} = number of split trays above the feed

N_{fB} = number of split trays below the feed

Hence, the total number of split-trays, $N_{f,\,Total}$ is

$$N_{f,Total} = N_{fT} + N_{fB} + 1 \tag{7.14}$$

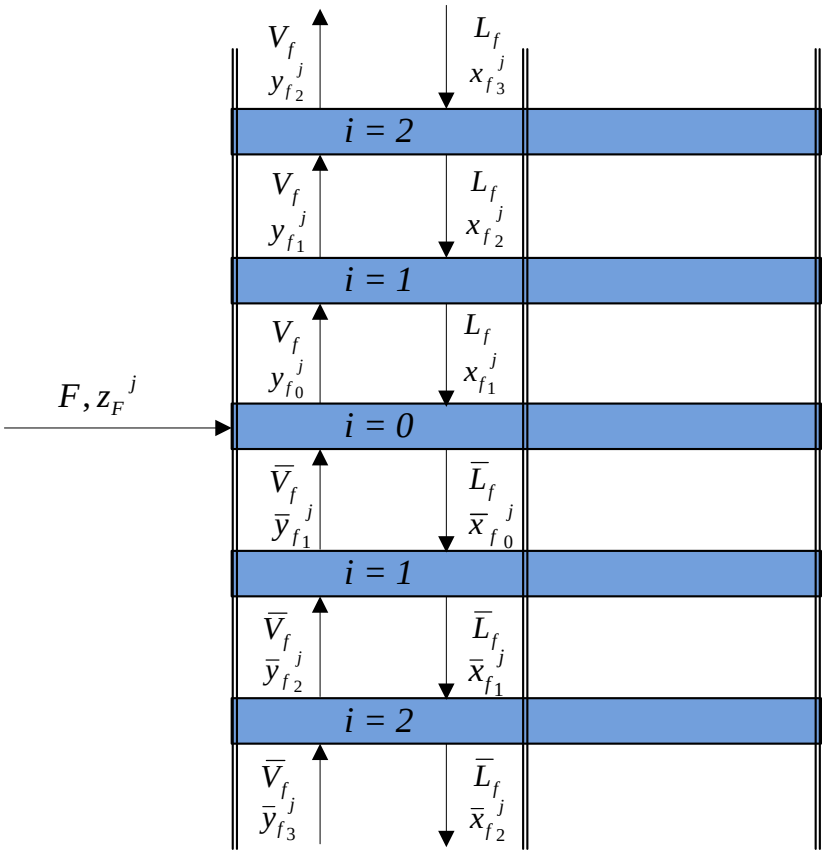


Figure 7.3 Stage model of DWC at Region 1 (feed side of dividing wall)

Figure 7.3 shows the stage-wise material balance at Region 1. The corresponding equations for the feed tray, trays above the feed and trays below the feed are discussed in Section 7.2.1.1 to 7.2.1.3.

7.2.1.1. Material balance at feed tray

From Figure 7.3, it can be seen that the feed tray is located at tray $i = 0$. Denoting j as the components in the feed, the component balance equation at the feed tray is:

$$Fz_F^{\,j} + L_f x_{f1}^{\,j} + \bar{V}_f \bar{y}_{f1}^{\,j} = V_f y_{f0}^{\,j} + \bar{L}_f \bar{x}_{f0}^{\,j} \tag{7.15}$$

Because of the assumptions made before: saturated liquid feed and liquid composition in the feed tray is similar to the composition of the feed, the liquid composition at feed tray is taken as:

$$\bar{x}_{f0}^{\,j} = z_F^{\,j} \tag{7.16}$$

Assuming vapour-liquid equilibrium condition,

$$y_{f0}^{\ j} = K_{f0}^{\ j} \bar{x}_{f0}^{\ j} \tag{7.17}$$

Where $K_{f0}^{\ j}$ denotes the vapour-liquid equilibrium constant corresponding to the feed tray.

After determining all the known parameters, there are still two unknowns left: $x_{f1}^{\ j}$ and $\bar{y}_{f1}^{\ j}$. Equation (7.15) can be rearranged to find $x_{f1}^{\ j}$:

$$x_{f1}^{\ j} = \frac{V_f}{L_f} y_{f0}^{\ j} + \frac{\bar{L}_f}{L_f} \bar{x}_{f0}^{\ j} - \frac{\bar{V}_f}{L_f} \bar{y}_{f1}^{\ j} - \frac{F}{L_f} z_F^{\ j} \tag{7.18}$$

In equation (7.18), the value of the vapour composition from the first tray below the feed, i.e. $\bar{y}_{f1}^{\ j}$ is used as an adjustable parameter to obtain $x_{f1}^{\ j}$ by altering the intersection point between the two top operating lines (or two bottom operating lines) of the feed and side stream sides in Regions 1 and 2 respectively. The setting of $\bar{y}_{f1}^{\ j}$ will be described in Section 7.3.1.

7.2.1.2. Material balance above feed tray

The material balance above the feed is performed from the feed tray upward by using the bubble-point calculation. As shown in Figure 7.3, the tray index in this section is numbering upward from the feed tray.

For *i = 1*,

$$V_f y_{f1}^{\ j} + L_f x_{f1}^{\ j} = L_f x_{f2}^{\ j} + V_f y_{f0}^{\ j} \tag{7.19}$$

which can be expressed as follows:

$$y_{f1}^{\ j} = \frac{L_f}{V_f} x_{f2}^{\ j} + y_{f0}^{\ j} - \frac{L_f}{V_f} x_{f1}^{\ j} \tag{7.20}$$

For *i = 2*,

$$y_{f2}^{j} = \frac{L_f}{V_f} x_{f3}^{j} + y_{f1}^{j} - \frac{L_f}{V_f} x_{f2}^{j} \tag{7.21}$$

After substituting equation (7.20) into equation (7.21), it gives the following equation:

$$y_{f2}^{j} = \frac{L_f}{V_f} x_{f3}^{j} + y_{f0}^{j} - \frac{L_f}{V_f} x_{f1}^{j} \tag{7.21}$$

The top operating line above the feed for $i = 1, 2, ..., N_{fT}$ can be written in a general form as below.

$$y_{fi}^{j} = \frac{L_f}{V_f} x_{fi+1}^{j} + y_{f0}^{j} - \frac{L_f}{V_f} x_{f1}^{j} \tag{7.22}$$

Alternatively, equation (7.22) can be rearranged for x_{fi+1}^{j} where $i = 1, 2, ..., N_{fT}$

$$x_{fi+1}^{j} = \frac{V_f}{L_f} y_{fi}^{j} - \frac{V_f}{L_f} y_{f0}^{j} + x_{f1}^{j} \tag{7.23}$$

Or, written in a general equation as

$$x_{fi+1}^{j} = \delta_{fT} y_{fi}^{j} + \varepsilon_{fT}^{j} \tag{7.24}$$

where the slop and intercept of the operating line are

$$\delta_{fT} = \frac{V_f}{L_f} = \frac{\beta(RD + F - S - B)}{\alpha RD} = \frac{\beta(RD + D)}{\alpha RD} = \frac{\beta(R+1)}{\alpha R} \tag{7.25}$$

$$\varepsilon_{fT}^{j} = x_{f1}^{j} - \frac{V_f}{L_f} y_{f0}^{j} = x_{f1}^{j} - \left[\frac{\beta(R+1)}{\alpha R}\right] y_{f0}^{j} \tag{7.26}$$

7.2.1.3. Material balance below feed tray

The material balance below the feed is performed from the feed tray downward by using the dew-point calculation. Referring to Figure 7.3, the tray index in this section is numbered downward from the feed tray.

For stage $i = 1$,

$$\bar{V}_f \bar{y}_{f\,2}^{\,j} + \bar{L}_f \bar{x}_{f\,0}^{\,j} = \bar{V}_f \bar{y}_{f\,1}^{\,j} + \bar{L}_f \bar{x}_{f\,1}^{\,j} \tag{7.27}$$

which can be simplified as

$$\bar{y}_{f\,2}^{\,j} = \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,1}^{\,j} + \bar{y}_{f\,1}^{\,j} - \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,0}^{\,j} \tag{7.28}$$

For $i = 2$,

$$\bar{y}_{f\,3}^{\,j} = \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,2}^{\,j} + \bar{y}_{f\,2}^{\,j} - \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,1}^{\,j} \tag{7.29}$$

By substituting equation (7.28) into equation (7.29)

$$\bar{y}_{f\,3}^{\,j} = \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,2}^{\,j} + \bar{y}_{f\,1}^{\,j} - \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,0}^{\,j} \tag{7.30}$$

For $i = 1, 2, ...N_{fB}$, equation (7.30) can be written in the following form:

$$\bar{y}_{f\,i+1}^{\,j} = \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,i}^{\,j} + \bar{y}_{f\,1}^{\,j} - \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,0}^{\,j} \tag{7.31}$$

Or, in a general form of linear equation

$$\bar{y}_{f\,i+1}^{\,j} = \delta_{fB} \bar{x}_{f\,i}^{\,j} + \varepsilon_{fB}^{j} \tag{7.32}$$

where the slope and intercept of the line are

$$\delta_{fB} = \frac{\bar{L}_f}{\bar{V}_f} = \frac{\alpha RD + F}{\beta(RD + F - S - B)} = \frac{\alpha RD + F}{\beta(RD + D)} = \frac{\alpha RD + F}{\beta D(RD + 1)} \tag{7.33}$$

$$\varepsilon_{fB}^{j} = \bar{y}_{f\,1}^{\,j} - \frac{\bar{L}_f}{\bar{V}_f} \bar{x}_{f\,0}^{\,j} = \bar{y}_{f\,1}^{\,j} - \left[\frac{\alpha RD + F}{\beta D(RD + 1)} \right] \bar{x}_{f\,0}^{\,j} \tag{7.34}$$

7.2.2. Region 2

Region 2 covers the side stream side of the dividing wall section of DWC. Consider the number of split-trays above and below the side withdrawal tray as:

N_{sT} = number of split trays above the side withdrawal

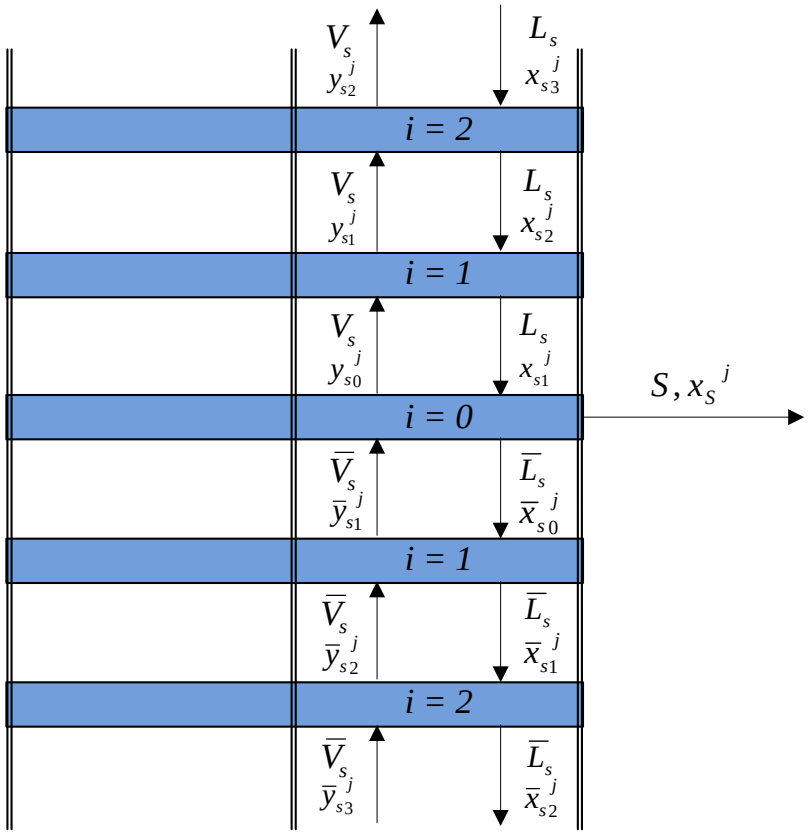


Figure 7.4 Stage model of DWC at Region 2 (side withdrawal section of dividing wall)

N_{sB} = number of split trays below the side withdrawal

Therefore, the total number of split-trays, $N_{s,\,Total}$ is

$$N_{s,Total} = N_{sT} + N_{sB} + 1 \tag{7.35}$$

The stage-wise material balance at Region 2 is given in Figure 7.4. The respective equations for the side withdrawal tray, trays above and below the side withdrawal stream are discussed in Section 7.2.2.1 to 7.2.2.3.

7.2.2.1. Material balance at side withdrawal tray

According to Figure 7.4, the side withdrawal tray is located at tray $i = 0$. Denoting j as the components, the component balance equation at tray $i = 0$ is:

$$\bar{V}_s \bar{y}_{s1}^{\,j} + L_s x_{s1}^{\,j} = S x_S^{\,j} + V_s y_{s0}^{\,j} + \bar{L}_s \bar{x}_{s0}^{\,j} \tag{7.36}$$

Like Region 1, as the liquid composition in the side withdrawal tray is similar to the composition of the side stream, hence the liquid composition at side withdrawal tray is

$$\bar{x}_{s0}^{\ j} = x_S^{\ j} \tag{7.37}$$

Assuming vapour-liquid equilibrium condition,

$$y_{s0}^{\ j} = K_{s0}^{\ j} \bar{x}_{s0}^{\ j} \tag{7.38}$$

where $K_{s0}^{\ j}$ denotes the vapour-liquid equilibrium constant for respective tray.

Rearranging equation (7.36) to find $x_{s1}^{\ j}$,

$$x_{s1}^{\ j} = \frac{S}{L_s} x_S^{\ j} + \frac{V_s}{L_s} y_{s0}^{\ j} + \frac{\bar{L}_s}{L_s} \bar{x}_{s0}^{\ j} - \frac{\bar{V}_s}{L_s} \bar{y}_{s1}^{\ j} \tag{7.39}$$

The value $\bar{y}_{s1}^{\ j}$ can be adjusted in the range of $\bar{x}_{s0}^{\ j} < \bar{y}_{s1}^{\ j} < y_{s0}^{\ j}$ to obtain a value for $x_{s1}^{\ j}$ so that a desired intersection point between the top (or bottom) operating lines in Regions 1 and 2 can be achieved. The setting of $\bar{y}_{s1}^{\ j}$ will be described in Section 7.3.2.

7.2.2.2. Material balance above side withdrawal tray

For the section above the side withdrawal, the material balance is performed by applying the bubble-point calculation from the side withdrawal tray in upward trend. The tray index numbering from above the side withdrawal tray toward the top as given in Figure 7.4 is referred in this section. Similar to the equations at the feed tray, for tray $i = 1, 2, ..., N_{sT}$,

$$V_s y_{si}^{\ j} + L_s x_{si}^{\ j} = L_s x_{si+1}^{\ j} + V_s y_{si-1}^{\ j} \tag{7.40}$$

which can be expressed as

$$y_{si}^{\ j} = \frac{L_s}{V_s} x_{si+1}^{\ j} + y_{s0}^{\ j} - \frac{L_s}{V_s} x_{s1}^{\ j} \tag{7.41}$$

Or

$$x_{s\,i+1}^{\ j} = \frac{V_s}{L_s} y_{s\,i}^{\ j} - \frac{V_s}{L_s} y_{s\,0}^{\ j} + x_{s1}^{\ j} \tag{7.42}$$

Or in a general linear equation form

$$x_{s\,i+1}^{\ j} = \delta_{sT} y_{s\,i}^{\ j} + \varepsilon_{sT}^{j} \tag{7.43}$$

Where the gradient and intercept of the operating line are

$$\delta_{sT} = \frac{V_s}{L_s} = \frac{(1-\beta)(RD+F-S-B)}{(1-\alpha)RD} = \frac{(1-\beta)(R+1)}{(1-\alpha)R} \tag{7.44}$$

$$\varepsilon_{sT}^{j} = x_{s1}^{\ j} - \frac{V_s}{L_s} y_{s\,0}^{\ j} = x_{s1}^{\ j} - \left[\frac{(1-\beta)(R+1)}{(1-\alpha)R}\right] y_{s\,0}^{\ j} \tag{7.45}$$

7.2.2.3. Material balance below side withdrawal tray

The material balance for the section below the side withdrawal is performed by applying the dew-point calculation from the side withdrawal tray in downward trend. The tray index numbered from below the side withdrawal tray toward the bottom in Figure 7.4 is referred in this section. Similar to the equations at the feed tray, for tray $i = 1, 2, ..., N_{sB}$,

$$\bar{V}_s \bar{y}_{s\,i+1}^{\ j} + \bar{L}_s \bar{x}_{s\,i-1}^{\ j} = \bar{V}_s \bar{y}_{s\,i}^{\ j} + \bar{L}_s \bar{x}_{s\,i}^{\ j} \tag{7.46}$$

which can be expressed as

$$\bar{y}_{s\,i+1}^{\ j} = \frac{\bar{L}_s}{\bar{V}_s} \bar{x}_{s\,i}^{\ j} + \bar{y}_{s1}^{\ j} - \frac{\bar{L}_s}{\bar{V}_s} \bar{x}_{s\,0}^{\ j} \tag{7.47}$$

Or in a general linear equation form

$$\bar{y}_{s\,i+1}^{\ j} = \delta_{sB} \bar{x}_{s\,i}^{\ j} + \varepsilon_{sB}^{j} \tag{7.48}$$

where

$$\delta_{sB} = \frac{\bar{L}_s}{\bar{V}_s} = \frac{(1-\alpha)RD - S}{(1-\beta)(RD+F-S-B)} = \frac{(1-\alpha)RD - S}{(1-\beta)(RD+D)} \tag{7.49}$$

$$\varepsilon_{sB}^{j} = \bar{y}_{s1}^{\ j} - \frac{\bar{L}_s}{\bar{V}_s}\bar{x}_{s0}^{\ j} = \bar{y}_{s1}^{\ j} - \left[\frac{(1-\alpha)RD - S}{(1-\beta)(RD+D)}\right]\bar{x}_{s0}^{\ j} \tag{7.50}$$

7.2.3. Region 3

Region 3 covers the section of the column above the top split trays. The component balance model at the top split-tray section, involving the last top split trays of Regions 1 and 2 and first tray of Region 3 numbering upward, is given in Figure 7.5.

For the tray just above the split-tray, i.e. *i=1* the corresponding component balance equation is

$$Lx_{d2}^{\ j} + V_f y_{f\,NfT}^{\ j} + V_s y_{s\,NsT}^{\ j} = Vy_{d1}^{\ j} + Lx_{d1}^{\ j} \tag{7.51}$$

The equation is rearranged as

$$x_{d2}^{\ j} = \frac{V}{L}y_{d1}^{\ j} + x_{d1}^{\ j} - \frac{V_f}{L}y_{f\,NfT}^{\ j} - \frac{V_s}{L}y_{s\,NsT}^{\ j} \tag{7.52}$$

As the composition of the split trays have to be close due to the irreversible mixing which will lower the thermodynamic efficiency of the column (Kim, 2005a; R. Smith, 2005), hence, it can be assumed that $y_{d0}^{\ j} = y_{f\,NfT}^{\ j} = y_{s\,NsT}^{\ j}$. Let the number of trays above the top split-tray section is N_T, the component balance equation can be expressed for $i = 1, 2, ..., N_T$ as

$$x_{d\,i+1}^{\ j} = \frac{V}{L}y_{d\,i}^{\ j} + x_{d1}^{\ j} - \frac{V}{L}y_{d0}^{\ j} \tag{7.53}$$

Or in a general linear equation form

$$x_{d\,i+1}^{\ j} = \delta_d y_{d\,i}^{\ j} + \varepsilon_d^{j} \tag{7.54}$$

Where

$$\delta_d = \frac{V}{L} = \frac{L+D}{L} = \frac{RD+D}{RD} = \frac{R+1}{R} \tag{7.55}$$

$$\varepsilon_d^{j} = x_{d1}^{\ j} - \frac{V}{L}y_{d0}^{\ j} = x_{d1}^{\ j} - \left(\frac{R+1}{R}\right)y_{d0}^{\ j} \tag{7.56}$$

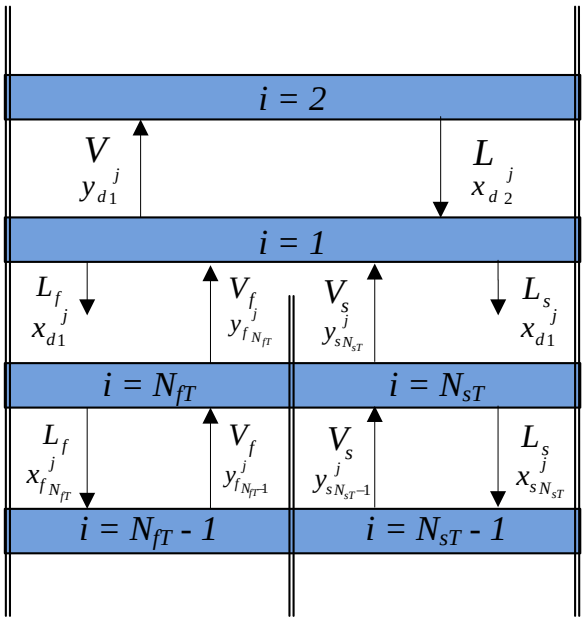


Figure 7.5 Stage model of DWC at the top split-tray section (Regions 1, 2 and 3)

The model at the condenser stage is provided in Figure 7.6. At the condenser stage, assuming $y_{d\,NT}^{\ j} = x_{d\,NT+1}^{\ j} = x_D^{\ j}$, the component balance equation is

$$(L+D)x_{d\,NT+1}^{\ j} - Vy_{d\,NT}^{\ j} = 0 \tag{7.57}$$

The duty of the condenser is calculated by utilizing the enthalpy balance as below:

$$(L+D)H_{L\,NT+1} - VH_{v\,NT} + Q_{cond} = 0 \tag{7.58}$$

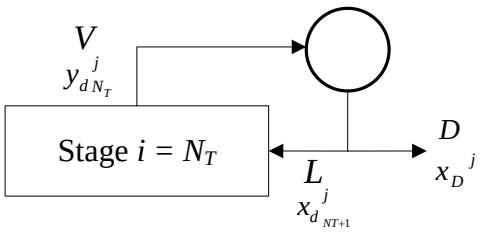


Figure 7.6 Stage model of DWC at the condenser stage

7.2.4. Region 4

The section of the column below the bottom split trays is covered in Region 4. The component balance model at the bottom split-tray section, which includes the last bottom split trays of Regions 1 and 2 and first tray of Region 4 numbered downward, is illustrated in Figure 7.7.

For the tray just below the split-tray, i.e. *i=1*, the corresponding component balance equation is as below.

$$\bar{V}\bar{y}_{b2}^{\,j} + \bar{L}_f \bar{x}_{f\,NfB}^{\,j} + \bar{L}_s \bar{x}_{s\,NsB}^{\,j} = \bar{V}y_{b1}^{\,j} + \bar{L}\bar{x}_{b1}^{\,j} \tag{7.59}$$

which can be put in the form of

$$\bar{y}_{b2}^{\,j} = \frac{\bar{L}}{\bar{V}}\bar{x}_{b1}^{\,j} + \bar{y}_{b1}^{\,j} - \frac{\bar{L}_f}{\bar{V}}\bar{x}_{f\,NfB}^{\,j} - \frac{\bar{L}_s}{\bar{V}}\bar{x}_{s\,NsB}^{\,j} \tag{7.60}$$

Like the top split tray, as the composition of the last split trays have to be close, hence, it can be assumed that $\bar{x}_{b0}^{\,j} = \bar{x}_{f\,NfB}^{\,j} = \bar{y}_{s\,NsB}^{\,j}$. Taking the number of trays below the bottom split-tray section as N_B, the component balance equation for *i = 1, 2, ...,*

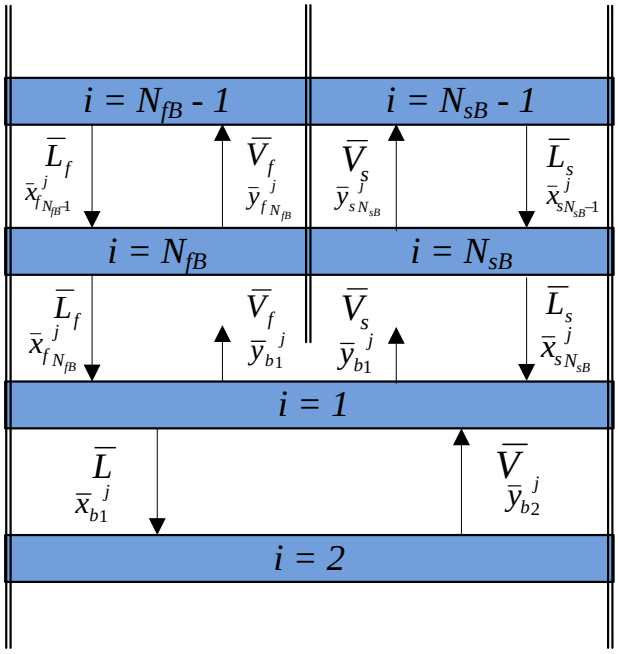


Figure 7.7 Stage model of DWC at the bottom split-tray section (Regions 1, 2 and 4)

N_B is

$$\bar{y}_{b\,i+1}^{\ j} = \frac{\bar{L}}{\bar{V}}\bar{x}_{bi}^{\ j} + \bar{y}_{b1}^{\ j} - \frac{\bar{L}}{\bar{V}}\bar{x}_{b0}^{\ j} \tag{7.61}$$

Or

$$\bar{y}_{b\,i+1}^{\ j} = \delta_b \bar{x}_{bi}^{\ j} + \varepsilon_b^j \tag{7.62}$$

where the slope and intercept of the line are

$$\delta_b = \frac{\bar{L}}{\bar{V}} = \frac{RD+F-S}{RD+F-S-B} = \frac{RD+F-S}{RD+D} \tag{7.63}$$

$$\varepsilon_b^j = \bar{y}_{b1}^{\ j} - \frac{\bar{L}}{\bar{V}}\bar{x}_{b0}^{\ j} = \bar{y}_{b1}^{\ j} - \left(\frac{RD+F-S}{RD+D}\right)\bar{x}_{b0}^{\ j} \tag{7.64}$$

The model at the reboiler stage is given in Figure 7.8. At the reboiler stage, the component balance equation is

$$Bx_B + \bar{V}\bar{y}_{b\,NB+1}^{\ j} - \bar{L}\bar{x}_{b\,NB}^{\ j} = 0 \tag{7.65}$$

The duty of the reboiler is determined from the enthalpy balance as stated below:

$$BH_B + \overline{VH}_{VNB+1} - \bar{L}\bar{H}_{LNB} - Qreb = 0 \tag{7.66}$$

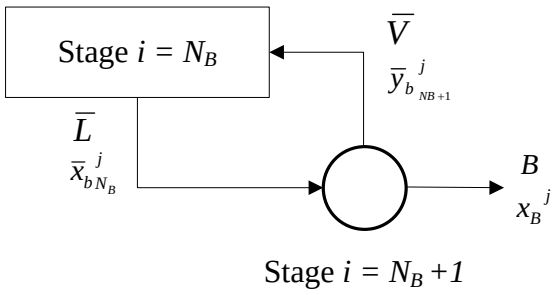


Figure 7.8 Stage model of DWC at the reboiler stage

7.3. Intersection Point Estimation

There are 6 crucial intersection points at: (1) feed location, (2) side stream location, (3) top split-tray section, (4) bottom split-tray section, (5) top column, and (6) bottom column. Note that, two of the intersections are fixed at the feed and side stream locations as point $\phi_f{}^j$ and $\phi_s{}^j$ respectively. These points are defined as follows.

7.3.1. Intersection point at feed location

The intersection point at the feed location for *n* components is

$$\phi_f{}^j = (\bar{x}_{f0}{}^j, \bar{y}_{f1}{}^j), \forall j \in (1,2,...,n)$$

where it has been mentioned previously in Section 7.2.1.1 that the liquid composition of feed tray is assumed to be equal to the feed composition, i.e.

$$\bar{x}_{f0}{}^j = z_F{}^j, \forall j \in (1,2,...,n) \tag{7.16}$$

Meanwhile, the vapour molar fractions from the tray immediately below the feed ($\bar{c}_{f1}{}^j$) are set as follows. A parameter, r_f, is introduced as the tuning parameter (i.e., adjusted to achieve convergence of solution) for specifying $\bar{y}_{f1}{}^j$. For a given value of r_f, calculate

$$\bar{c}_{f1}{}^j = r_f (y_{f0}{}^j - z_F{}^j) + z_F{}^j, \forall j \in (1,2,...,n), \forall r_f \in (0,1) \tag{7.67}$$

Then, the vapour molar fractions are obtained by normalizing the values above

$$\bar{y}_{f1}{}^j = \frac{\bar{c}_{f1}{}^j}{\sum_{j=1}^{n} \bar{c}_{f1}{}^j}, \forall j \in (1,2,...,n) \tag{7.68}$$

Note that, $y_{f0}{}^j = K_{f0}{}^j \bar{x}_{f0}{}^j$ where $K_{f0}{}^j$ denotes the vapour-liquid equilibrium constant corresponding to the feed tray.

7.3.2. Intersection point at side withdrawal location

For *n* components, the intersection point at the side stream is

$$\phi_s{}^j = (\bar{x}_{s0}{}^j, \bar{y}_{s1}{}^j), \forall j \in (1,2,...,n)$$

As mentioned in Section 7.2.2.1, the liquid composition in the side stream tray is taken to be equal to the liquid composition in the side stream withdrawal, i.e.

$$\bar{x}_{s0}{}^j = x_S{}^j, \forall j \in (1,2,...,n) \tag{7.37}$$

The molar fraction of vapour from the split-tray immediately below the side withdrawal is

$$\bar{c}_{s1}{}^j = r_s(y_{s0}{}^j - x_S{}^j) + x_S{}^j, \forall j \in (1,2,...,n), \forall r_s \in (0,1) \tag{7.69}$$

Then, the above equation is normalized as below.

$$\bar{y}_{s1}{}^j = \frac{\bar{c}_{s1}{}^j}{\sum_{j=1}^{n} \bar{c}_{s1}{}^j}, \forall j \in (1,2,...,n) \tag{7.70}$$

where $y_{s0}{}^j$ can be computed using equation (7.38). Identical to the role of r_f, the role of the r_s is to be used as the tuning parameter to specify a value for $\bar{y}_{s1}{}^j$.

Note that, $y_{s0}{}^j = K_{s0}{}^j \bar{x}_{s0}{}^j$ where $K_{s0}{}^j$ denotes the vapour-liquid equilibrium constant corresponding to the side stream tray.

7.3.3. Intersection point at top split-tray section

The intersection point at the top of split-tray section is obtained by matching the tray compositions which are computed in stage-by-stage manner (upward trend) from feed and side withdrawal trays. The idealized intersection point corresponds to tray $i = N_{fT}$ for Region 1 and tray $i = N_{sT}$ for Region 2 as shown in Figure 7.5 is selected based on the trays with the minimum composition difference. Since the trays with the minimum composition difference usually have close temperature, thus, in practice the minimum temperature difference between the liquids entering the topmost of the split-tray is used as the convergence criterion for the ease of computation in Matlab. The idealized intersection point for *n* components is taken as

$$\phi_{st}{}^j = (x_{d1}{}^j, y_{d0}{}^j), \forall j \in (1,2,...,n)$$

where $x_{d1}^{\ j}$ is the liquid molar fraction coming from the first tray immediately above the split-tray section and $y_{d0}^{\ j}$ is the vapour molar fraction coming from the split trays.

To initiate the computation of the top column (Region 3), the following equations are applied.

$$x_{d1}^{\ j} = \frac{x_{f\ NfT+1}^{\ j} L_f + x_{s\ NsT+1}^{\ j} L_s}{L} \tag{7.71}$$

$$y_{d0}^{\ j} = \frac{y_{f\ NfT}^{\ j} V_f + y_{s\ NsT}^{\ j} V_s}{V} \tag{7.72}$$

7.3.4. Intersection point at bottom split-tray section

For the bottom split-tray section, the same procedure as the top split-tray section is exercised. The idealized intersection point at the section is found by performing the calculation in downward trend and choosing the trays ($i = N_{fB}$ for Region 1 and $i = N_{sB}$ for Region 2). In practice, around this point the convergence of solution is achieved with a minimum temperature difference between vapour entering the bottommost of the split-tray. Let take the intersection point for *n* components as

$$\phi_{sb}^{\ j} = (x_{b0}^{\ j}, y_{b1}^{\ j}), \forall j \in (1,2,...,n)$$

where $x_{b0}^{\ j}$ is the liquid molar fraction coming from the last split trays and $y_{b1}^{\ j}$ is the vapour molar fraction coming from the first tray immediately below the split-tray section.

The intersection point required in order to start the computation for Region 4 can be obtained via the following equations.

$$\bar{x}_{b0}^{\ j} = \frac{\bar{x}_{f\ NfB}^{\ j} \bar{L}_f + \bar{x}_{s\ NsT}^{\ j} \bar{L}_s}{\bar{L}} \tag{7.73}$$

$$\bar{y}_{b1}^{\ j} = \frac{\bar{y}_{f\ NfB+1}^{\ j} \bar{V}_f + \bar{y}_{s\ NsB+1}^{\ j} \bar{V}_s}{\bar{V}} \tag{7.74}$$

7.3.5. Intersection point at top-most tray and bottom-most tray

The intersection point in Region 3 (top-most tray) is obtained through stage-by-stage calculation from top interlinking tray toward the top until the top product specification is met. Same condition applies to the determination of the point at bottom-most tray, i.e. performing the calculation from bottom interlinking tray in downward manner till the bottom product specification is reached.

7.4. Process Design Algorithm

Take a note that, in the proposed procedure there are 3 convergence criteria to achieve the design solution. These criteria are applied in sequence rather than simultaneously. The three criteria applied in sequence are as follows:

1. Minimum temperature differences at the interlinking trays at the topmost and bottommost of Regions 1 and 2 with either Region 3 or 4.
2. Number of split-trays - similar number of trays in Regions 1 and 2.
3. Product specifications - top and bottom compositions meet the specifications.

Figure 7.9 presents the steps required in the proposed design algorithm. Before the start of the stage-by-stage computation, several known input parameters are required. These input parameters are the feed conditions and the product distributions estimated based on the specifications. The product distributions here include the compositions and flow rates of the distillate, side stream or bottom products; which two out of the three streams have to be specified. Besides that, the key components involved are also identified.

To initiate the calculation, the design variables are identified and their values have to be assumed. There are five design variables involved:

(a) Column reflux ratio (R),

(b) Liquid split ratio (α),

(c) Vapour split ratio (β),

(d) Composition tuning parameters for Region 1 (r_f) and Region 2 (r_s).

The initial values for the variables must be set at their corresponding limits. The limit for the reflux, liquid split and vapour split ratios can be determined using the Underwood equations as discussed in Section 6.3.3. The tuning parameters for Regions 1 and 2 must fall between 0 and 1.

Based on the given input parameters and design variables, the internal vapour and liquid flow rates for all of the four regions can be computed using equations (7.5) to (7.13) in Section 7.2. Next, with the assumed feed stage liquid composition similar to the feed composition in Region 1, the liquid and vapour compositions for the feed stage are found via component balance as given in Section 7.2.1.1. Same procedure is applied for the Region 2 using equations covered in Section 7.2.2.1.

Later, the stage-by-stage calculations are performed from the stage above the feed tray for Region 1 and the side withdrawal tray for Region 2 towards the top of the column until a minimum temperature difference is achieved (first criterion mentioned above). The tray with the minimum temperature difference is taken as the first tray in Region 3. In this proposed method, the minimum temperature difference is considered instead of composition difference for the ease of computation in Matlab. Similar procedure is applied to the calculation from the trays below the feed tray and side withdrawal tray towards the bottom of the column using dew-point calculation.

Then, the number of trays at Regions 1 (N_f) and 2 (N_s) are calculated and checked if they achieve same number of trays (second criterion). If the number of trays obtained for both regions is different, the computation has to be repeated with updated design variables until the convergence (same number of trays) is reached. It is interesting to note that, only two tuning parameters are needed for adjustment in order to fulfil the second criterion. In other words, no variation of other input parameters is required. Because of this, this algorithm can speed up the entire design calculation when compared with several other existing methods.

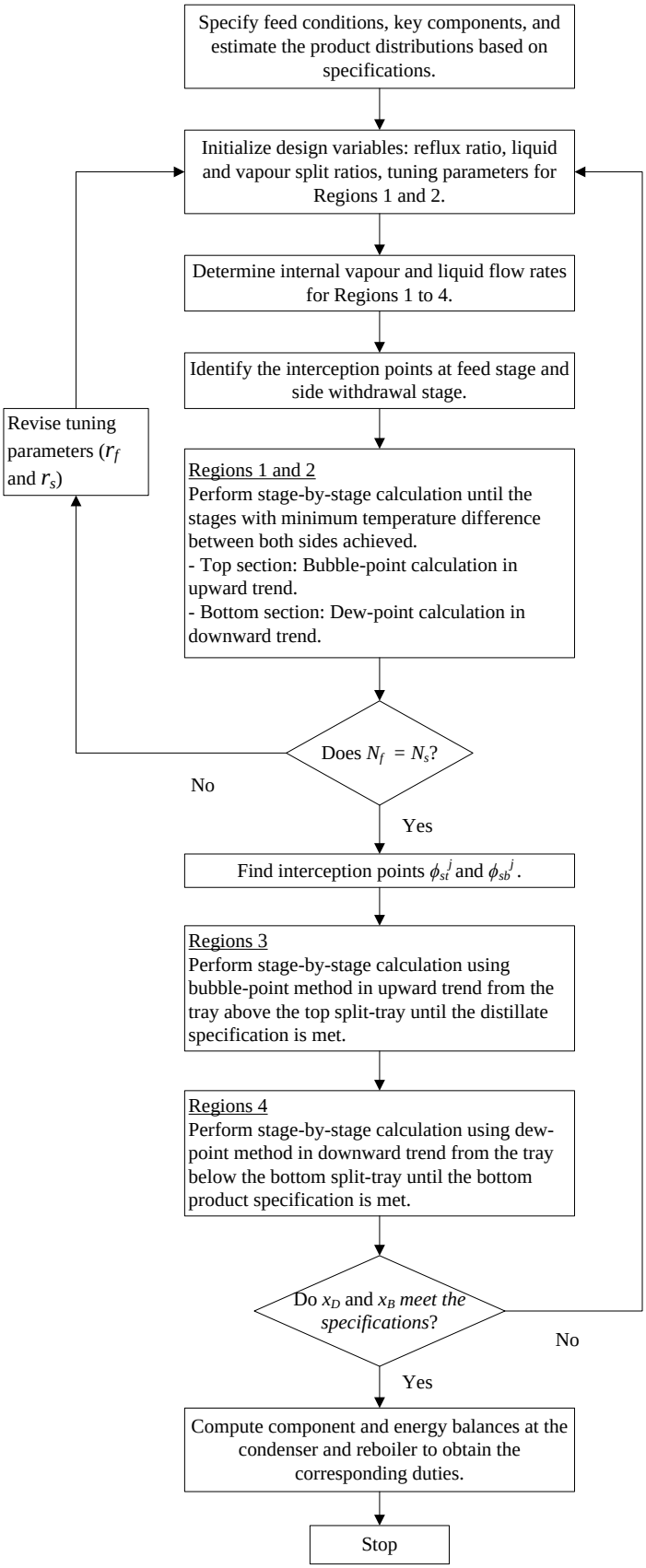


Figure 7.9 Flow chart for the design algorithm of the proposed semi-rigorous model

Once the second convergence criterion is achieved, the liquid and vapour compositions below the first tray of Region 3 ($\phi_{st}{}^{j}$) and above the first tray of Region 4 ($\phi_{sb}{}^{j}$) are found by using the equations covered in Sections 7.3.3 and 7.3.4. After that, the stage-by-stage calculation is performed for Region 3 using bubble-point method in upward trend from the tray above the top split-tray until the specified product specification is reached. It is then followed by the computation of stage-by-stage calculation in downward trend from the tray below the bottom split-tray until the bottom product specification is met. If the product specifications cannot be achieved (i.e., third convergence criterion cannot be achieved) due to the pinch condition, the computation is repeated with updated design variables. In that case, the reflux ratio can be adjusted. Then, the previous calculations are repeated to meet the first and second criteria. Finally, the component and energy balances at the condenser and reboiler are performed to obtain their corresponding duties. This completes the design calculations based on the algorithm shown in Figure 7.9.

7.5. Case Study

To ensure the feasibility of the design model and algorithm proposed, the algorithm is applied to a case study of a three-component feed system. The ternary mixture which consists of Propane, n-Butane and n-Pentane is to be separated in a DWC with Propane as the light key component, n-Butane as the middle key component, and n-Pentane as the heavy key component. The mixture is fed into the column at a flow rate of 100 kmol/h basis. The feed quality (q_F) is taken as 1 due to the assumption of saturated liquid. The column is assumed to operate at 17 bar. The feed conditions of the hydrocarbon system are presented in Table 7.1.

To validate the model, the rigorous process design is carried out based on the proposed semi-rigorous design algorithm as illustrated in Figure 7.9. The proposed design algorithm is solved using Matlab (Appendix B.4) with the given initial values for the design variables: R = 5, α = 0.40, β = 0.55, r_f = 0.9 and rs = 0.95. The value of r_s is varied until the same number of tray is obtained for Regions 1 and 2 (second criterion after the first criterion is met). The value obtained for r_s in this condition is 0.8220. The structural variables obtained are presented in Table 7.2.The results from

the computation are then used as the input parameters to perform the simulation using Aspen HYSYS. As there is no standard model for the simulation of a DWC in commercial software, a 2-column model with prefractionator will be applied to represent the DWC in Aspen HYSYS. The 2-column model is commonly applied in various literature studies (Premkumar & Rangaiah, 2009; Rangaiah et al., 2009) because it is much easier to setup in Aspen HYSYS if compared with the 4-column and pump-around models. Moreover, it gives satisfactory representation of the real-life Petlyuk column sequence and the results can be inspected easily (Dejanović et al., 2010). The method on how to perform the simulation has been covered in Chapter 4.

Table 7.1 Feed and products conditions of the depropanizer

Components	Mole Fraction
Propane (C_3)	0.3333
n-Butane (nC_4)	0.3334
n-Pentane (nC_5)	0.3333
Total Molar Flow (kmol/h)	100
Feed Pressure (bar)	17
Feed liquid fraction, q_F	1
Minimum purity of C_3 at top stream (Mole fraction)	0.95
Minimum purity of nC_4 at side stream (Mole fraction)	0.95
Minimum purity of nC_5 at bottom stream (Mole fraction)	0.95

Table 7.2 Structural variables obtained from the proposed design model for Aspen HYSYS simulation

Parameters	Value
Number of stages, NT	28
Number of stages in Region 1 and 2	14
Number of stages in Region 3	7
Number of stages in Region 4	7
Feed stage location, Nf	19
Withdrawal stage location, Ns	14

Table 7.3 Comparison of the results between the proposed semi-rigorous design model and Aspen HYSYS simulation

Components	Proposed Model (Mole Fraction)			HYSYS Simulation (Mole Fraction)		
	Top Product	Side Product	Bottom Product	Top Product	Side Product	Bottom Product
Propane (C_3)	0.9524	0.0141	0.0002	0.9499	0.0285	0.0001
n-Butane (nC_4)	0.0374	0.9564	0.0151	0.0499	0.9500	0.0499
n-Pentane (nC_5)	0.0103	0.0295	0.9847	0.0002	0.0215	0.9500
Total Molar Flow (kmol/h)	34.5	33	33.5	35.22	32.18	34.00
Temperature (^oC)	53.8897	107.66	157.62	51.46	104.00	150.40
Condenser Duty, Qcond (MW)		1.496			1.526	
Reboiler Duty, Qreb (MW)		1.511			1.649	

Finally, the results obtained from Aspen HYSYS are used as the basis to compare with the proposed model. From the Table 7.3, it can be observed that the results from the rigorous simulation, which include the condenser and reboiler duties, the compositions, the total molar flow, and the temperature for the top, side and bottom products, agree well with the results computed from the proposed model. The deviations of the values are caused by different equilibrium models and distillation model applied. The distillation model utilized in Aspen HYSYS involves the energy balance equations in the stage calculations (rigorous method), whereas for the proposed semi-rigorous method, the energy balance equations are eliminated (due to constant molar overflow assumption).

7.6. Summary

A semi-rigorous stage-by-stage modelling procedure based on the McCabe-Thiele method and Lewis-Matheson (LM) design approach has been developed for the design of a DWC for the fractionation of ternary component mixtures. The semi-rigorous nature of this procedure is due to the CMO assumption (exclusion of energy balance equations). However, this procedure can also be applied to the rigorous

design by incorporating the energy balance equations to the stage-by-stage calculation. This method is different from most of the previous works done by researchers in terms of: (1) Fenske, Underwood and Gilliland equations are not needed in the design procedure, (2) introduction of three convergence criteria applied in sequence, and (3) introduction of two tuning parameters to quickly achieve the second convergence criterion (same number of trays in both Regions 1 and 2). The design procedure starts at the feed and side withdrawal points and the calculations are performed towards the top and the bottom of the column. This procedure can avoid the tedious iterations encountered in matching the composition on the feed, side withdrawal and interlinking trays in other semi-rigorous models (Amminudin et al., 2001), which may lead to very slow convergence problem. Besides capable of generating the results of the structural variables and the final product streams like in most of the previous design methods, the proposed design algorithm can also produce the compositions and temperature profiles for quick review purpose without any need for tedious simulating using process conventional simulators, for example Aspen HYSYS. The feasibility of the model has been successfully tested using a ternary hydrocarbon mixture and the results are validated using Aspen HYSYS. It is worth noting that, since the algorithm can be written in Matlab, this will help a lot in the complex computations involving equation solving and optimization steps. Different numerical equation solvers and optimization techniques can be adopted with ease, hence making the design more flexible than in Aspen HYSYS in terms of the computational effort.

CHAPTER 8: EQUIPMENT SIZING AND HYDRAULIC DESIGN OF DWC

This chapter describes a methodology for the mechanical design of a dividing-wall column (DWC). The methodology is developed based on the conventional design procedure of a single column. Furthermore, the methodology is tested for its practicability via a case study, i.e., a DWC applied to depropanizer/debutanizer process. It is interesting to note that, all the calculations for the mechanical design are carried out using Matlab. The rest of this chapter is laid down as follows. Section 8.1 gives an overview of the chapter. In Section 8.2, the design procedure for the column and tray hydraulics of DWC is discussed in detail. The application of the design procedure is demonstrated on a case study provided in Section 8.3. Lastly, a summary of the chapter is given in Section 8.4.

8.1. Overview

The design of major equipment for the distillation system starts once the external process design is established (number of stages, feed location and side stream location are known). Similar to the design of conventional distillation unit, the DWC design consists of a vertical shell, column internals (either trays or packings), a condenser and a reboiler. The only difference from the conventional column design is the existence of the dividing wall section within the given column. As a consequence, the basic concepts for the column sizing and hydraulic designs as described in Chapter 5 can be adapted to the case of DWC mechanical design. Nevertheless, it is vital to perform the column sizing with hydraulic test for the DWC design where some modification have to be made to the procedure outlined in Figure 5.5 to suit the DWC model. The hydraulic test is crucial as to ensure the feasibility of the determined column size and tray features. The type of tray selected for this work is the sieve tray because of its well established design procedure, low capital and maintenance costs, high capacity, and ease of cleaning. But a minor drawback of the sieve tray is that it has a smaller turndown ratio (Kister, 1992), hence this may limit

the operational range of the DWC system. With respects to the designs of condenser and reboiler for the DWC, the same procedure as that of the conventional column can be applied (see Section 5.2.2).

8.2. Column and Tray Hydraulics Design Procedure for DWC

The design procedure of the column with tray hydraulics is shown in Figure 8.2. The steps involved in the procedure are summarized as follows.

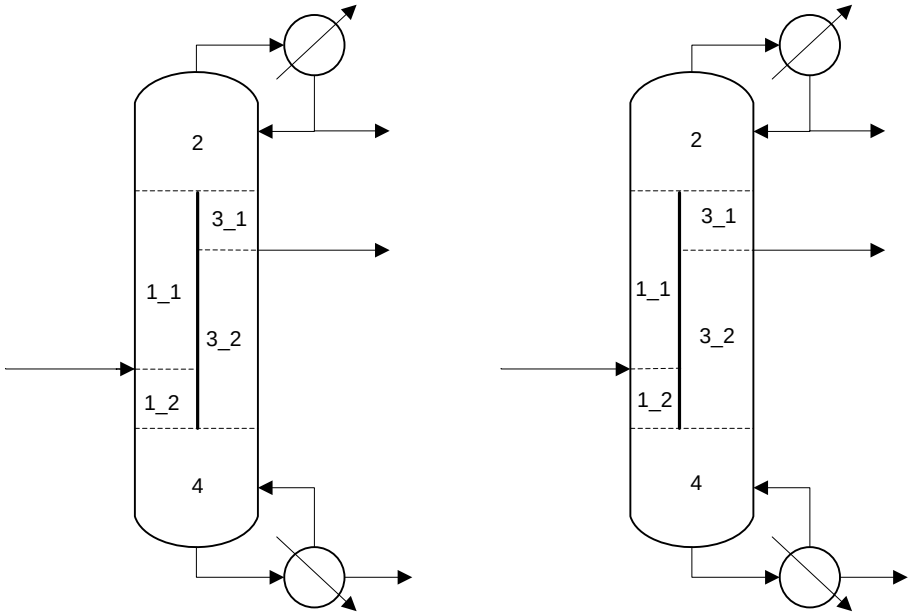
Step 1: Firstly, the column is divided into six sections as shown in Figure 8.1. Since the feed and qualities are assumed to be saturated liquid (q =1), the internal vapour flow rates across the trays in each section should be constant. Hence, a centrally or off-centre arrangement of the dividing wall should be considered for the DWC.

Step 2: For each section (sections 1 to 4), the trays with maximum and minimum throughput (vapour load) are selected for analysis.

Step 3: With the computed physical properties and flow rates, the diameters for each section of the column are calculated based on the preliminary specifications of the tray. The tray specifications proposed for initial design (Kister, 1992; Turton et al., 2009) are:

- Tray spacing of 600 mm (24 in),
- Hole diameter of 12.7 mm (0.5 in),
- Clear liquid height at the transition from the froth to spray regime of 63.5 mm (2.5 in),
- Flooding factor of 0.8, and foaming factor of 0.9.

Note that, the computation of the diameters for Sections 2 and 4 are similar to that of the conventional column. For the top section above the dividing wall, the tray diameter computed is corresponding to sum of those in Sections 1_1 and 3_1 as each stage at both of the sections practically share the same tray (trays are divided by a wall). The same condition applies to the trays in Sections 1_2 and 3_2.



(a) (b)

Figure 8.1 Dividing-wall column with divided sections: (a) Centrally arranged dividing wall; (b) Off-centre arranged dividing wall

As stated by Rangaiah et al. (2009), the diameter of the bottom section of the DWC is usually larger than that of the top section. Here, a step column is considered since the economic advantage is a major concern. It is however, according to Kister (1992), different diameters for the top and bottom sections are likely to be economical if the calculated diameter difference exceeds 20 percent. Therefore, in this work, a uniform column with the diameter equal to the largest diameter of all four sections (Sections 2, 1_1 and 3_1, 1_2 and 3_2, and 4) is used if the diameter difference is within the 20 percent.

Step 4: After the diameter of the column is selected, the same steps as proposed for the hydraulic design of a conventional column are used to determine the tray layouts for Sections 2 and 4. If the respective tray layout does not satisfy the hydraulic test, these steps have to be repeated with a new tray layout or diameter. Then, the revised diameter and total area of the column obtained from this part of computation are used to determine the location of the dividing wall.

Step 5: The location of the dividing wall is determined by computing the areas individually for all sections in the dividing wall part of the column. As indicated by

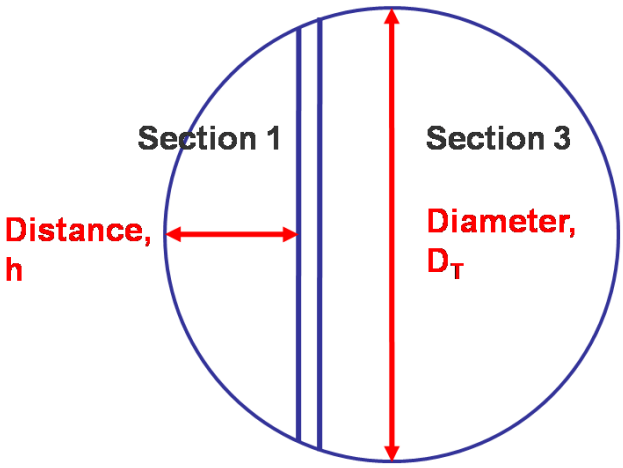


Figure 8.2 Tray layout at dividing wall section (Sections 1 and 3)

Rodr ́guez-Ángeles et al. (2015), the sum of area of the matching trays at the feed side and side draw side of the dividing wall part shall be the same as the area of a single tray at the top and bottom of the column (assuming diameter difference is less than 20%). The distance of the wall from the shell should be proportional to the fractional area occupied by a section equivalent to the prefractionator column. Thus, in this work, the area of Section 1 is calculated by assuming it as a single column. The same assumption and calculation are applied to Section 3.

Next, the fractional area for Section 1 as shown in Figure 8.2 is calculated. The calculated value is then used to find the segment area required for the shared tray, whose diameter shall be similar to the total area computed at top and bottom sections (2 and 4) of the column. Once the area is obtained, the location of the wall can be determined using the equation of a circular segment as given below.

$$Area = (D_T/2)^2 \cos^{-1}\left(\frac{D_T/2-h}{D_T/2}\right) - (D_T/2-h)\sqrt{2D_T h/2 - h^2} \qquad (8.1)$$

where D_T is the diameter of the column and h is the distance of the dividing wall from the shell of Section 1. It is important to note that the result of the $\cos^{-1}$ function in the formula (8.1) is given in radian unit.

Step 6: After Step 5 is completed, the tray layout specification and hydraulic tests are iteratively performed on the trays at each section until the results satisfy the hydraulic constraints. Otherwise, the computation is repeated with re-location of the

dividing wall by adjusting the fractional area of Section 1 or revision of the tray layout. The output from the sizing and hydraulic design is then used to compute the efficiency, followed by the calculations on height, area and volume of the column. The procedure on how to carry out these steps is quite the same as those for the conventional column which has been discussed in Section 5.2.1. The procedure for the column sizing with the hydraulic tests of the DWC is summarized in Figure 8.3.

8.3. Case Study

Extending the results obtained from the proposed DWC process design model described in Chapter 6, the proposed design procedure (Figure 8.3) is applied to the DWC (depropanizer/debutanizer unit) in order to determine the column internal design taking into account the hydraulic trays, reboiler and condenser. To initialize the mechanical design of the trays, the mass and volumetric flow rates for both phases across the stages have to be known. Although the molar flow rates computed for each section of the DWC are constant across the stages due to the semi-rigorous nature (constant molar overflow assumption) of the proposed design model, the mass and volumetric flow rates throughout the column can be different because of the variation in the vapour compositions. Therefore, the trays with minimum and maximum throughputs for each section have to be selected for the design. The liquid and vapour loads for the respective sections of DWC are presented in Table 8.1.

As mentioned in previous section of this chapter, the hydraulic design of the column is carried out by performing the hydraulic tests iteratively until the conditions meet the operable design criteria. At the dividing-wall section, the location of the dividing wall is adjusted until the trays at both sides of wall passes the hydraulic tests. The thickness of the dividing wall for DWC is assumed to be 5 mm (Kaibel et al., 1999). All the tests are performed in Matlab (Appendix B.5) and the results of the final design are presented in Table 8.2. The overall efficiency obtained is acceptable, that is 73.5%, which falls within the range of 60 to 90% as given by Turton et al. (2009).

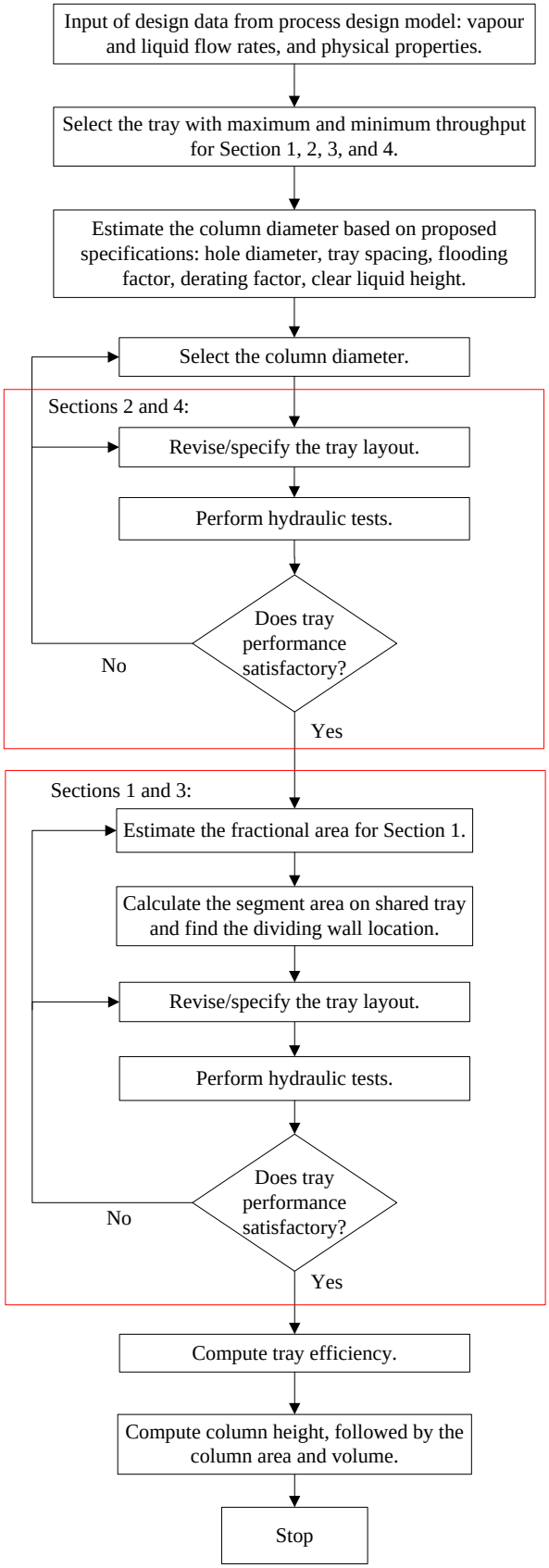


Figure 8.3 Procedure for column sizing with hydraulic tests for the DWC

Table 8.1 Selected trays with liquid and vapour loads for the hydraulic calculations for respective sections of DWC

Sections	Type	Stage Number	Vapour Mass Flow (kg/h)	Vapour Volumetric Flow (m^3/h)	Liquid Mass Flow (kg/h)	Liquid Volumetric Flow (m^3/h)
1_1	Maximum	33	268,934	5,650	140,754	184
	Minimum	14	261,524	5,613	133,343	177
1_2	Maximum	43	315,000	6,210	383,900	506
	Minimum	34	269,524	5,654	351,118	458
2	Maximum	13	504,768	10,902	417,232	546
	Minimum	1	437,679	10,284	355,982	468
3_1	Maximum	23	287,946	5,800	322,291	426
	Minimum	14	254,766	5,413	297,692	391
3_2	Maximum	43	303,171	5,934	254,443	335
	Minimum	25	286,960	5,812	238,577	315
4	Maximum	54	728,546	13,204	745,800	987
	Minimum	44	636,019	12,326	665,543	877

Table 8.2 Final design of the tray overcoming the hydraulic test

Parameters	Sections					
	1_1	1_2	2	3_1	3_2	4
Diameter, DT (m)	5.0242	5.0242	5.0292	5.0242	5.0242	5.0292
Section area, AT (m^2)	10.3163	10.3163	19.8650	9.5236	9.5236	19.8650
Active area, AA (m^2)	7.8595	7.6089	15.0974	7.2214	7.2379	14.5357
Tray spacing, S (mm)	533.4	533.4	533.4	533.4	533.4	584.2
Type of tray	Sieve	Sieve	Sieve	Sieve	Sieve	Sieve
Number of passes	1	2	2	2	2	4
Hole diameter, dH (mm)	5	5	5	5	5	5
Plate thickness, tp (mm)	3.429	3.429	3.429	3.429	3.429	3.429
Downcomer type	Straight	Straight	Straight	Straight	Straight	Straight
Downcomer area, AD (m^2)	1.2410	1.3663	2.3838	1.1511	1.1428	2.6646
Average downcomer width, wdc (m)	0.6427	0.3990	0.5106	0.3556	0.3535	0.3132
Average weir length, Lwav (m)	2.7771	5.9799	8.1903	5.6760	5.6709	16.5324
Outlet weir height, hw (mm)	50.8	50.8	50.8	50.8	50.8	50.8
Downcomer clearance, hcl (mm)	38.1	38.1	38.1	38.1	38.1	38.1
Flow path length, FPL (m)	2.3432	1.2045	1.7304	1.1951	1.1982	0.8537

Table 8.3 Summary of equipment design for the DWC

Parameters	Value
Actual number of trays	75
Actual feed tray location	47
Actual side withdrawal tray location	33
Actual top interlinking tray location	18
Actual bottom interlinking tray location	59
Column efficiency (%)	73.5
Column area, AT (m^2)	19.87
Column volume, VT (m^3)	919.44
Dividing wall location from the shell of feed side (m)	2.59
Condenser area, Acond (m^2)	2340.1
Reboiler area, Areb (m^2)	2539.7

By using the actual number of trays estimated based on overall efficiency and the tray spacing obtained for the top, dividing-wall and bottom sections, the column height is calculated by taking into account of the extra feed space, disengagement space (top and bottom) and skirt height. The height obtained for the column is 46.28 m. A single column would be sufficient for the DWC to achieve the separation as that of a combined conventional depropanizer and debutanizer units. This is so because the column height computed does not exceed the limit given by Turton et al. (2009), that is maximum of 53 m. Excessively tall column is not desirable because of its vulnerability to the wind load and foundation considerations. If the column height is above the recommended value, then the column has to be re-designed or split into two columns. Of course, there is no need to redesign or split the obtained column since its height is well below the recommended maximum height. Overall, the results of the actual number of trays, stage locations and equipment design for the column, reboiler, and condenser are summarized in Table 8.3. The parameters listed in the table are essential for the estimation of the capital cost.

8.4. Summary

The main contribution of this chapter is to establish a systematic procedure for the mechanical design (column internal design) of the DWC based on that of the

conventional column design. So far, very limited work has been published to address this matter. In this chapter, the condenser and reboiler for the DWC are sized with the same procedure as applied to the single column. For the column unit, the column sizing and tray design have to be conducted at each section of the column, i.e., Sections 1, 2, 3, and 4. The top and bottom sections have the same sizing and tray design procedure as the conventional column. Assuming a uniform column, the total area for the matching trays at Sections 1 and 3 has to be equal to the area of a single tray in Sections 2 and 4. The fractional area occupied by Section 1 on the shared tray is calculated by assuming it as a single column. The fractional area or the tray layout specifications will be the adjustable variables to determine the location of the dividing wall until the trays at both of the sections pass the hydraulic tests. The difference of this work with the methodology proposed by Rodr ́guez-Ángeles et al. (2015) is that the fractional area is the main adjustable variables in determining the location of dividing wall instead of tray layout specifications, which is often more tedious and time-consuming. The design procedure has been successfully tested on the DWC unit (depropanizer/debutanizer system) using Matlab. The proposed methodology is important to ensure the viability and operability of the column size and tray layout before the estimation of the capital cost is carried out.

CHAPTER 9: OPTIMIZATION AND ECONOMIC EVALUATION

In this chapter, a general procedure for the optimization of dividing-wall column (DWC) is presented. By using the proposed procedure, the optimization and economic evaluation for the DWC are performed. Note that, the optimization procedure is applied to a case study using Matlab. The organization of this chapter is as follows. A summary of the overall design procedure which has been discussed in previous chapters is given in Section 9.1. In Section 9.2, the optimization procedure is presented along with the formulation of the optimization problem and its optimization variables and constraints. The detail on the economic evaluation is provided in Section 9.3 and a case study is given in Section 9.4. Lastly, a summary of the chapter is given in Section 9.4.

9.1. Overall Design Procedure

The overall design procedure (including both column external and internal parts) for the dividing-wall column (DWC) is illustrated in Figure 9.1. From the figure, it can be clearly seen that the overall design procedure can be divided into two sections: process design procedure and equipment design procedure. The former is performed to obtain the data necessary for the operating cost calculations and equipment design, while the latter is required for the computation of the total capital cost. The main purpose of the overall design model is to obtain the operating cost and the capital cost for the calculation of the total annualized cost (TAC), which is used for economic analysis. The output data required from each part of the model necessary for the computation of the equipment design and costs are summarized in Figure 9.1. The computation of the TAC for DWC is obtained using Matlab (Appendix B.6).

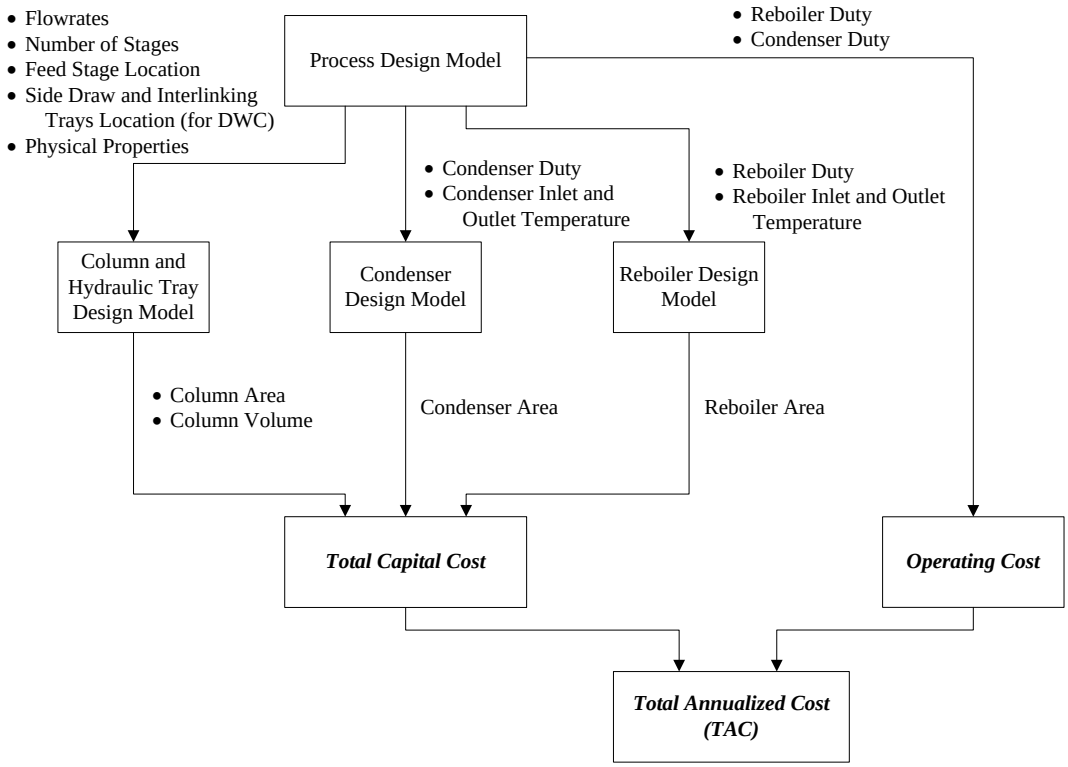


Figure 9.1 Overall design procedure for a dividing wall column (DWC)

9.2. Optimization Procedure

Once the initial design for the DWC is produced, the final step of the design is to perform the optimization based on the preliminary design. For the DWC, the design variables required for the proposed process design model are as discussed in Chapter 6: reflux ratio and liquid split ratio. However, the reflux ratio of the column is the only degree of freedom considered as the optimization variable because the liquid split ratio is used as the adjusting variable to ensure equal number of stages is obtained on the both sides of the dividing wall. If semi-rigorous analytical method in Chapter 7 is used, the composition tuning parameters are used as the adjusting variables to achieve equal number of stages at the dividing wall section, whereas the liquid and vapour split ratios are varied to ensure the feasibility of the point estimated at the top and bottom split trays. The boil-up ratio is also no longer to be considered as the optimization variable because it can be determined from the reboiler duty which is directly calculated from the overall column enthalpy balance.

In this work, the optimization problem for the DWC is a steady state non-linear program (NLP). The problem can be formulated in the form of

$$\begin{aligned} \min_{u} \quad & J(x,u) \\ \textit{subject to} \quad & f(x,u) = 0 \\ & g(x,u) \le 0 \end{aligned} \tag{9.1}$$

where J is the objective function, f is the DWC model equations and g are the operational constraints. x are the state variables in the process model and u are the independent variables which can be manipulated.

A cost function can be formulated to define the problem. The main objective function for the optimization in this work is to minimize the total annualized cost (TAC). The TAC to be minimized, comprises of both capital and operating costs, which can be written as

$$J = OPC + A_F CAP \tag{9.2}$$

where OPC denotes the operating cost, CAP the capital cost, and A_F the annualized factor for the capital cost. The constraints involved in the column optimization are product specifications and other related operating conditions such as vapour flow equalization condition. These constraints have been implicitly defined in the earlier steps of the process model. The details on the computation of capital cost, operating cost and TAC are covered in Section 9.3. The complete procedure for the design and optimization as summarized in Figure 8.2 are as follows.

Step 1: Firstly, the input parameters required for solving the DWC are specified. These parameters are feed conditions and specifications of three product streams.

Step 2: The design variables required for the initialization of the calculation are provided. For modified Lewis-Matheson (LM) method as proposed in Chapter 6, the design variables are reflux ratio and liquid split ratio. On the other hand, the design variables for the method proposed in Chapter 7 are reflux ratio, liquid and vapour split ratios and composition tuning parameters at both sides of dividing wall.

Step 3: The process design model for DWC is solved using the process design algorithm as proposed in Chapter 6 or 7. If the feed system comprises more than 3

components, the process model as proposed in Chapter 6 is applied. Otherwise, the process model as proposed in Chapter 7 is applied.

Step 4: Then, equipment design with hydraulic tests is performed on the DWC unit, which consists of condenser, reboiler and column with trays (Chapter 8).

Step 5: The total annualized cost (TAC) is then computed using equation 9.2, which consists of operating cost and annualized capital cost. The operating cost is calculated based on the reboiler and condenser duties. On the other hand, the capital cost is calculated using the results obtained from equipment design.

Step 6: The computed TAC is checked if a minimum value of TAC is achieved. If it is not yet acheived, the calculation is repeated by adjusting the optimization parameter, which is reflux ratio (return to Step 2).

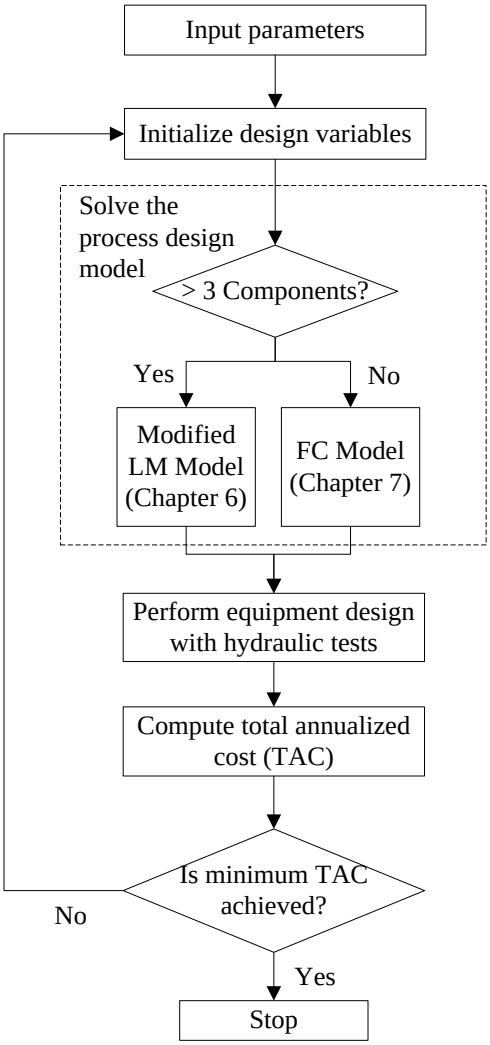


Figure 9.2 Design and optimization procedure for DWC design

9.3. Economic Evaluation

The total annualized cost (TAC) is defined as the sum of the operating cost and the capital cost with annualized factor. The operating cost estimated for the plant daily operation comprised of the raw material cost and utilities cost. However, in this study, only the total utilities cost is considered because the raw material cost is relatively independent of the design of the distillation unit. The total cost of the utilities was evaluated according to the utilities cost data as suggested by Turton et al. (2009), presented in Table 9.1. In the present work, two types of utilities considered are: (1) steam for the reboiler and (2) cooling water for the condenser. Therefore, the operating cost for the column is the sum of the costs of cooling water and steam based on the condenser and reboiler duties.

To estimate the bare module costs of the equipment in the distillation system, the cost correlations proposed by Turton et al. (2009) are employed. For the DWC, some additional assumptions are required to take into consideration of its characteristics. The cost of the vessel is assumed to be 20% higher than the cost corresponding to the conventional column, whereas the cost of the sieve trays at the dividing wall section is assumed to be 30% higher than the standard trays (Gómez-Castro et al., 2011). The Chemical Engineering Plant Cost Index (CEPCI) of 541.7 for year 2016 is utilized for cost updating to account for changes that result from inflation. The annualized factor, A_F, is calculated using the equation (9.3) as given below by adopting the life period (n) and interest rate (ir) of 10 years and 15% respectively (Sinnott & Towler, 2009):

$$A_F = \frac{ir(1+ir)^n}{(1+ir)^n - 1} \tag{9.3}$$

Table 9.1 Utilities Cost Data

Utility	Price [$/(kW.year)]
Low Pressure Steam (5 barg)	421.1
Cooling Water	10.8

9.4. Case Study

Using the proposed process model and equipment sizing model established in Chapters 6 and 8, the optimization is carried out on the DWC, which is designed to replace the depropanizer and debutanizer units in a gas plant. The same case study as covered in Chapters 6 and 8 is used for optimization in this chapter. All of the design and optimization solution for the DWC design are solved using Matlab.

From Chapter 6, the minimum value of R obtained for the proposed process design model to be operable is 3.48. The way on how to obtain this value has been covered in Section 6.4.3. Therefore, this value is taken as the lower bound for the optimization. The upper bound for the reflux ratio is set as 4.4, which is 25% higher than the lower bound. This estimated upper bound is found to be sufficient for the optimization in this work. This can be observed in Figure 9.3, which illustrates on the relationship between the costs (operating cost, capital cost and TAC) and the reflux ratio. The figure shows that the TAC for the DWC increases when the reflux ratio increases. Since the objective of the optimization is to achieve minimum TAC, thus,

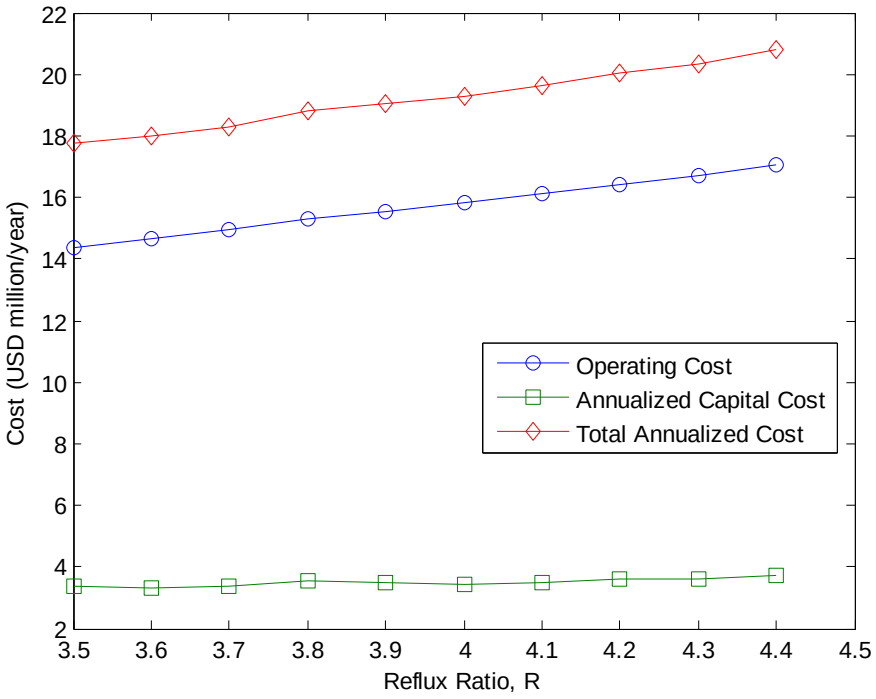


Figure 9.3 Variations in operating, annualized capital and total annualized costs with the reflux ratio

the costing obtained beyond the upper bound of reflux ratio will be at the expense of diminishing profit.

From the figure, it can also be seen that the annualized capital cost does not vary significantly with the rising reflux ratio. On the other hand, the operating cost gives ascending profile when the reflux ratio increases. Moreover, it is also observed from the figure that the operating cost for the column is much higher than the annualized capital cost. Therefore, it can be concluded that the operating cost is the determining factor in the optimization of the DWC because it gives the most contribution to the TAC calculation without considering the purity constraint.

Bear in mind that, the solution of the proposed design model will provide the structural variables or parameters of the DWC. Therefore, the structural parameters for this design model are dependent on the reflux ratio. This is different from the rating model, in which the structural parameters have to be specified via the initial calculations. This can be seen from Figure 9.4 that the total number of trays (NT_{act}) and the number of trays at the dividing wall section (Ndw_{act}) decrease with

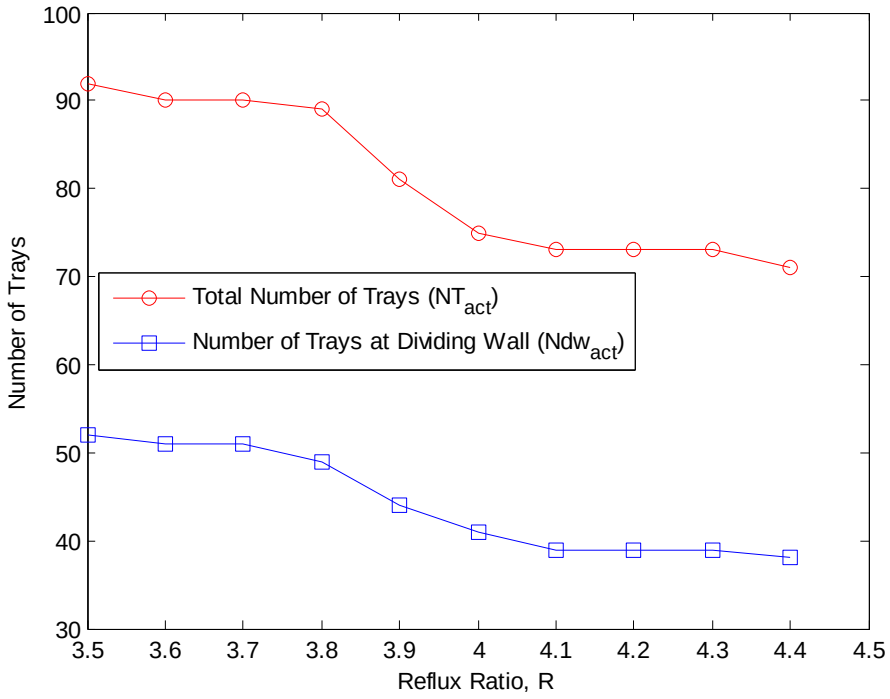


Figure 9.4 Variations of total number of trays in the column and at the dividing wall section with the reflux ratio

increasing reflux ratio. It is found out that with a 2.8% increase of the reflux ratio, the number of trays at the dividing wall section reduces on an average of 3.4%.

For the liquid split ratio, it is found that there is a certain range of the ratio which can give the same number of trays at the dividing wall section at different reflux ratio. The range of the liquid split ratio is very narrow, only up to 4% of difference between minimum and maximum values is obtained. The value of the liquid split ratio for different reflux ratio will affect the number of trays at the dividing wall section. However, the effect is not very significant as only on an average of two-tray difference is achieved with the minimum and maximum values of the liquid split ratio. Therefore, within this design and optimization model, the liquid split ratio which gives the smallest number of trays at the dividing wall section is selected for each reflux ratio. The relationship between the liquid and vapour split ratios and the reflux ratio is shown in Figure 9.5. As seen in the figure, both of the split ratios show the non-linear characteristic of their respective profiles with increasing reflux ratio. The liquid split ratios obtained for different reflux ratio are found to vary around 0.31, whereas the vapour split ratios obtained are fluctuating around 0.51.

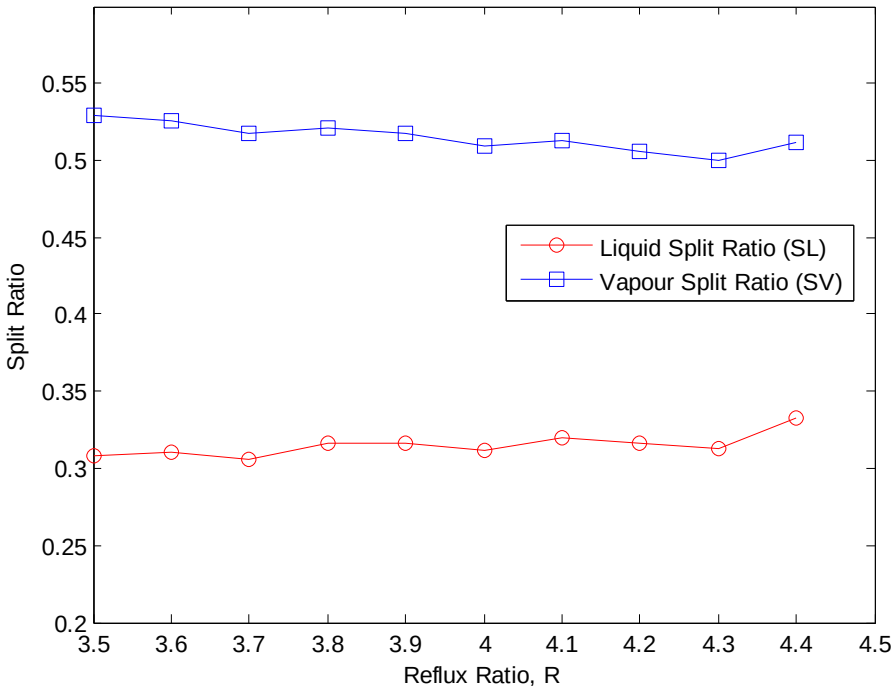


Figure 9.5 Variations of liquid and vapour split ratios with the reflux ratio

As given in Table 6.1, the specifications for the propane in the distillate, the butane in the side draw product and the pentane in the bottom product are 0.91, 0.97, and 0.98 respectively. These specifications are defined as the constraint for this optimization problem. From Figure 9.6, it can be noticed that the purities for the light key in the distillate and the middle key in the side-stream product fall within their respective product specifications with increasing reflux. Therefore, the purities of the both product stream are not a major concern in this study. The condition is different for the heavy key composition in the bottom product as it shows obvious increment with rising reflux ratio. At low reflux ratio, the purity of the bottom product falls outside the required specification. Therefore, the minimum reflux ratio obtained in this case study to satisfy the product specifications is 3.8. Table 9.2 presents the comparison of energy performance and operating cost between conventional column sequence and DWC. The results show that the DWC can give about 18% operating cost savings when compared with the conventional column sequence. The final results obtained from the optimization are summarized in Table 9.3. The TAC obtained for the DWC is USD 18.798 million/year.

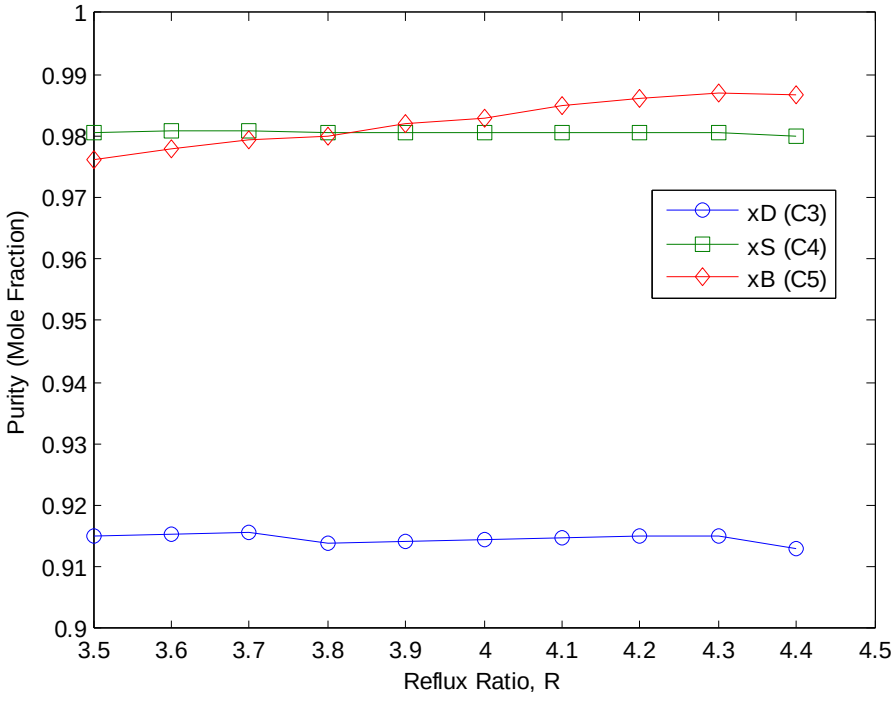


Figure 9.6 Variations in purities for the top, middle and bottom product streams with the reflux ratio

Table 9.2 Comparison of energy performance and operating cost between conventional column sequence and DWC

	Conventional Column Sequence		Dividing wall column (DWC)
	Depropanizer	Debutanizer	
Condenser Duty (MW)	23.10	23.75	32.79
Reboiler Duty (MW)	24.84	18.10	35.47
Operating Cost (USD million/year)	18.588		15.277
Operating Cost Saving (%)	0.00		17.81

Table 9.3 Summary of the optimization results for the DWC

Parameters	Value
TAC (USD million/year)	18.798
Reflux ratio, R	3.8
Total number of stages, NT_{act}	89
Number of stages at dividing wall, Ndw_{act}	49
Purity of C_3 in top stream (Mole fraction)	0.9140
Purity of C_4 in side stream (Mole fraction)	0.9804
Purity of C_5 in bottom stream (Mole fraction)	0.9801
Distillate flow rate (kmol/h)	2030.8
Intermediate product flow rate (kmol/h)	1449.9
Bottom product flow rate (kmol/h)	288.3
Condenser duty, Q_{cond} (MW)	32.79
Reboiler duty, Q_{reb} (MW)	35.47

9.5. Summary

The overall design and optimization procedure for the DWC is presented in this chapter. The purpose of this chapter is to establish an optimization methodology combining both process design and equipment design (including trays) of DWC. By considering the hydraulic conditions in the optimization procedure, a feasibility and reliability of the design of the DWC can be obtained. The methodology which has been presented in greater detail can serve as a guideline on how to incorporate various design models into the optimization procedure to achieve optimum design of DWC.

The optimization problem for DWC, which is typically a non-linear program (NLP), can be formulated with the objective function to minimize the total annualized cost TAC) subject to the product specifications of top, middle, and bottom products. The parameter defined for the optimization of the DWC is reflux ratio. The overall procedure for the optimization starts with the input of known parameters, followed by initialization of design variables, solution of the process model and equipment design model, and calculation of the TAC. The procedure is repeated until a minimum value of TAC is achieved. Otherwise, the procedure is repeated with new reflux ratio. This model solution procedure has been implemented in Matlab environment and it has been applied successfully to the design of the DWC unit to replace the depropanizer/debutanizer system in a gas plant.

Although in a DWC design there appears to have more input variables (degree of freedoms) than in a conventional distillation column, only very few input variables can be used in the optimization phase. In this study, only one input variable (i.e., reflux ratio) is used in the DWC optimization phase. The reason for the limited number of the optimization variables is that most of the input variables available have been used to achieve the requirements in the first two phases – process and equipment designs. For example, the liquid and vapour split ratios are used in the process design to ensure equal number of stages is achieved in the feed and side stream sides of the dividing wall zone (physical requirement). Meanwhile, the column diameter and fractional area (dividing wall) are used in the equipment design to meet the requirements imposed by flooding and weeping. Moreover, the high degree of interrelationships among those input variables, which are partly induced by the assumptions made, is another reason for the limited number of input variable in the optimization phase. For example, in the modified theta procedure the liquid split ratio can be shown to be dependent on the vapour split ratio; thus one variable can be expressed in terms of another. Such interrelationships that exist among several input variables have no doubt imposed a big challenge in the DWC optimization.

CHAPTER 10: CONCLUSION AND FUTURE WORK

The research efforts reported in this dissertation represent a solid contribution towards the advancement in the area of design and optimization of dividing-wall column (DWC). This chapter shall highlight some concluding remarks and possible future works in the DWC research.

10.1. Concluding Remarks

In this dissertation, the complete procedure for the design and optimization of a dividing-wall column (DWC) is established. In general, the design of the DWC can be divided into three major phases, which are (1) process design, (2) equipment design and (3) optimization. In this work, the process design phase is covered in Chapters 4 to 7, equipment design phase in Chapter 5 and 8, and lastly optimization in Chapter 9.

In chapter 4, the sequential procedures on how to carry out the process design of DWC using Aspen HYSYS are illustrated based on the application to a ternary separation, i.e., depropanizer/debutanizer system. The design of the DWC using Aspen HYSYS is found to be a tedious process because short-cut simulation is required prior to starting the rigorous simulation of the DWC. As the design toolbox for DWC does not exist in the existing library of operations in Aspen HYSYS, the DWC is then represented by three short-cut columns for the short-cut simulation and the Petlyuk column arrangement for the rigorous simulation. Due to the different configuration and calculation models, the transfer of the data from the short-cut columns to the rigorous model (Petlyuk column) often leads to the severe convergence issue. Therefore, a tedious trial and error running is necessary to achieve the convergence of solution to the system model equations. Despite this convergence issue, it is undeniable that Aspen HYSYS is a powerful tool in producing reliable results for the process design. Hence, Aspen HYSYS is used as a basis to validate any new design model and method proposed in the chapters covering the process design part (Chapters 5 to7).

In Chapter 5, a rigorous stage-by-stage modelling of the DWC together with the model solution procedure is presented. The procedure involved is based on the Lewis-Matheson (LM) design approach for the multi-component separation (NGLs fractionation unit) of a conventional column. The purpose of this chapter is to build the fundamental model for the design of a DWC. The main contribution of this work is the improvement in the computational procedure for solving the existing LM design problem by incorporating: (1) Fenske equation and (2) modified theta method in the design procedure. Fenske equation is incorporated in earlier steps of the design procedure to enhance the estimation of the non-key component distributions, and thus avoiding infeasible solutions to the stage-by-stage system of equations of mass and energy balances. A modified theta method, of which a ratio of the liquid compositions (at feed stage) is introduced to the conventional theta method, is included in the design procedure to increase the accuracy of the composition matching at the feed stage for both rectifying and stripping sections. Besides that, to avoid the confusion caused by the availability of several previous works on the equipment design, the procedure for the equipment sizing with tray hydraulic calculations is also provided as the guideline for two important purposes:

(1) The way to perform the equipment designs.

(2) The criteria involved in the design.

The proposed model solution procedure has been successfully used in the design of an industrial-scale depropanizer column using Matlab software.

In Chapter 6, a new design algorithm for the design of a DWC is developed based on the modified LM design approach presented in Chapter 5. The modified Lewis-Matheson (LM) stage-by-stage method as suggested in Chapter 5 is applied as the foundation of this new design model. One of the salient features of this algorithm is the reduction of the degrees of freedom of the design via the derivation of some equations to relate the variables which interact with each other in the design. Thus, only two design variables are required to initialize the calculations: (1) reflux ratio and (2) liquid split ratio. The liquid split ratio is used in the design procedure to ensure that equal number of stages at both sides of the dividing wall is accomplished. The second feature is the introduction of modified theta method to enhance the speed

of the composition matching at the connecting trays. A different convergence criterion at the feed and interlinking trays is also recommended for simplifying the computation. This proposed model can also reduce the tedious work required in developing a more rigorous design model of the DWC. Instead of applying the rigorous design model in conjunction with the short-cut model or semi-rigorous model, this proposed model can be used independently because it can generate the profiles throughout the column, such as temperature and composition profiles, besides providing the operational and structural variables of the DWC. Although the model used in this chapter is semi-rigorous in nature, the design algorithm is also applicable to the rigorous model by including the energy balance equations into the existing algorithm.

To overcome the tedious and ad-hoc trial-and-error procedures commonly used to achieve convergence of solutions at selected locations, e.g., the feed and side-stream trays, a new design algorithm is proposed in Chapter 7. This stage-by-stage modelling procedure is developed based on the concepts of McCabe-Thiele method and Lewis-Matheson (LM) design approach. This algorithm can eliminate the convergence at selected locations by initiating the calculation at the feed and side withdrawal trays. Two new tuning parameters are introduced to speed up the convergence of the solution, i.e. matching tray numbers between the feed and side-stream sides of the dividing wall sections. The proposed design algorithm can also produce the compositions and temperature profiles for quick review purpose without any need for tedious simulation using conventional process simulators. The feasibility of the model has been successfully tested using a ternary hydrocarbon mixture and the results are validated using Aspen HYSYS. It is worth noting that, since the algorithm can be written in Matlab code, this will make the design to be more flexible and efficient than in Aspen HYSYS in terms of the reduced trial-and-error computational effort.

Chapter 8 describes a methodology for the equipment design of a DWC which is developed based on the conventional design procedure of a single column as recommended in Section 5.2 of Chapter 5. This chapter is important because currently there are only a limited number of papers published on this matter. So far, to the best of the author's knowledge, there is only one paper presented on the

methodology of the mechanical design with hydraulic consideration (Rodr ́guez-Ángeles et al., 2015). Therefore, based on the general idea provided by the authors, more detailed steps on how to perform the column design of DWC with hydraulic trays are outlined in this chapter. In their work, in determining the location of the dividing wall, the optimization to achieve the objective of minimum total diameter at the dividing wall section via a systematic adjustment of several parameters, such as weir area and holes size, is required. Therefore in the present work, for the ease of computation, the fractional area is selected as the main adjustable variable to determine the location of the dividing wall until the trays at both of the sections pass the hydraulic tests. The tray layout specifications will only be revised if the fractional area does not satisfy the hydraulic test criteria.

In Chapter 9, the overall procedure of the optimization and economic evaluation for the DWC are presented. The main contribution of this chapter is to establish an optimization methodology for both process and equipment design (including trays) of DWC. This is important to ensure the feasibility of the column design which shall satisfy weeping, flooding and entrainment conditions. The process design model used for the optimization is the one as proposed in Chapter 6 because it is developed with the feature of reduced number of degrees of freedom. Alternatively, the procedure and model developed in Chapter 7 can also be used in the optimization. The economic performance criterion in the optimization used in this work is the total annualized cost (TAC) of the DWC.

10.2. Future Works

Derived from the works presented in this thesis, some of the future works and interesting research ideas to improve the current state-of-the art in DWC research are listed as follows.

- The process models as proposed in Chapters 6 and 7 can be converted to rigorous design by considering energy balance equations in the design.
- The type of DWC used in this work is middle-type arrangement of DWC. Extended study can be done by applying the design algorithm to upper-type

DWC and lower-type DWC. In particular, the algorithm developed in Chapter 7 can be extended to these different arrangements of DWC.

- The feed mixture used in this work is mainly hydrocarbon system, which is considered as not highly non-ideal mixture. Thus, further study is required on the extensions of the design algorithms to non-ideal and azeotropic mixture.

- Both of the design algorithms (Chapters 6 and 7) proposed in this work are applicable to the design of a new DWC. Hence, further work has to be done on how to apply the design methods in retrofit cases.

- The study related to controllability issue is another important topic for further research. Therefore, in future study, a methodology for addressing both steady-state economic and controllability performances in the design should be proposed.

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APPENDIX

A. Thermodynamic Models

A.1 Equation of state

The equation of state chosen to predict the vapour-liquid equilibrium (VLE) of the proposed models in this study is Peng-Robinson (PR) equation. This equation of state has long been recognized as the most popular equation of state for natural gas systems in refinery plant. Thus, it would be sufficient to apply this equation in predicting the equilibrium of light hydrocarbon mixtures used in this study (Aspen Technology, 2011). The PR equation written in polynomial (cubic) form is

$$Z^3 - (1-B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \qquad \text{(A1)}$$

To predict the equilibrium of a multi-component mixture, the mixing and combining rules have to be applied to the parameters of the equation of state (Nasri & Binous, 2009):

$$A = \sum_{i=1}^{C}\sum_{j=1}^{C} y_i y_j A_{ij} \qquad \text{(A2)}$$

$$A_{ij} = (A_i A_j)^{0.5}(1 - k_{ij}) \qquad \text{(A3)}$$

$$A_i = 0.45724\left(\frac{R^2 T_{ci}^2}{P_{ci}}\right)\alpha \qquad \text{(A4)}$$

$$\alpha^{1/2} = 1 + m\left(1 - (T/T_{ci})^{1/2}\right) \qquad \text{(A5)}$$

$$m = 0.37464 + 1.54226\,\omega - 0.26992\,\omega^2 \qquad \text{(A6)}$$

$$B = \sum_{i=1}^{C} y_i B_i \qquad \text{(A7)}$$

$$B_i = 0.07780\left(\frac{RT_{ci}}{P_{ci}}\right) \qquad \text{(A8)}$$

Where ω is acentric factor of the species, T_{ci} is the critical temperature in *K*, P_{ci} is the critical pressure in *bar*, *R=8.314e-5 m^3.bar/mol.K* is the universal gas constant and *Z=PV/(RT)* is the compressibility factor. The values for acentric factor, critical temperature and pressure for each species are taken from Perry and Green (1997) are The binary interaction parameters, k_{ij} can be obtained from Aspen HYSYS. Then, the equilibrium constants are computed using the equations as below.

$$k_i = \frac{\varphi_{il}}{\varphi_{iv}} \tag{A9}$$

$$\varphi_{li} = \exp\left[(Z_l - 1)\frac{B_i}{B} - \ln(Z_l - B) - \frac{A}{2\sqrt{2}B}\left[\frac{2\sum_j y_j A_{ij}}{A} - \frac{B_i}{B} \right] \ln\left[\frac{Z_l + (1+\sqrt{2})B}{Z_l + (1-\sqrt{2})B} \right] \right] \tag{A10}$$

$$\varphi_{vi} = \exp\left[(Z_v - 1)\frac{B_i}{B} - \ln(Z_v - B) - \frac{A}{2\sqrt{2}B}\left[\frac{2\sum_j y_j A_{ij}}{A} - \frac{B_i}{B} \right] \ln\left[\frac{Z_v + (1+\sqrt{2})B}{Z_v + (1-\sqrt{2})B} \right] \right] \tag{A11}$$

A.2 Enthalpy

The calculation of enthalpies for vapour and liquid mixtures is required to complete the energy balance of the distillation system. From the energy balance, the duties for the condenser and reboiler for the corresponding system can be obtained. These parameters are necessary in determining the capital and operating costs.

To compute the enthalpy of vapour phase mixture, the following equations are applied (Biegler et al., 1997).

$$\Delta H_V(T, y) = \sum_{k=1}^{C} y_k H^0_{f,k} + \int_{T_0}^{T} y_k C^0_{p,k}(T)\,dT \tag{A12}$$

where y_k is the vapour composition of component *k*, $H^0_{f,k}$ is the heat of formation for component *k* at reference temperature T_0 = *298 K* and $C^0_{p,k}(T)$ is the temperature dependent heat capacities for component *k*. The equation of the heat capacity for each component is

$$C_{p,k}^{0}(T) = C_{pA,k} + C_{pB,k}T + C_{pC,k}T^{2} + C_{pD,k}T^{3} \qquad \text{(A13)}$$

where $C_{pA,k}$, $C_{pB,k}$, $C_{pC,k}$ and $C_{pA,k}$, are constants in the ideal gas heat capacity equation.

On the other hand, the enthalpy for the liquid mixture can be computed as follows.

$$\Delta H_{L}(T,x) = \sum_{k=1}^{C} x_{k}\left[H_{f,k}^{0} + \int_{T_0}^{T} y_{k} C_{p,k}^{0}(T)dT - \Delta H_{vap,k}(T) \right] \qquad \text{(A14)}$$

where x_k is the liquid composition of component k, $H^{0}_{f,k}$ is the heat of formation for component k at reference temperature $T_0 = 298$ K, $C^{0}_{p,k}(T)$ is the temperature dependent heat capacities for component k and $\Delta H_{vap,k}$ is the heat of vaporization of component k which is estimated using Watson correlation as below (Biegler et al., 1997).

$$\Delta H_{vap,k}(T) = \Delta H_{vap,k}(T_{b,k})\left[\frac{T_{c,k} - T}{T_{c,k} - T_{b,k}} \right] \qquad \text{(A15)}$$

where T_{ck} is the critical temperature of component k, $T_{b,k}$ is the atmospheric boiling temperature for component k and $\Delta H_{vap,k}(T_{b,k})$ is the known heat of vaporization at the atmospheric boiling temperature for respective components. The data for the critical temperature for each component is obtained from Perry and Green (1997), whereas the data for the boiling point, heat of vaporization at atmospheric boiling point, heat of formation and constants in the ideal gas heat capacity equation is taken from (Sinnott (2005)).

B. Matlab Programmes for Simulation

Due to confidentiality concern, only selected Matlab codes are presented in the following sections.

B.1 Process design of simple column

```
% % Process design model of simple column (Chapter 5)
% Initialized parameters
R = 2.2;

%-------------------------------------------------------------------
% % Input parameters/Initial Estimation
% Temperature in deg K
% Pressure in bar
% Flowrate in kmol/hr
% Condenser/Reboiler Duty in MW

% Identify Light key (LK) & heavy key (HK) components
LK = 2;
HK = 3;

% Feed condition
[F,xf,Tf,n] = Feed;

% Distillate condition
[D,xD,P0,T0] = Distillate;

% Bottom stream product condition
B = F - D;
b = xf*F - xD*D;
xB = b/B;

%-------------------------------------------------------------------
% % Dewpoint/Bubblepoint calculations of product streams

% Pressure estimation
[PD,PB,Pf] = ColumnP(P0,xD,xB,T0);

% K-value estimation
[Kf,Kt,Kb] = K_Value(Pf,xf,Tf,T0,P0,y,PB,xB);

%-------------------------------------------------------------------
% % Feasible product distribution
% Fenske equation
d = xD*D;
[Nmin,xD,D,xB,B] = Fenske(Kt,LK,HK,xf,F,d,b);

%-------------------------------------------------------------------
% % Solution model

% Top column
[y,x,K,T,P,V,L,L0,Qc,HV,HL,HL0,n,Nf] = ...
      topcolumn(xD,D,R,T0,P0,F,xf,Tf,Pf,LK,HK);

% Bottom column
HLD = HL0;
Qreb = (D*HLD + B*HLB - F*HLf)/3600 + Qc;
```

```
xfeedT = x(Nf,LK);
[y_B,x_B,T_B,KB,VB,LB,HV_B,HL_B,P_B,NfB] = ...
      bottomcolumn(xB,B,R,TB0,PB0,Qreb,F,xf,Tf0,Pf0,LK,HK,xfeedT);

% Correction to meet at feed stage for top and bottom sections
[y,x,K,T,P,V,L,L0,Qc,HV,HL,HL0,n,...
      y_B,x_B,T_B,KB,VB,LB,HV_B,HL_B,P_B] = ...
      topcolumn(xD,D,R,T0,P0,F,Nf,q, xB,B,R,F,TB0,PB0,Qreb,NfB);

% Total number of stages (excluded reboiler & condenser)
NT = Nf + (NfB-1) - 1;

%-------------------------------------------------------------------
end
```

B.2 Equipment design of simple column (Chapter 5)

```
function [Acol,Vcol,Acond,Areb,P,Qc,Qreb] = Size_SC (R)
% % Equipment design model of SC (Chapter 5)

% % Input data from process design
[x,y,T,P,NTop,NBot,T0,TB,Qc,Qreb,L,V,Stage,n] = ...
      Inputpara_SC(R);

%-------------------------------------------------------------------
% % Physical properties for selected trays with minimum and maximum
throughputs
[sigmaLm_max,rho_vmix_max,rho_lmix_max,Vmass_max,Lmass_max,Qvmax,...
      Qlmax,Cs_ANmax,sigmaLm_min,rho_vmix_min,rho_lmix_min,...
      Vmass_min,Lmass_min,Qvmin,Qlmin] = propsSC(Stage,n,T,P,x,y,...
      L,V);

%-------------------------------------------------------------------
% Column design
% Column diameter (DT) & height (HT) in m
% Column area (Acol) in m2 & Column volume (Vcol) in m3

% Estimation and selection of largest column diameter
DT = ColumnDiameter(sigmaLm_max,rho_vmix_max,rho_lmix_max,...
      Vmass_max,Lmass_max,Qvmax,Qlmax)

% Solution for top and bottom sections of column
[DT,ST,SB] = hydraulicTest(Qlmax,Qvmax,Qlmin,Qvmin,...
      rho_vmix_min, rho_lmix_min,sigmaLm_min,sigmaLm_max,...
      rho_vmix_max,rho_lmix_max,Cs_ANmax,Vmass_max,Lmass_max);

% Column Area & Volume
[HT,Acol,Vcol] = ColumnSize_SC(Stage,T,P,DT);

%-------------------------------------------------------------------
% Condenser design
% Total area (Acond) in m2
T1 = T(1,2)+273.15;
Acond = CondenserSize(T0,T1,Qc);

%-------------------------------------------------------------------
```

```
% Reboiler design
% Total area (Areb) in m2
TNT = T(end,2)+273.15;
Areb = ReboilerSize(TNT,TB,Qreb);

%---------------------------------------------------------------------
end
```

B.3 Process design of DWC (Chapter 6)

```
% % Process design model of DWC (Chapter 6)
% Initialized parameters
R2all = 4;
SL = 0.315;

%---------------------------------------------------------------------
% % Input parameters/Initial Estimation
% Temperature in deg K
% Pressure in bar
% Flowrate in kmol/hr
% Condenser/Reboiler Duty in MW

% Identify Light key (LK), middle key (MK) & heavy key (HK)
components
LK = 2;
MK1 = 3;
MK2 = 4;
HK = 5;

% Feed condition
[F,xf,Tf,n] = Feed;

% Distillate condition
[D,xD,P0,T0] = Distillate;

% Bottom product condition
[B,xB] = Bottom_Product;

% Side stream product condition
S = F - D - B;
s = xf*F - xD*D - xB*B;
xS = s/S;

% Prefractionator
[xD1,D1,d1,xB1,B1,b1] = Prefractionator;

%---------------------------------------------------------------------
% % Dewpoint/Bubblepoint calculations of product streams

% Pressure estimation
[PD,PB,Pf,PD1,PB1,~] = ColumnP(P0,xD,xB,T0);

% K-value estimation
[Kf,Kt1,Kb1,Kt,KtS,Kb] = K_Value(Pf,xf,Tf,T0,PD1,yD1,PB1,xB1,P0,...
      y,PB,xB,xS);

%---------------------------------------------------------------------
```

```
% % Feasible product distribution
% Fenske equation
[Nmin1,yD1,D1,xB1,B1] = Fenske(Kt1,Kf,Kb1,LK,HK,xf,F,d1,b1);
s1 = yD1*D1 - d;
s2 = xB1*B1 - b;
[Nmin2,xD,D,xS1,S1] = Fenske(Kt,Kt1,KtS,LK,MK1,yD1,D1,d,s1);
[Nmin3,xS2,S2,xB,B] = Fenske(KtS,Kb1,Kb,MK2,HK,xB1,B1,s2,b);

%--------------------------------------------------------------------
% % Solution models

% Sections 2 and 3_1
[R2,xD,D,y,x,K,T,P,V,L,L0,Qc,HV,HL,HL0,Nf,n,y_S1,x_S1,T_S1,KS1,...
      VS1,LS1,HV_S1,HL_S1,P_S1,Qreb2,NfS1] = ...
      DWC_CMOcol2(xD,D,T0,P0,D1,yD1,LK,MK1,HK,xS1,S1,TS1,Pf,TD1,...
      PD1,MK2,R2all,SL);

% Sections 3_2 and 4
[HLf,HLS,HLB] = Enthalpy(Pf,Tf,xf,n,xS,xB,PB,T0);

[R3,xS2,S2,y_S2,x_S2,K_S2,T_S2,P_S2,VS2,LS2,L0_S2,Qc3,HV_S2,...
      HL_S2,HL0_S2,NfS2,n,y_B,x_B,T_B,KB,VB,LB,HV_B,HL_B,P_B,...
      NfB,Qreb3] = ...
      DWC_CMOcol3(xS2,S2,TS2,B1,xB1,TB1,PB1,EmL,MK2,HK,xB,B,R2all,TB
      ,PB,F,D,Nf,NfS1,P,VS1,HL0,S,HLS,HLf,HLB,Qc,MK1,S1,HL_S1);

% Section 1
x0 = x(Nf,:);
y1 = y(Nf+1,:);
L1_1 = L(Nf) - LS1(NfS1+1);
V1_1 = V(Nf+1) - VS1(NfS1);
R1 = L1_1/(V1_1 - L1_1);

[y1_1,x1_1,K1_1,T1_1,P1_1,V_1_1,L_1_1,HL01_1,Nf1_1,n,y1_2,x1_2,...
      T1_2,K1_2,V_1_2,L_1_2,Nf1_2,P1_2] = ...
      DWC_CMOsec1_1(y1,V1_1,x0,L1_1,T(Nf),P(Nf),F,xf,Tf0,Pf,EmL,...
      LK,HK, xB1,L1_2,yB0,V1_2,T_B(NfB),P_B(NfB),xfeedT);

%--------------------------------------------------------------------
end
```

B.4 Process design of DWC (Chapter 7)

```
% % Process design model of DWC (Chapter 7)

% % Initialized parameters and input parameters
% Temperature in deg C
% Pressure in bar
% Flowrate in kmol/hr
% Condenser/Reboiler Duty in MW

% Identify Light key (LK), middle key (MK) & heavy key (HK)
components
LK = 1;
MK = 2;
HK = 3;
```

```
[rf,rs,ar,br,R,F,D,S,B,P,Kef,zf,Kes,ws,Tbpf,Tbps,Xsc] = startvalues;
n = length(zf);

%---------------------------------------------------------------------
% % Internal flows and intersection points estimation
[ybf1,ybs1,xf1,xs1,ynu,xbnf,xd1,yb1,xD,yB,Kef,Kes,Tbpf,Tbps,...
    Lflow,Vflow,yf0,xf0,xs0,ys0,P,F,D,S,B,Xsc] = ...
    precalcDWC(ar,br,R,F,D,S,B,P,Kef,zf,Kes,ws,Tbpf,Tbps,Xsc);

%---------------------------------------------------------------------
% % Solution models

% Dividing wall section (Region 1 and 2)
[xf,xs,yf,ys,Tf,Ts,xbf,xbs,ybf,ybs,Tbf,Tbs,NfT,NsT,Nf,Ns] = ...
      dividingwall(Lflow,Vflow,P,xf0,yf0,xf1,ybf1,xs0,ys0,xs1,ybs1);

% Region 3 and condenser stage
% Flow rates and top interlinking tray compositions
LT = Lflow(1) + Lflow(3);
VT = Vflow(1) + Vflow(3);
xd1 = (Lflow(1)*xf(1,:) + Lflow(3)*xs(1,:)) / LT;
yd0 = (Vflow(1)*yf(1,:) + Vflow(3)*ys(1,:)) / VT;
[~,Td0, ~] = dewpoint(yd0,P);
[xd,yd,Td,NT,xD,TD,Qc] = Region3(LT,VT,P,xd1,yd0,Xsc(1,1:n));

% Region 4 and reboiler stage
LB = Lflow(2) + Lflow(4);
VB = Vflow(2) + Vflow(4);
xb0 = (Lflow(2)*xbf(NfB,:) + Lflow(4)*xbs(NsB,:)) / LB;
yb1 = (Vflow(2)*ybf(NfB+1,:) + Vflow(4)*ybs(NsB+1,:)) / VB;
[Tb0, ~] = bubblepoint(xb0,P);
[xb,yb,Tb,NB,xB,TB,Qr] = Region4(LB,VB,P,xb0,yb1,Xsc(3,1:n));

%---------------------------------------------------------------------
end
```

B.5 Equipment design of DWC (Chapter 8)

```
function [Acol,Vcol,Acond,Areb,P,Qc,Qreb] = Size_DWC (R,SL)
% % Equipment design model of DWC (Chapter 7)

% % Input data from process design
[x,y,T,P,NTpre,NTside,NTop,NBot,T0,TB,Qc,Qreb,L,V,Stage,n] = ...
      inputpara_DWC(R,SL);

%---------------------------------------------------------------------
% % Physical properties for selected trays with minimum and maximum
throughputs
[sigmaLm_max,rho_vmix_max,rho_lmix_max,Vmass_max,Lmass_max,Qvmax,...
      Qlmax,Cs_ANmax,sigmaLm_min,rho_vmix_min,rho_lmix_min,...
      Vmass_min,Lmass_min,Qvmin,Qlmin] = propsDWC(Stage,n,T,P,x,y,...
      L,V);

%---------------------------------------------------------------------
% Column design
% Column diameter (DT) & height (HT) in m
% Column area (Acol) in m2 & Column volume (Vcol) in m3
```

```
% Estimation and selection of largest column diameter
DT = ColumnDiameter(sigmaLm_max,rho_vmix_max,rho_lmix_max,...
      Vmass_max,Lmass_max,Qvmax,Qlmax)

% Solution for Sections 2 and 4
[DT,ST,SB] = hydraulicTest(Qlmax(3),Qlmax(6),Qvmax(3),...
      Qvmax(6),Qlmin(3),Qlmin(6),Qvmin(3),Qvmin(6),...
      rho_vmix_min(3),rho_vmix_min(6),rho_lmix_min(3),...
      rho_lmix_min(6),sigmaLm_min(3),sigmaLm_min(6),...
      sigmaLm_max(3),sigmaLm_max(6),rho_vmix_max(3),...
      rho_vmix_max(6),rho_lmix_max(3),rho_lmix_max(6),...
      Cs_ANmax(3),Cs_ANmax(6),Vmass_max(3),Vmass_max(6),...
      Lmass_max(3),Lmass_max(6));

% Solution for Sections 1 and 3
[DTdw,h,AT1,AT3,Sdw] = hydraulicTestdw(Qlmax,Qvmax,Qlmin,Qvmin,...
      rho_vmix_min, rho_lmix_min,sigmaLm_min,sigmaLm_max,...
      rho_vmix_max,rho_lmix_max,Cs_ANmax,Vmass_max,Lmass_max);

% Column Area & Volume
[HT,Acol,Vcol] = ColumnSize_DWC(Stage,T,P,DT);

%-------------------------------------------------------------------
% Condenser design
% Total area (Acond) in m2
T1 = T(1,2)+273.15;
Acond = CondenserSize(T0,T1,Qc);

%-------------------------------------------------------------------
% Reboiler design
% Total area (Areb) in m2
TNT = T(end,2)+273.15;
Areb = ReboilerSize(TNT,TB,Qreb);

%-------------------------------------------------------------------
end
```

B.6 Costing of DWC (Chapter 9)

```
function [TAC,OP,CAP] = totalcost_DWC(R,SL)

% Annualised capital cost ($/y)
ir = 0.15; % Fractional interest rate
nyr = 10; % Number of years
[Acol,Vcol,Acond,Areb,P,Qc,Qreb] = Size_DWC (R,SL);
BMC = BareModuleCost_DWC(R,SL, Acol,Vcol,Acond,Areb,P,Qc,Qreb);
CAP = BMC*(ir*(1+ir)^nyr)/((1+ir)^nyr - 1);

% Operating Cost ($/y)
OP = operatingcost(Qc,Qreb);

% Total Annualised Cost ($/y)
TAC = OP + CAP;

end
```