DESIGN OF MULTICOMPONENT HEAT INTEGRATED DISTILLATION SYSTEMS

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A project report submitted in partial fulfilment of the requirements for the award of the degree of Bachelor of Engineering (Hons.) of Chemical Engineering

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DECLARATION

I hereby declare that this project report is based on my original work except for citations and quotations which have been duly acknowledged. I also declare that it has not been previously and concurrently submitted for any other degree or award at UTAR or other institutions.

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APPROVAL FOR SUBMISSION

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ABSTRACT

Conventional distillation is energy intensive and remains important to the industry. A more efficient column is necessary to reduce this high energy consumption. One of the most prospective alternative is the internally heat integrated distillation column (i-HIDiC). The design of the internally heat integrated distillation column for an alcohol mixture feed (ethanol, isopropanol, *n*-propanol, isobutanol and *n*-butanol) was performed using the commercial software Aspen Plus together with ChemSep. ChemSep was used to perform the Fenske-Gilliland-Underwood-Kirkbride calculations to obtain the necessary parameters such as number of stages, feed location and reflux ratio for Aspen Plus. The reboiler and condenser duties, operation, capital and total annualized costs of the i-HIDiC were compared with the conventional column. In order to have better long term savings, the lowest operation costs was used to determine the optimal compressor pressure. The optimal compressor pressure obtained was 200, 160, 150 and 150 kPa for column C1, C2, C3 and C4 respectively. Results of the simulation showed that the reboiler and condenser duties for the distillation train reduced by 78.54 % and 74.04 % respectively when the i-HIDiC was used, with column C1 contributing the least and columns C2 and C4 contributing the most reductions. The operation, capital and total annualized costs were reduced by 50.01 %, 49.73 % and 49.77 % respectively when the i-HIDiC was used for the distillation train. Column C1 did not contribute to any costs reduction but resulted in an increase in overall costs. The largest contributors for the reduction in costs were columns C2 and C4.

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LIST OF SYMBOLS / ABBREVIATIONS

A	heat transfer area, m²
A_{cond}	condenser heat transfer area, m²
A_{HP}	heat panel area, m²
A_{HP}	total heat panel area, m²
A_{reb}	reboiler heat transfer area, m²
b	bottom flow rate, kmol/hr
C	cost, $
$C_{capital}$	Capital cost, $
C_{compr}	compressor cost, $
C_{HE}	heat exchanger cost, $
$C_{operation}$	Operation costs, $/yr
C_p	specific heat capacity of water, kJ/kg·°C
C_{TAC}	Total annualized cost, $/yr
d	distillate flow rate, kmol/h
D	largest diameter of distillation column, m
d_{rec}	diameter of rectifying section, m
d_{str}	diameter of stripping section, m
H	height of distillation column, m
i	light key
j	heavy key
L	latent heat of vaporisation, kJ/kg
$\dot{m}$	mass flow, kg/h
N	number of trays
N_{HP}	number of heat panels
N_{min}	minimum number of stages
Q_{cond}	condenser duty, kJ/h
Q_{reb}	reboiler duty, kJ/h

Q_{stage}	heat transfer rate per stage, kJ/h
SA_{HP}	sum of all heat panel areas, m²
TA_{HP}	total area of heat panels, m²
T_R	temperature at the rectifying stage, °C or K
T_S	temperature at the stripping stage, °C or K
U	overall heat transfer coefficient (~1 kW/m²·°C)
U_{cond}	condenser overall heat transfer coefficient, kW/m²·°C
U_{reb}	reboiler overall heat transfer coefficient, kW/m²·°C
V	vapour flow rate, kmol/s
α	relative volatility
γ	payback period, yr
ΔT_{stage}	temperature difference between the rectifying and stripping stage
ΔT_{min}	minimum temperature difference or pinch temperature
i-HIDiC	internally/ideal heat integrated distillation column
CO_2	carbon dioxide
DWC	divided wall column
NEDO	New-Energy and Industrial Technology Development Organization
FUG-K	Fenske-Gilliland-Underwood-Kirkbride method
TAC	total annualized cost

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CHAPTER 1

INTRODUCTION

1.1 Background

The distillation process is used to separate 95% of all fluid separations in the chemical industry and accounts for 3% of global energy consumption (Hernández, Segovia-Hernández & Rico-Ramírez, 2005). This large energy consumption will increase the operating cost as energy costs are rising due to the increase in crude oil prices. It is also a known fact that large energy consumption contributes to large amount of carbon dioxide (CO_2) emissions due to the burning of fossil fuels. In an industry, 70% of operation costs are due to energy expenses in which 19 % is from distillation (Schaller, 2007).

Distillation is the most important method used for separation. However, there is a major drawback that is the high energy consumption. In order to improve the energy efficiency, the concept of heat integration was introduced to the distillation process in 1970 (Mascia et. al., 2007). Heat integration is the heat transfer between the hot and cold streams without addition or removal of energy through external sources. Many researches on the heat integrated distillation column (HIDiC) have been performed during the past few decades to investigate its feasibility and practicality in real world applications (Huang, Shan, Zhu & Qian, 2007; Iwakabe et. al., 2006).

All of these researches has led to the creation of various improved distillation columns such as the Petlyuk column, divided-wall column, heat pump assisted column, diabatic distillation column, ideal HIDiC (i-HIDiC) and others (Jana, 2010). However, these columns are not without its drawbacks and they only exist as models and in simulations.

1.2 Problem Statement

Conventional distillation columns require large amounts of energy to perform the desired separations. Though there are various alternative column types that were proposed, the industry has yet to adopt the proposed technology. In a heat integrated distillation system, additional unit operations (i.e. flash column, compressor, heat transfer mediums) may be present. These additional units may incur higher operation and capital costs as well as additional maintenance. These factors may be the reasons why the industry has yet to adopt them.

Besides that, distillation systems become more complex as more components are present in the system. By applying heat integration to a multicomponent system, the complexity will increase even further. This complexity is evident as researchers face issues such as finding an optimal design, lack of accurate models that predict process characteristics precisely and the difficulty of column control (Jana, 2010). On top of that, multicomponent distillation will also produce different distillation sequences that affect the cooling and heating duties (Mascia, Ferrara, Vacca, Tola & Errico, 2007).

1.3 Objectives

The objectives of this project are listed as follows:

1. To design a multicomponent, heat integrated distillation train using the internally heat integrated distillation column.
2. To study the effect of compressor pressure on the internally heat integrated distillation column.
3. To study and compare the heating and cooling duties of the internally heat integrated column with the conventional design.
4. To study and compare the operation, capital and total annualized cost (TAC) of the internally heat integrated column with the conventional column.

1.4 Scope

The distillation columns are first designed based on the popular and established Fenske-Underwood-Gilliland-Kirkbride (FUG-K) method. Information from this pre-design will be used and simulated in the commercial software Aspen Plus. Column sizing will also be performed and feasibility of the column will be performed according to Gadalla (2009). Cost calculations will be based on the work by Chen, Huang and Wang (2010).

CHAPTER 2

LITERATURE REVIEW

2.1 Background

Humans have performed and developed separation techniques since early civilizations. These separations include extraction of metals from ores, perfumes from flowers, dyes and distil liquors (Kirk & Othmer, 1982). Today, separation techniques are not only used in the industry, but also in the laboratories. An example of an analytical separation method is chromatography. Industrial scale separation methods include distillation, absorption, stripping and extraction (Seader & Henley, 2006).

In the industry, distillation is the most important in fluid separations. 95 % of fluids are separated via this method (Hernández, Segovia-Hernández & Rico-Ramírez, 2005). Distillation is performed by using a distillation column. The distillation column produces coexisting zones that differ in temperature, pressure composition and/or phase state. The components that are to be separated will behave differently in different conditions in these zones. When equilibrium is achieved, different composition of the components will exist in these zones thus separation will be achieved between the components. In order to produce these zones, a distillation column usually contains trays or packings for fluids to come into contact (Doherty, Fidkowski, Malone & Taylor, 2008).

2.2 Conventional Distillation

In a conventional distillation column, fluid that is to be separated will be fed into the column. The liquid portion of the feed will cascade down each tray while the vapour will bubble through the trays. This flow scheme will allow the liquid and vapour to come into contact with each other and mass transfer will occur.

Liquid reaching the bottom of the column will enter the reboiler where it is partially vaporised to provide a boil-up, which is sent back to the column. The remaining liquid in the reboiler will be withdrawn as a bottoms. On the other hand, vapour that reaches the top of the column will be condensed in a condenser. Part of the condensed vapour will be returned to the column as a reflux while the remaining liquid will be withdrawn as a distillate.

The separability of the fluid depends mainly on the relative volatility between the components, number of trays and the ratio of flow rates of the liquid phase to the vapour phase. Lighter components (lower boiling point) will concentrate in the vapour phase while heavier components (higher boiling point) will concentrate in the liquid phase.

A distillation column is separated into two sections (Figure 2.1). The section below the feed is known as the stripping section whereas the section above the feed is known as the rectifying section. Multiple distillation columns may be combined together to form a distillation train to separate a multicomponent feed. In this conventional system, heat is supplied at the reboiler and removed at the condenser. This usually results in low energy efficiency especially when the removed heat is wasted. (Doherty, Fidkowski, Malone & Taylor, 2008)

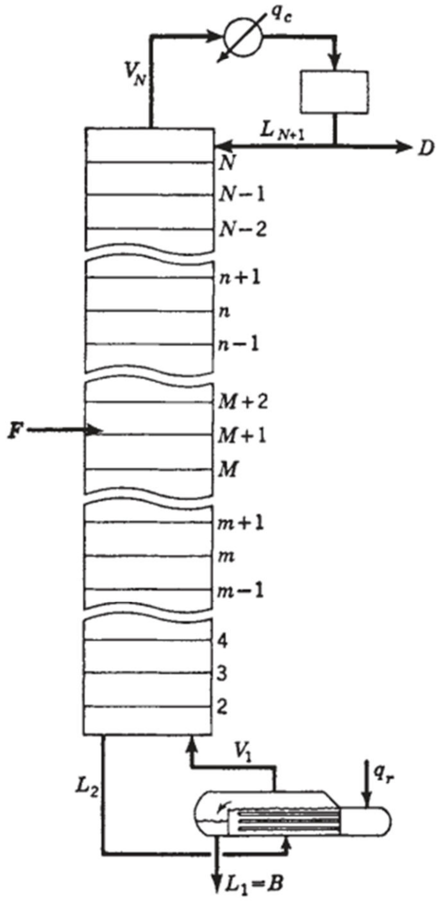

Figure 2.1: Schematic Diagram for a Simple Continuous Distillation Column with One Feed.

2.3 Heat Integrated Distillation Columns (HIDiC)

Due to the low energy efficiency and high energy consumption of conventional distillation columns, new columns have been developed that incorporates the heat integration concept to reduce energy input and increase energy efficiency. These columns are also known as thermally coupled columns. Various designs have been researched and proposed but very few have been adopted by the industry.

2.3.1 Petlyuk Column

The Petlyuk column is one of the thermally coupled columns that have been researched. It was proposed by Petlyuk and his team in 1965 and also known as a fully thermally coupled column. A variation to the Petlyuk column is the divided wall column (Tung, 2004). Both columns are thermodynamically equivalent despite the difference in configuration. Figure 2.2 shows the distillation scheme for both Petlyuk and divided wall column (DWC).

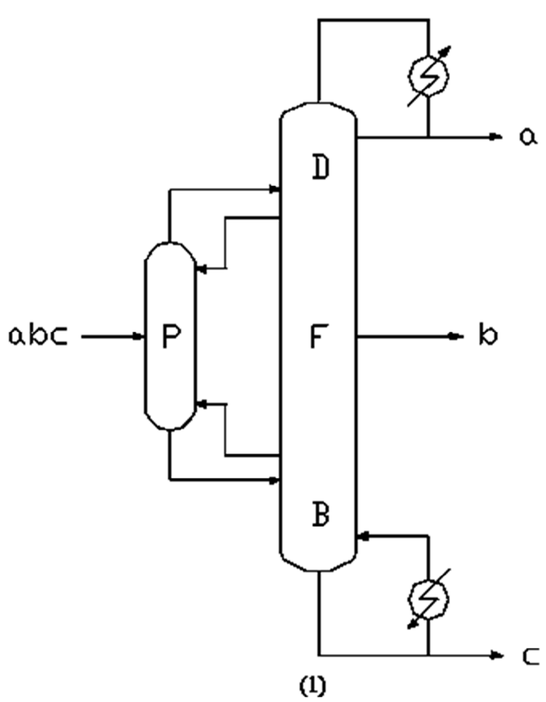

Figure 2.2: General Scheme of the Petlyuk (1) and the Divided Wall (2) Column. Notations: a, b, c – Components; P – Prefractionator; F – Fractionator; D – Distillate; B – Bottoms

These two schemes are normally used to separate ternary mixtures. The Petlyuk scheme uses an external prefractionator linked by two recycle streams from the main fractionation column. Various literatures have reported energy savings of the Petlyuk scheme of up to 30 – 50 % (Hernández & Jiménez, 1999; Halvorsen & Skogestad, 2003). The same effect of the use of an external prefractionator can be achieved by installing a wall into the main column. Energy savings for the divided wall column of up to 30 % is comparable to the Petlyuk scheme as reported by Kaibel and Schoenmarkers (2002). The high energy efficiency of both columns is achieved through efficient use of vapour and liquid to run the full course of the stages for vapour/liquid contact and the elimination of remixing in the main column. These two schemes requires the least amount of reboiler duty for a given operating pressure, number of stages, feed composition and product specification (Tung, 2004; Hernández, Pereira-Pech, Jiménez & Rico-Ramírez, 2003).

The main drawback of both schemes is the difficulty in control. For the Petlyuk column, the fully interconnected structure that results in vapour interconnections flowing back and forth between the columns poses a design challenge as neither column can be at a uniformly higher pressure than the other (Segovia-Hernández, Hernández & Jiménez, 2005). On the other hand, the divided wall column suffers from the lack of control of the split liquid and vapour flows. Controlling the liquid split using only hydrostatic head and controlling the amount of pressure drop to prevent downcomer backup is the main challenge faced by this column. Due to these difficulties, the operating and control range of this column is very limited (Tung, 2004). Despite these drawbacks, it has been reported that BASF has adopted and implemented the DWC in the production plants (Kaibel & Schoenmarkers, 2002; Calzon-McConville, Rosales-Zamora, Segovia-Hernández, Hernández & Rico-Ramírez, 2006). Other than BASF, it has also been reported that Linde AG has built the largest DWC for Sasol in South Africa (Parkinson, 2007).

2.3.2 Ideal and Internally Heat Integrated Distillation Column (i-HIDiC)

A more recent distillation column configuration that have received much attention is the ideal heat integrated distillation column and the internally heat integrated distillation column. This distillation column configuration has yet to be adopted by any industry but currently there are pilot plants that have been built in Japan and Netherlands using this column (Olujić, Jödecke, Shilkin, Schuch & Kaibel, 2009). In Japan, the research on the internally heat integrated distillation column is funded by the New-Energy and Industrial Technology Development Organization (NEDO).

Figure 2.3 shows the configurations for both ideal and internally heat integrated distillation columns. The only difference between both configurations is that the ideal HIDiC does not have any reboiler and condenser while the internally HIDiC still contains a reboiler and a condenser. As the name suggest, the ideal HIDiC may not be achievable in real world applications and the presence of the reboiler and condenser may still be necessary for the start-up of the column.

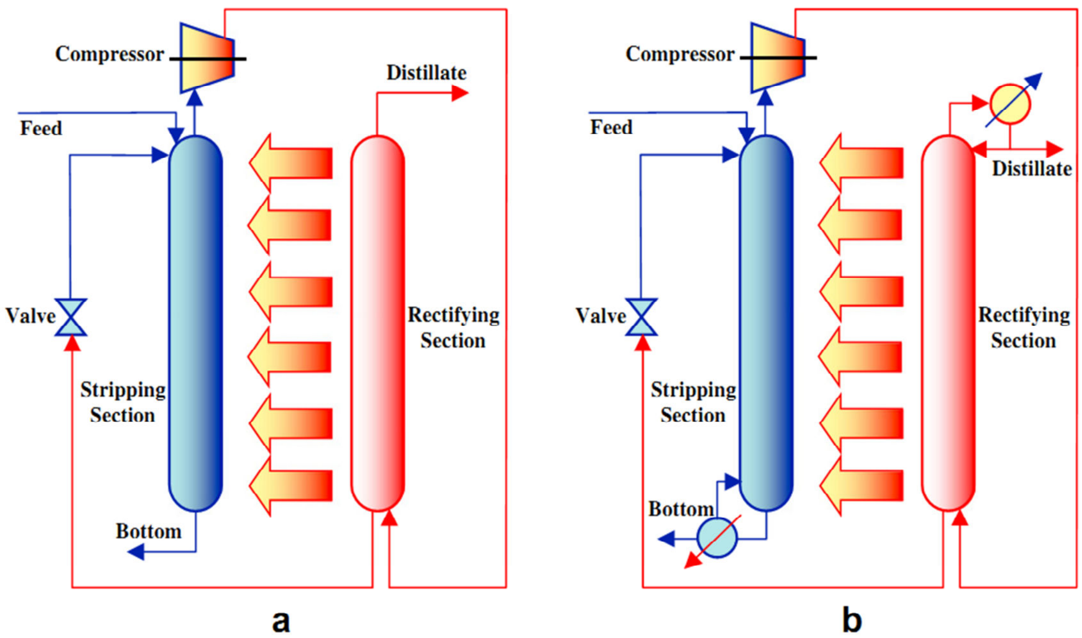

Figure 2.3: Ideal HIDiC (a) and the Internally HIDiC (b)

The operation of both columns is similar. Both configurations contain a stripping section, a rectifying section, a compressor and a throttling valve. Feed is usually fed at the top of the stripping section. Vapour from the stripping section is compressed to raise the pressure hence the temperature and fed into the rectifying section. Pressure of the liquid from the bottom of the rectifying section is reduced by the throttling valve and recycled to the stripping section. If the pressure of the rectifying section is sufficiently higher than the stripping section, the temperature of the rectifying section will also be higher than of the stripping section. Thus, heat transfer will occur. This heat transfer will result in lower or even zero reboiler and condenser duties which results in significant energy savings (Iwakabe et. al., 2006; Gadalla, 2009).

To facilitate heat transfer between the stripping and rectifying sections, various methods have been proposed. There is the plate-fin device, plate-fin heat exchanger, vertical shell and tube heat exchanger, sieve tray, heat transfer panels/elements, multitube, split, two concentric cylinders, multi concentric cylinders and three internal heat exchangers. Table 2.1 summarises the proposed heat transfer methods.

Table 2.1: Summary of Proposed Heat Transfer Methods for Ideal and Internally Heat Integrated Distillation Column

Heat Transfer Method	Reference
Plate-fin device	Tung, Davis & Mah, 1986
Plate-fin heat exchanger	Hugill, 2005
Vertical shell and tube heat exchanger	Naito et. al., 2000
Sieve tray	Kaeser & Pritchard, 2005
Heat transfer panels/elements	Schmal, Van Der Kooi, Rijke, Olujić & Jansens, 2006
Multitube	Gadalla, Jiménez, Olujić & Jansens, 2007
Split configuration	Gadalla, Jiménez, Olujić & Jansens, 2007
Two concentric cylinders	Gadalla, Jiménez, Olujić & Jansens, 2007
Multi concentric cylinders	Gadalla, Jiménez, Olujić & Jansens, 2007
Three internal heat exchangers	Huang, Chen & Wang, 2010

Energy savings for the ideal and internally HIDiC have been reported in various literatures of up to 60 % compared to the conventional distillation column (Chen, Huang & Wang, 2010; Naito et. al, 2000; Iwakabe et. al., 2006). This energy savings is comparable if not better than the energy savings reported by the Petlyuk and the divided wall column scheme. Despite having a compressor in the configuration, the amount of energy required or consumed by the compressor is significantly smaller compared to the amount of energy savings from the low reboiler and condenser duties as reported by Huang, Chen and Wang (2010). The control of the ideal HIDiC does not present a very large problem as it has been reported that the control performance is comparable to conventional distillation columns (Huang, Shan, Zhu & Qian, 2007).

However, there are various drawbacks and reasons on the lack of adoption from the industry. Firstly, most of the research that have been done regarding to the ideal and internally HIDiC have been focused on binary mixtures. Theoretical and simulated results that have been verified are also only for binary mixtures in a pilot plant (Iwakabe et. al., 2005). For a multicomponent system, results have only been reported for simulations. The literatures had reported energy savings for a multicomponent system is of 30 – 50 % (Iwakabe et. al., 2005; Kim, 2011). Secondly, most of the research that have been performed lacked the necessary design aspects as they are mostly focused on simulation, experimental studies, operational studies and operational aspects. Any design suggestions, modelling or simulation aspects and design procedures are not included in the works (Gadalla, 2009).

Thirdly, there were no general approaches or methods to deal with new design problems and application of i-HIDiCs at the process design level, simulation and design aspects. Fourthly, design feasibility and hydraulic capacity viable for heat exchange were not defined. (Gadalla, 2009). Thermodynamic feasibility is the availability of quality heat for heat transfer to occur. To determine this, temperature profiles are required for both sections of the column. Three types of temperature profiles can be obtained; parallel, variable and decreasing or increasing. Figure 2.4 shows an example of a temperature profile. The temperature difference (ΔT) in Figure 2.4 is at a minimum value and is known as the minimum temperature difference for the i-HIDiC (ΔT_{min}). This value has an effect on the energy cost which can be optimised by adjusting the pressure increase. A large ΔT_{min} value indicates less heat will be exchanged thus a large reboiler and condenser duty and vice versa. From Figure 2.4 also, we can partly determine the limiting stages for heat transfer. A hydraulic design is required to fully determine the limiting stages. On the other hand, the hydraulic design feasibility is to determine whether there is adequate space available for the installation of the heat transfer medium (i.e. heat panels).

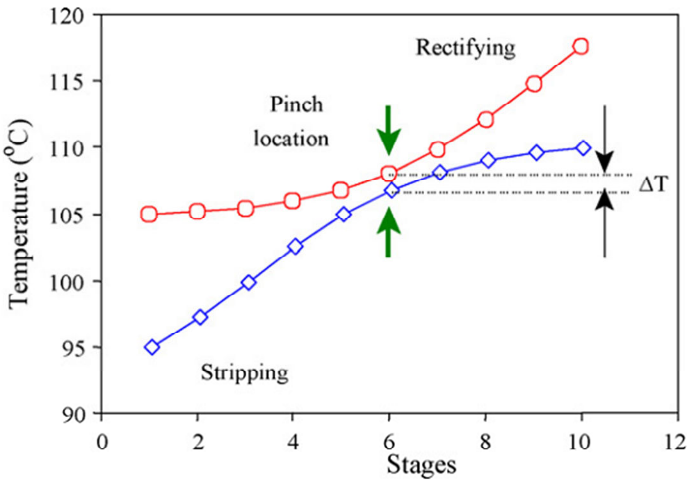

Figure 2.4: Temperature Profile Plot

Lastly, the inclusion of a compressor, which is difficult to operate and maintain, was said to be preventing the adoption of the i-HIDiCs in the industry (Kim, 2011). To address the presence of the compressor, Kim (2011) proposed a scheme that removed all compressors. Figure 2.4 shows the proposed scheme. This scheme basically heat integrates the rectifying section of the second column with the stripping section of the first and the stripping section of the second with the rectifying of the third.

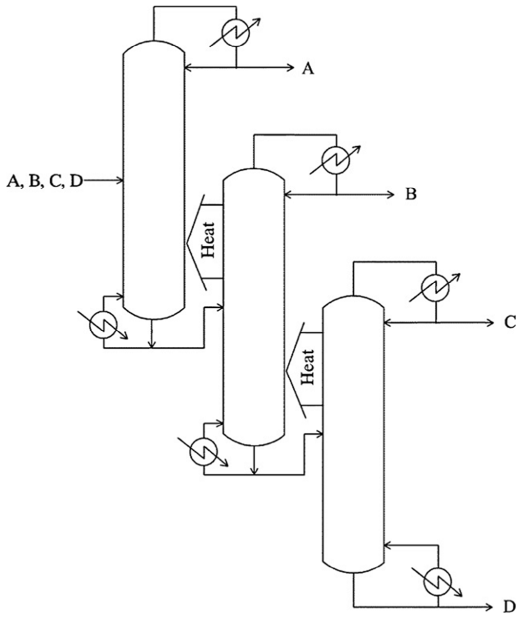

Figure 2.5: The Proposed i-HIDiC Scheme by Kim (2011)

Despite the drawbacks that may be present, the ideal and internally HIDiC has a great potential to replace current distillation columns due to the significant energy that may be saved. Further research needs to be performed on its feasibility and practicality to encourage adoption by the industry.

2.3.3 Multi-effect Column

The multi-effect column is also known as the pressure-staged column. In this distillation scheme, column pressures are adjusted such that the cooling of one column can be used a heating in another column (Engelien & Skogestad, 2005). In other words, the overhead vapour from one column is used as a heat source in the reboiler of the next column. Figure 2.5 shows one of schemes that have been proposed. Multi-effect columns may be heat integrated in the direction of mass flow (forward integration) or in the opposite direction (backward integration) (Jana, 2010).

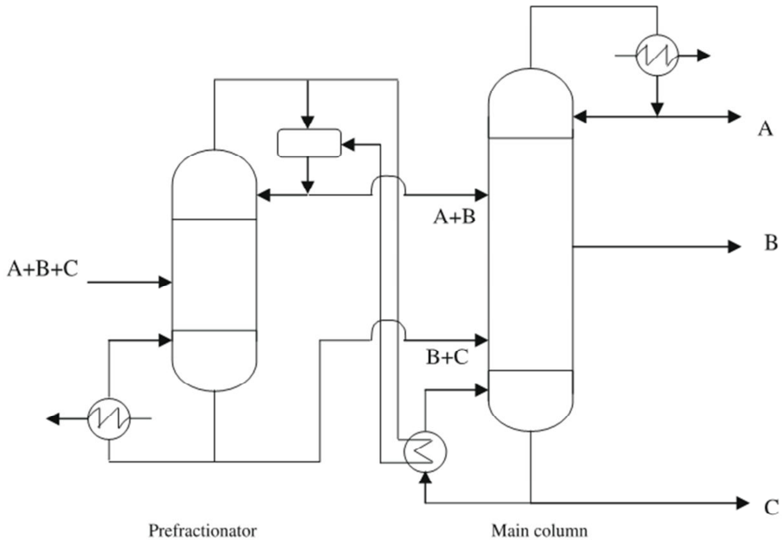

Figure 2.6: Schematic Representation of a Multi-effect Column for Ternary Separation

The advantage of this scheme other than energy savings is in the revamp of existing plants. This scheme allows for the reduction of heat consumption without major replacement of columns (Halvorsen & Skogestad, 2011). Energy savings have been reported to be much better than conventional distillation column (up to 55 %) as well as the Petlyuk scheme (up to 25 %) (Engelien & Skogestad, 2005). The disadvantage of this scheme which is also the main reason of lack of adoption and interest is control of the column. Han and Park (1996) have reported that controlling the system in this scheme is very difficult as the system is nonlinear, multivariable and interacting. Until a solution is found to overcome the control issue, it is highly unlikely to be adopted. Besides that, more work has to be done in regards to optimal design and economics in addition to controllability of the column (Jana, 2010).

2.3.4 Diabatic Column

The diabatic distillation column is a column where a heat exchanger is present in each tray. Figure 2.6 shows a representation of this scheme. Instead of having all the heat being supplied at the reboiler, the heat is redistributed through the heat exchangers that are integrated with each tray. Most researches focuses on the reduction of entropy of this system (Røsjorde & Kjelstrup, 2005; Koeijer, Røsjorde & Kjelstrup, 2004) as the addition of heat exchangers to the system will increase the entropy. According to an experiment by Rivero (1993), the entropy production rate of the diabatic column is significantly lower than conventional columns.

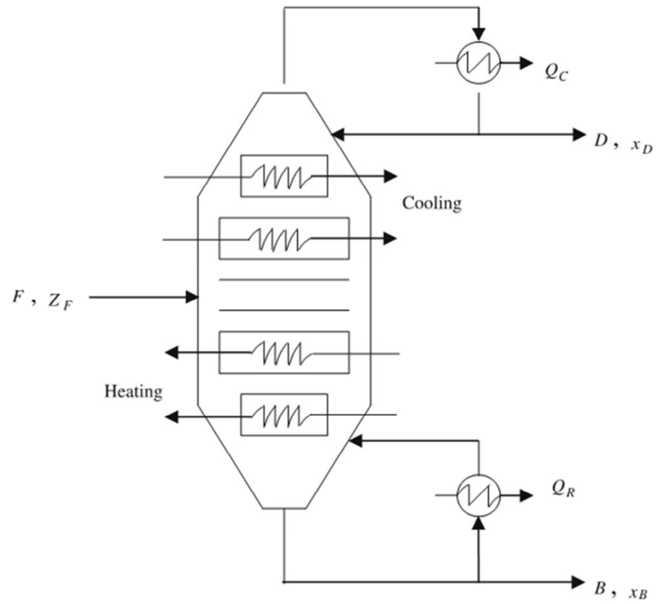

Figure 2.7: Schematic Representation of a Diabatic Distillation Column

Despite its potential to perform much more efficiently compared to conventional columns, this column remains theoretical. So far, the only extensive study on a pilot plant has only been done by Rivero (1993). Besides that, although capital cost may decrease due to the smaller reboiler and a condenser, the addition of heat exchangers and more trays will increase the cost. More work needs to be done in terms of determining optimal temperature and heating profiles at minimum entropy production before being adopted widely (Jana, 2010).

CHAPTER 3

METHODOLOGY

To design the distillation train, each column needs to be designed individually using various correlations that have been developed and then combine the columns together. This design step applies to both conventional and heat integrated columns. However, to design the ideal or internally HIDiC, data such as number of stages, reflux ratio must be obtained from the conventional design.

3.1 Conventional Distillation Column Design

The feed used is an alcohol mixture consisting of ethanol, isopropanol, n-propanol, n-butanol and isobutanol with compositions of 0.25, 0.15, 0.35, 0.15 and 0.1 respectively (King, 1971; Andrecovich & Westerberg, 1985; Yuan & An, 2002; Hasebe, 2009). Initial calculations of column parameters were determined using the Fenske-Underwood-Gilliland-Kirkbride (FUG-K) method. A 98 % recovery for top and bottom products was used to obtain the necessary column parameters from the FUG-K correlations. To perform the calculations for FUG-K, the free software, ChemSep V6.84 Lite, was used to obtain the feed location, reflux ratio and number of stages.

3.2 Simulation of Conventional Column

All simulations were carried out using the commercial software Aspen Plus V7.2 from AspenTech. Before proceeding to the HIDiC design, initial simulations were first carried out on a conventional distillation column using the design parameters obtained from ChemSep.

The optimal distillation sequence was based on the work by Hasebe (2009) and the saturated liquid feed flow rate was based on a basis of 100 kmol/h at 393 K. The fluid package, UNIQUAC, was selected based on the recommendations from Aspen Plus for alcohol feed. According to Meier, Leistner and Kobus (2006), the pressure drop per tray is 3 to 6 mbar. Therefore a pressure drop of 5 mbar was selected to ease in column pressure drop calculations. Once a convergence is obtained, the result from the simulations will be saved and recorded for use in the HIDiC design.

3.3 i-HIDiC Design and Simulation

The i-HIDiC design was based on the design methodology proposed by Gadalla (2009). Column parameters and data computed from the conventional design were reused for the i-HIDiC design. The conventional column was split at the feed location into two separate columns. The relative feed location remains unchanged as it is fed at the top stage of the stripping section. The number of stages or trays remains unchanged with the corresponding stripping and rectifying sections of the conventional column.

According to Gadalla (2009), the pressure for the rectifying section is assumed to be as high as the pressure at the bottom of the conventional column while the pressure of the stripping section is assumed to be equal to the pressure at the top of the conventional column. From this pressure difference, a pressure or compression ratio can be obtained that will provide the necessary driving force for heat transfer. For simplicity of this study, the pressures for both stripping and rectifying sections remain unchanged and a pressure increase was selected for the compressor so that the rectifying section has a higher temperature than the stripping section. The pressure increase specified or selected at the lowest or optimal operational costs.

The split column was simulated without any energy transfer between the stages to ensure that it converges. It should be expected that the reboiler and condenser duties obtained will be similar to those in a conventional column (maximum). To complete the simulation for the i-HIDiC, energy streams were added from the rectifying section to a corresponding stage in the stripping section.

At this point, there are two methods to determine how the energy should be transferred. The first method is to have a constant heat transfer area per stage and the second is a constant heat transfer rate per stage. Both parameters (heat transfer area or heat transfer rate) can be determined using Equation 3.1.

$$A = \frac{Q_{stage}}{U\Delta T_{stage}} \tag{3.1}$$

$$T_{stage} = T_R - T_S \tag{3.2}$$

Where,
A = heat transfer area, m²
Q_{stage} = heat transfer rate per stage, kJ/h
U = overall heat transfer coefficient (~1 kW/m²·°C)
ΔT_{stage} = temperature difference between the rectifying and stripping stage
T_R = temperature at the rectifying stage, °C or K
T_S = temperature at the stripping stage, °C or K

From Equation 3.1, the only parameters that could be manipulated were the heat transfer area and heat transfer rate per stage. The heat transfer area was limited by column hydraulics (refer Section 3.1.4) while the heat transfer rate depended on the amount of heat transfer area available. In this work, the heat transfer area will be determined in the feasibility study (Section 3.1.4) followed by the heat transfer rate.

The output of the simulation was saved or recorded. Important parameters such as reboiler and condenser duties were then compared to the duties obtained from the conventional column.

3.4 Design Feasibility

According to Gadalla (2009), most works do not include the thermodynamic and hydraulic designs to verify the feasibility of the i-HIDiC. Therefore, in this project feasibility study was performed based on Gadalla's (2009) work.

The temperature profile data were obtained from the simulation results (from Aspen Plus) of the i-HIDiC before performing any heat transfer. The temperature profile data were then plotted according to the stages with varying compressor pressures.

The hydraulic design feasibility is to determine whether there is adequate space available for the installation of the heat transfer medium (i.e. heat panels). By using a concentric layout (two cylinders) together with heat panels, necessary calculations to determine the amount of area available was performed according to the work by Gadalla, Jiménez, Olujić, & Jansens (2007).

$$\sigma = \frac{d_{str} - d_{rec}}{2} \tag{3.3}$$

$$\delta = \frac{0.10\pi d_{str}^2}{2(d_{str} - d_{rec})} \tag{3.4}$$

$$L = \sigma - \varepsilon \tag{3.5}$$

$$L1 = \pi d_{rec} - \delta \tag{3.6}$$

$$L2 = \pi d_{str} - \delta \tag{3.7}$$

$$A_{HP} = 0.30L \tag{3.8}$$

$$N_{HP} = \frac{L1}{0.03} \tag{3.9}$$

$$TA_{HP} = N_{HP}A_{HP} \tag{3.10}$$

Where,

d_{str} = diameter of stripping section, m

d_{rec} = diameter of rectifying section, m

A_{HP} = heat panel area, m²

N_{HP} = number of heat panels

TA_{HP} = total area of heat panels

*Refer Figure 3.2 for other notations

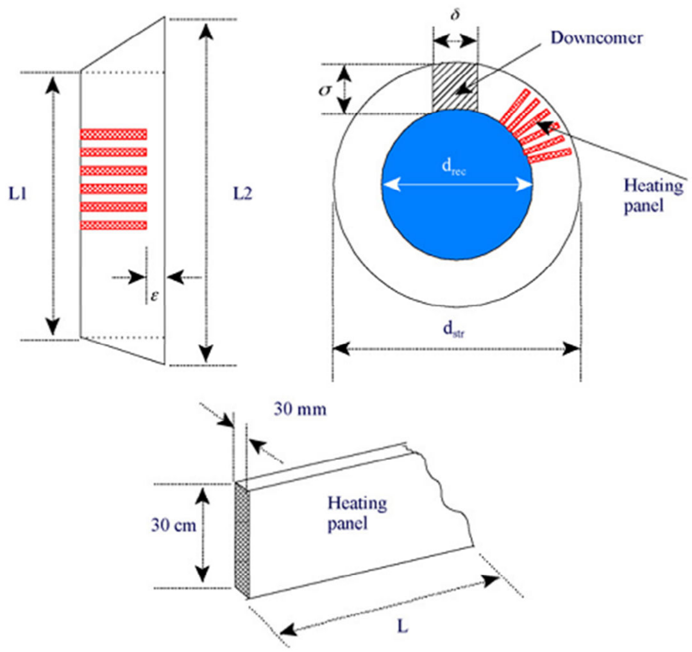

Figure 3.1: Geometric Analysis of Concentric i-HIDiC Configuration

To fully use the physical areas available for heat transfer, additional calculations are needed.

$$N'_{HP} = \frac{L2 - L1}{2(0.03)} \tag{3.11}$$

$$TA'_{HP} = N'_{HP} A'_{HP} \tag{3.12}$$

$$SA_{HP} = 2(TA_{HP} + TA'_{HP}) \tag{3.13}$$

Where,

SA_{HP} = sum of all heat panel areas, m²

*Refer Figure 3.3 for layout of additional panels.

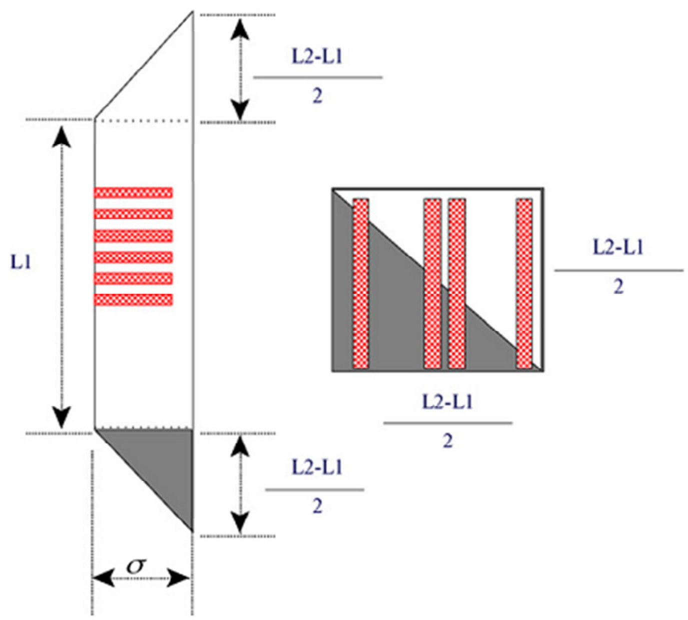

Figure 3.2: Layout of Extra Heat Panels in a Concentric i-HIDiC

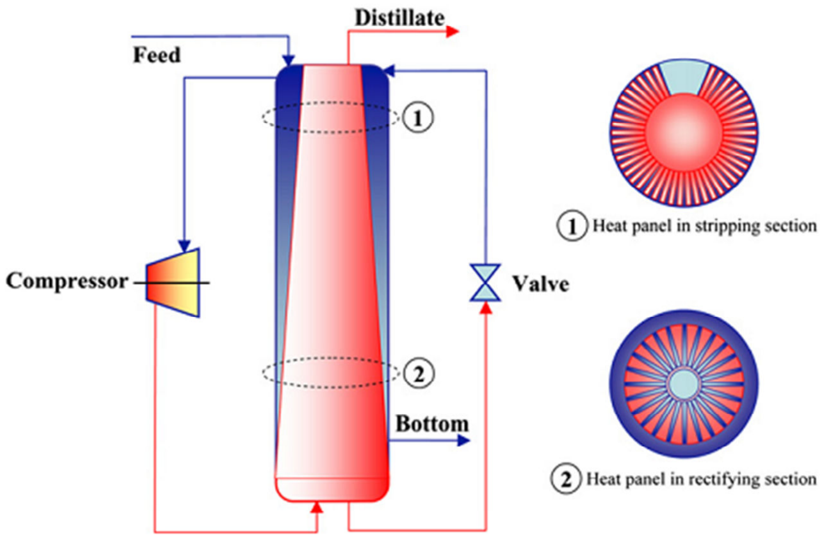

Figure 3.3: Possible Heat Panel Installation at Different Location Along the Concentric Column

This method to calculate the amount of heat transfer area gives the maximum area available in the column and the heat transfer rate is also the maximum based on the given area. The column diameter required for this calculation was obtained from Aspen Plus by using the tray sizing parameter. The trays in the column were assumed to be sieve trays and the Kister and Haas correlation was used instead of the default Fair correlation. The decision to use the former correlation was more realistic column diameters that can be obtain compared to the latter (Olujić, Sun, de Rijke & Jansens, 2006).

3.5 Capital and Operation Costs

Formulas used for the calculation of capital costs were based on the work by Chen, Huang and Wang (2010). The capital costs will only take into account the distillation column, heat exchangers and compressor.

To calculate the cost of the distillation column, the following formula is used:

$$H = N \times 2 \times \frac{1.2}{3.281} \tag{3.14}$$

$$C_{shell} = 17\,640 \times D^{1.066} \times H^{0.802} \tag{3.15}$$

$$C_{tray} = 229 \times D^{1.55} \times N \tag{3.16}$$

Where,

H = height of distillation column, m

N = number of trays

D = largest diameter of distillation column, m

C = cost, $

For heat exchangers (reboiler, heat panels, and condenser) and compressor, the following equations will be used:

$$A_{reb} = \frac{Q_{reb}}{U_{reb} \times \Delta T} \tag{3.17}$$

$$A_{cond} = \frac{Q_{cond}}{U_{cond} \times \Delta T} \tag{3.18}$$

$$C_{HE} = 7\,296\left(A_{reb}^{0.65} \times A_{cond}^{0.65} \times A_{HP}^{0.65}\right) \tag{3.19}$$

$$C_{compr} = 0.345 \times V^{0.82} \times 10^{6} \tag{3.20}$$

Where,

A_{reb} = reboiler heat transfer area, m²

A_{cond} = condenser heat transfer area, m²

A_{HP} = total heat panel area, m²

V = vapour flow rate, kmol/s

C_{HE} = heat exchanger cost, $

C_{compr} = compressor cost, \$

Q_{reb} = reboiler duty, kJ/h

Q_{cond} = condenser duty, kJ/h

U_{reb} = reboiler overall heat transfer coefficient, kW/m²·°C

U_{cond} = condenser overall heat transfer coefficient, kW/m²·°C

The overall heat transfer coefficient for reboiler and condenser was assumed to be at 1 000 and 800 W/m²·°C respectively (Olujić, Sun, de Rijke & Jansens, 2006).

Operation costs will only take into account steam (reboiler), cooling water (condenser) and electricity (compressor) consumption. Cost for steam, cooling water and electricity are summarised in Table 3.1. Other assumption for operating costs calculations is the column operates for 330 days or 7 920 hours per year.

Table 3.1: Summary of Utility Costs (Adapted from Seider, Seader, Lewin & Widagdo, 2010)

Utility	Cost
Steam (450 psi)	\$ 14.50 /1000 kg
Steam (150 psi)	\$ 10.50 /1000 kg
Steam (50 psi)	\$ 6.60 /1000 kg
Cooling water	\$ 0.02 /m³
Electricity	\$ 0.06 /kWh

The mass flow of steam was calculated based on the following formula by assuming that the energy is transferred only due to the condensation of the saturated steam:

$$\dot{m}_{steam} = \frac{Q_{reb}}{L} \tag{3.21}$$

Where,
$\dot{m}$ = mass flow, kg/h
L = latent heat of vaporisation, kJ/kg

The mass flow of cooling water is calculated based on the following formula by assuming that cooling water enters and leaves the condenser with a temperature difference of 16.67 °C.

$$\dot{m}_{cw} = \frac{Q_{cond}}{C_p \Delta T} \tag{3.22}$$

Where,
C_p = specific heat capacity of water, kJ/kg·°C

The total annualized cost (TAC) is given by,

$$C_{TAC} = \frac{1.2(C_{capital})}{\gamma} + C_{operation} \tag{3.23}$$

Where,
C_{TAC} = Total annualized cost, \$/yr
$C_{capital}$ = Capital cost, \$
$C_{operation}$ = Operation costs, \$/yr
γ = payback period, yr

The 20 % additional capital costs only applies to the HIDiC and the payback period can be assumed to be three years. This additional capital costs is due to the additional installation costs required for the heat panels (Nakaiwa et. al., 2003).

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Conventional Column

The optimal column sequence based on work by Hasebe (2009) is shown in Figure 4.1. The first column (C1) performs a separation between isopropanol and *n*-propanol. Next, the second column (C2) separates ethanol and isopropanol. Finally, the third (C3) and fourth (C4) column performs a separation between propanol and isobutanol, and isobutanol and *n*-butanol respectively.

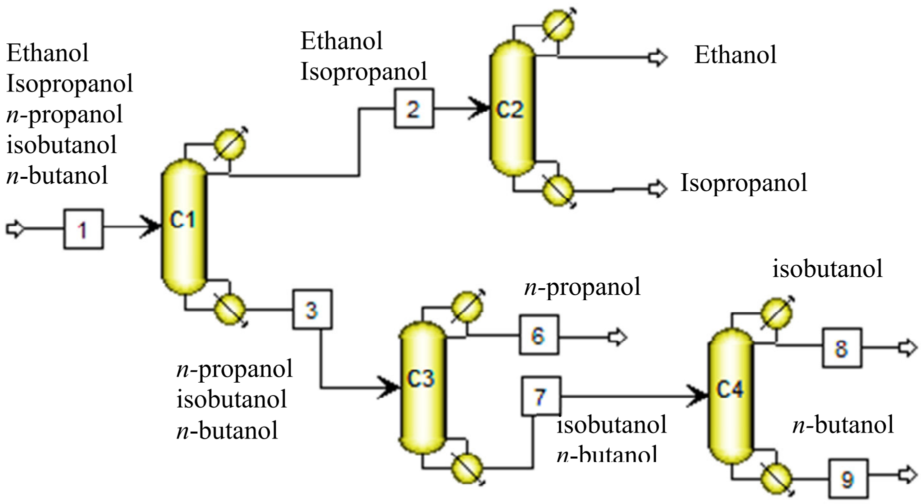

Figure 4.1: Optimal Sequence Based on Hasebe (2009)

FUG-K calculations from ChemSep resulted in 30, 95, 51 and 36 stages for columns C1, C2, C3 and C4 respectively. For column C1, saturated liquid feed at 278.6 kPa and 393 K enters at stage 11. The top product from column C1 at 273 kPa and 380 K enters column B2 at stage 48 while the bottom product from column C1 enters stage 18 of column C3 at 289 kPa and 407.6 K. Column C4 is fed at stage 19 using the bottom product of column C3 at 307 kPa and 421.4 K. Table 4.1 summarises these column parameters.

Table 4.1: Summary of Column Parameters for the Conventional Column

Column	Number of Stages	Feed Stage	Feed Condition	
			Temperature (K)	Pressure (kPa)
C1	30	11	393.0	278.6
C2	95	48	380.0*	273.0*
C3	51	18	407.6*	289.0*
C4	36	19	421.4*	307.0*

* - obtained from Aspen Plus

Reboiler and condenser duties are summarised in Appendix A (Table A.1) and shown in Figure 4.2. Figure 4.2 shows the typical thermodynamics of a distillation column where almost all of the energy input at the reboiler is removed at the condenser.

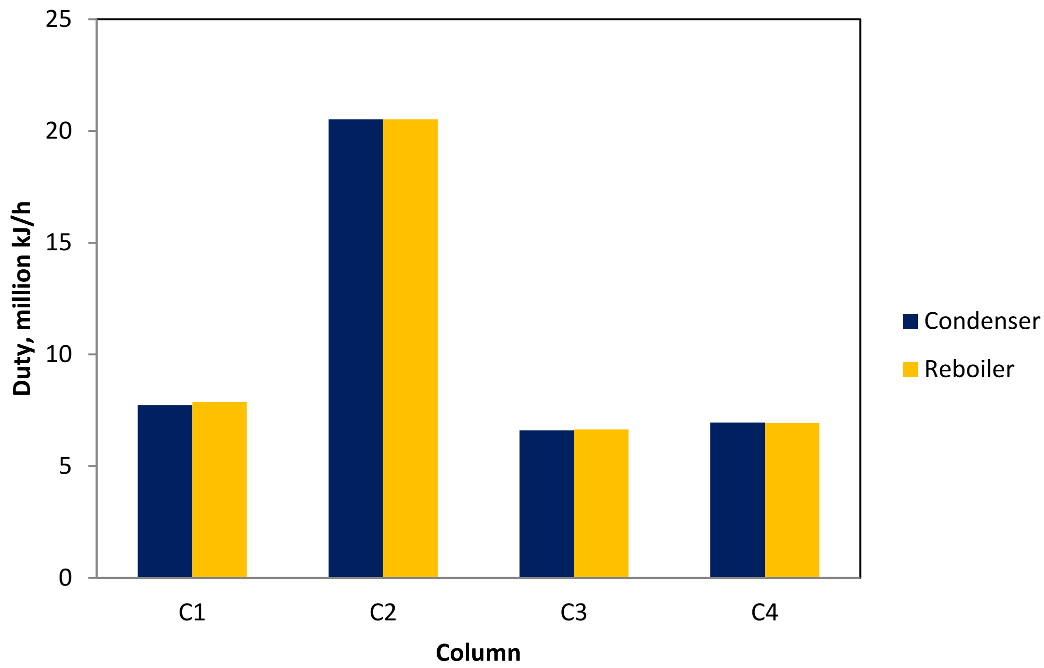

Figure 4.2: Reboiler and Condenser Duties for the Conventional Column

Columns C1, C3 and C4 have much lower number of stages as well as a much lower duties compared to column C2. This phenomenon is due to the low relative volatility, α, between ethanol and isopropanol. A low relative volatility will result in a larger number of stages as given by the Fenske equation (Equation 4.1). The large reboiler duty is due to the increase of energy required to produce enough vapour to flow through the large number of stages.

$$N_{min} = \frac{\log\left(\left(\frac{d_i}{d_j}\right)\left(\frac{b_j}{b_i}\right)\right)}{\log \alpha_m} \tag{4.1}$$

Where,

N_{min} = minimum number of stages

d = distillate flow rate, kmol/h

b = bottom flow rate, kmol/hr

α = relative volatility

i = light key

j = heavy key

4.2 Internally Heat Integrated Distillation Column (i-HIDiC)

As in the conventional column, the same distillation sequence is used. Figure 4.3 shows the configuration used in Aspen Plus. The pressure increase by the compressor is 200, 160, 150 and 150 kPa for columns C1, C2, C3 and C4 respectively. Each i-HIDiC column is represented by 4 blocks. For example, the first column (C1) consists of blocks B1 to B4. The column parameters are summarised in Table 4.3.

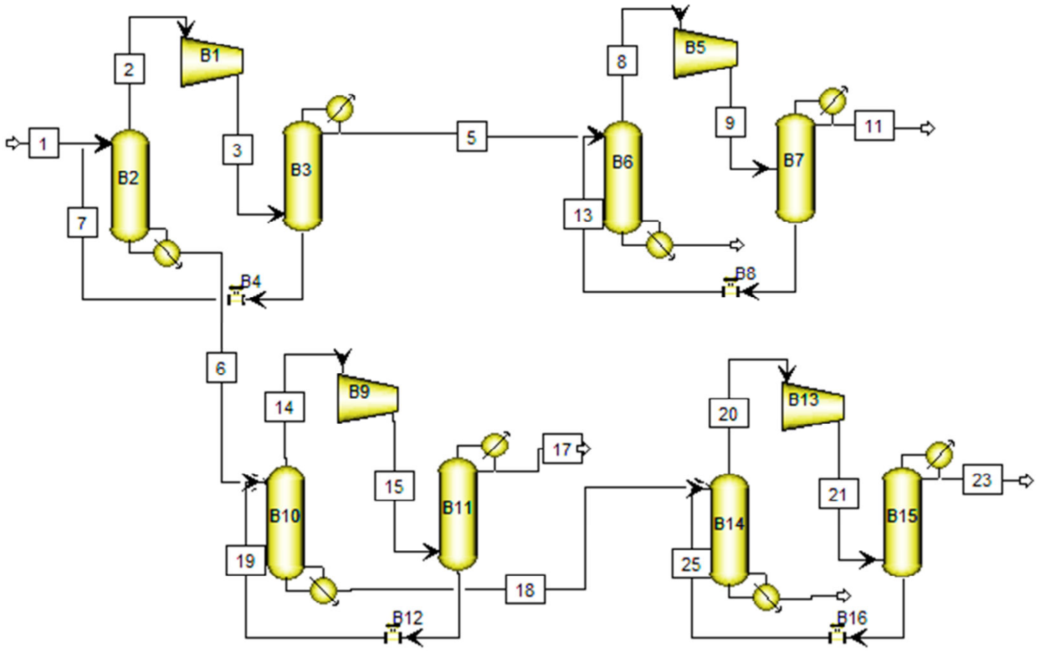

Figure 4.3: The i-HIDiC Sequence; C1 – B1 to B4, C2 – B5 to B8, C3 – B9 to B12, C4 – B13 to B15

Table 4.2: Summary of Column Parameters for the i-HIDiC

Column	Number of Rectifying Stages	Number of Stripping Stages	Feed Condition Temperature (K)	Feed Condition Pressure (kPa)	Compressor Pressure Increase (kPa)
C1	10	20	393.0	278.6	200
C2	47	48	398.3*	472.5*	160
C3	17	34	407.6*	289.1*	150
C4	18	18	421.4*	307.0*	150

* - obtained from Aspen Plus

4.2.1 Reboiler and Condenser Duties

Reboiler and condenser duties for the i-HIDiC varied greatly from column to column unlike the conventional column where almost similar magnitude of duties is observed for column C1, C3 and C4. Appendix A (Table A.2) and Figure 4.4 summarises the duties for the reboiler and condenser for the i-HIDiC.

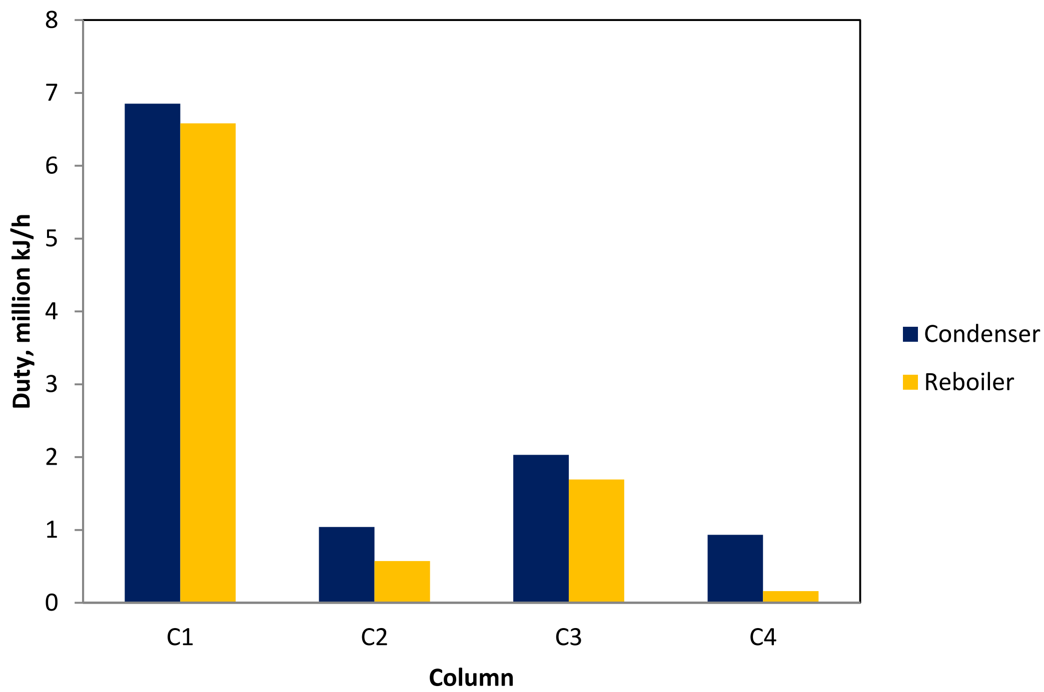

Figure 4.4: Reboiler and Condenser Duties for the i-HIDiC

From Figure 4.4, it was observed that condenser duties are higher than reboiler duties unlike the conventional column where reboiler and condenser duties are almost equal (Figure 4.2). This is due to larger vapour that is present in the column that is being condensed in the total condenser (liquid from condenser) compared to the amount of liquid that is being vaporised in the reboiler (vapour from reboiler) (Appendix A; Table A.3 and A.4). Besides that, it is also observed that column C1 has much higher duties compared to the other three. This is due to the lower heat transfer area available compared to the other three columns and smaller temperature difference compared to columns C2 and C3 (Table 4.3).

Table 4.3: Summary of Heat Transfer Area and Minimum Temperature Difference at the Optimum Compressor Pressure Increase for the i-HIDiC

Column	Heat Transfer Area, m^2	Minimum Temperature Difference, K
C1	173.65	4.38
C2	2 425.65	6.06
C3	239.20	9.03
C4	371.56	0.79

4.2.2 Effect of Compressor

The compressor present in the i-HIDiC controls the driving force for heat transfer between the rectifying and stripping sections. Inadequate compression will not provide the required driving force whereas over-compression will result in a large compressor and compressing cost (Gadalla, 2009). Figures 4.5 to 4.8 show the effect of the increase in compressing pressure on the temperature of the rectifying section for all the four columns.

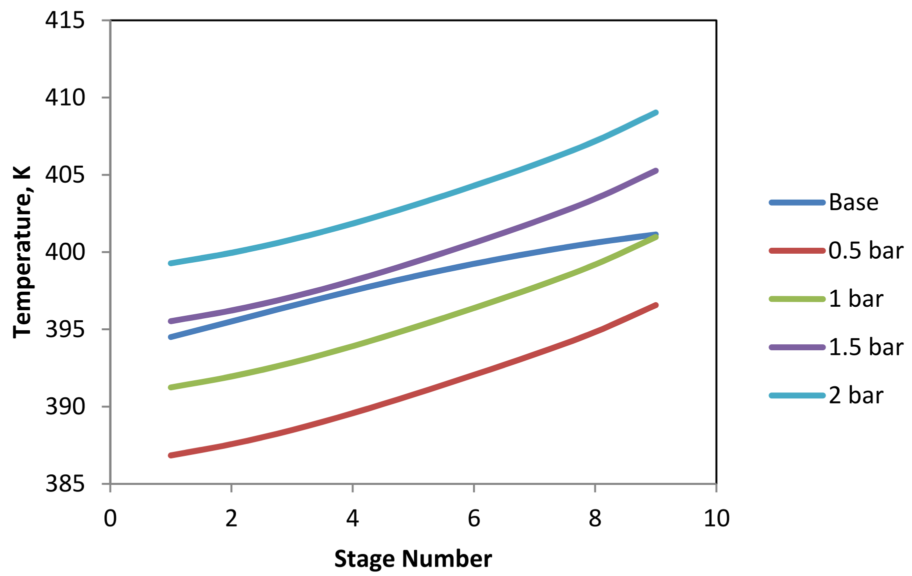

Figure 4.5: Temperature Profile Plot with Increasing Compressor Pressures for Column C1

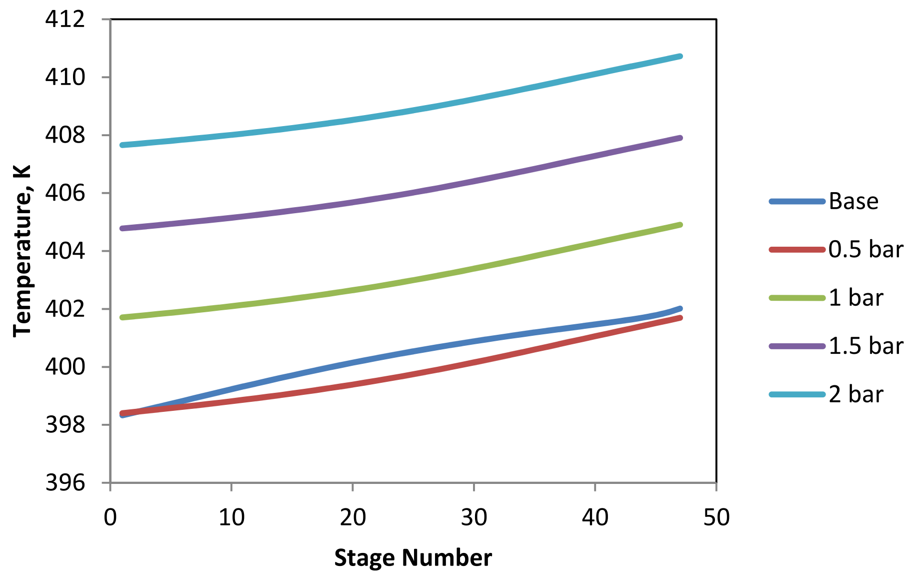

Figure 4.6: Temperature Profile Plot with Increasing Compressor Pressures for Column C2

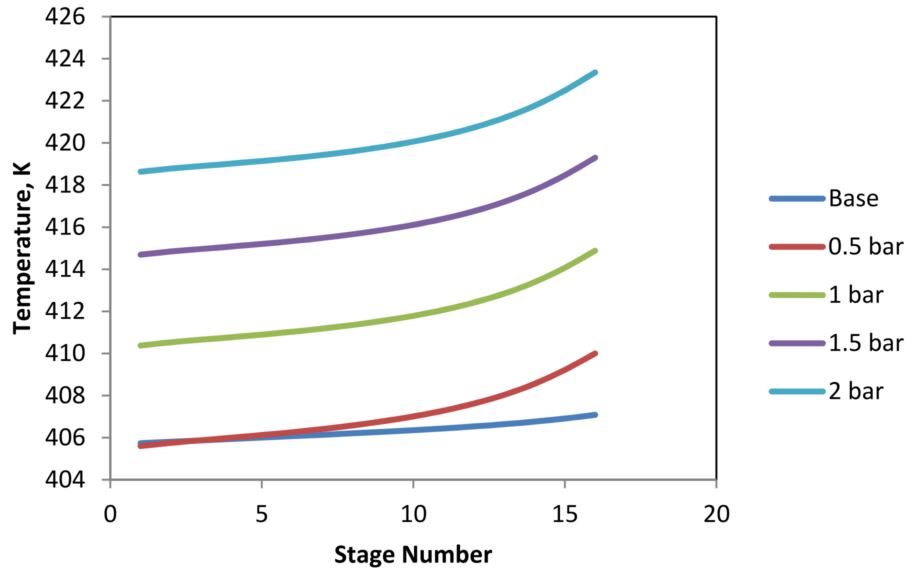

Figure 4.7: Temperature Profile Plot with Increasing Compressor Pressures for Column C3

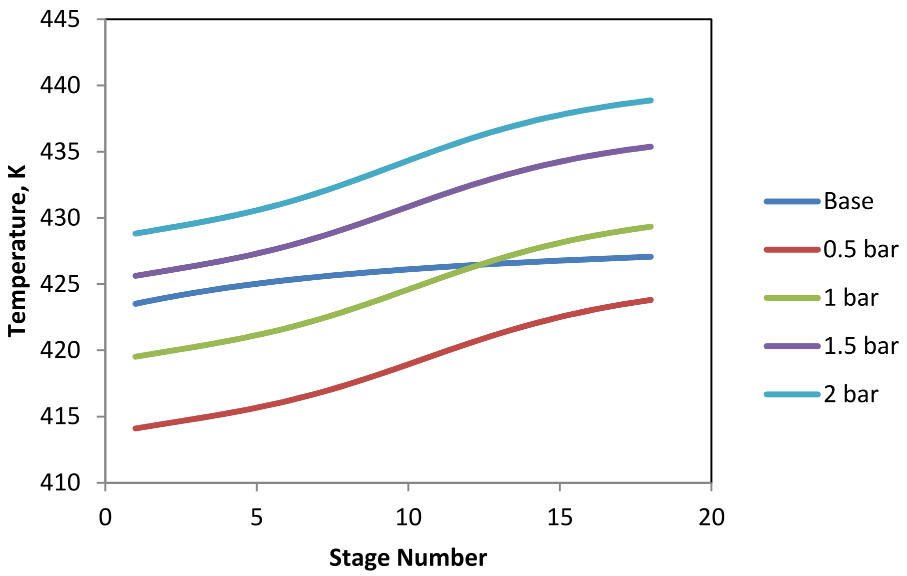

Figure 4.8: Temperature Profile Plot with Increasing Compressor Pressures for Column C4

In Figures 4.5 to 4.8 the "Base" line corresponds to the temperature profile of the stripping column. This temperature profile remains unchanged regardless of compression pressure. As the compression pressure increases, the temperature in the rectifying column also increases. As the temperature difference between the stripping and rectifying increases, the driving force or amount of energy that can be transferred also increases. By plotting the temperature profiles, it allows us to identify the pinch location or the limiting stages. Besides that, it also provides us with a preliminary feasibility study as suggested by Gadalla (2009). For a HIDiC column to be feasible, the temperature of the rectifying section has to be higher than the stripping section. If the opposite occurs, heat will transfer from stripping to rectifying resulting in higher duties. Table 4.4 summarises the estimated pinch stages and minimum pinch temperature difference at the minimum pressure for each column based on Figures 4.5 to 4.8. The minimum pressure increase in the table is the estimated required pressure increase to obtain a positive temperature difference.

Table 4.4: Summary of Column Pinch Stages for the i-HIDiC

Column	Estimated Pinch Location (Stage)	Minimum Pinch Temperature Difference, K	Estimated Minimum Pressure Increase, kPa
C1	3 – 4	0.56	150
C2	20 – 30	0.21	65
C3	1 – 7	0.1-0.2	63
C4	1 – 5	0.79	150

Other than the increase in temperatures, increasing compression pressures will also cause the increase the compression and compressor costs. The annual operation costs (steam, cooling water and electricity only) were the main factors in determining the optimum compressor pressure increase instead of capital cost as lower operating costs will provide better savings in the long run. Figures 4.9 to 4.11 show the change in operation costs due to the changes in pressure. No data is available for column C4 due to the temperature profile of the column (Figure 4.8) which has a very large variation between the highest and lowest stages. A slight decrease in pressure (10 kPa) will result in a negative temperature difference at the pinch while an increase in pressure (10 kPa) will result in a failed convergence due to "dried up stage". For column C2, no data is available for pressure increase above 160 kPa as an increase of 10 kPa will too result in a failed convergence due to "dried up stage".

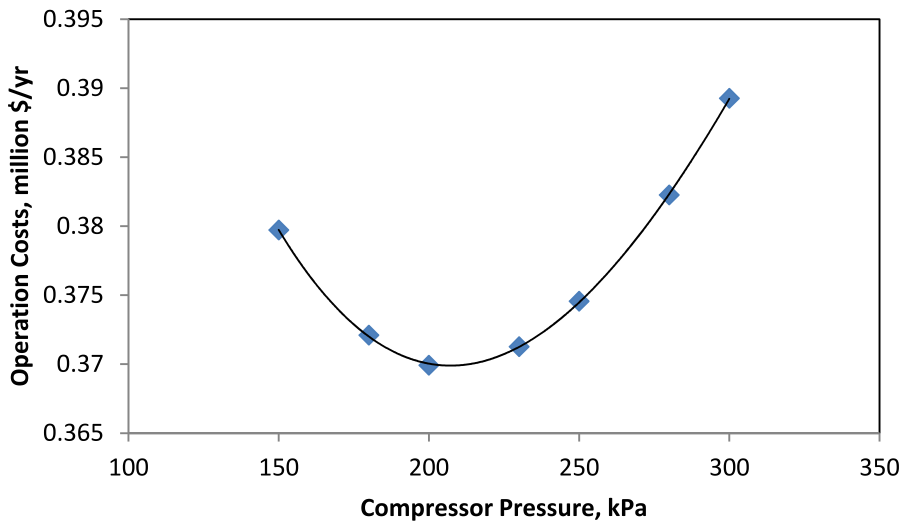

Figure 4.9: Operation Costs with Increasing Compressor Pressures for Column C1

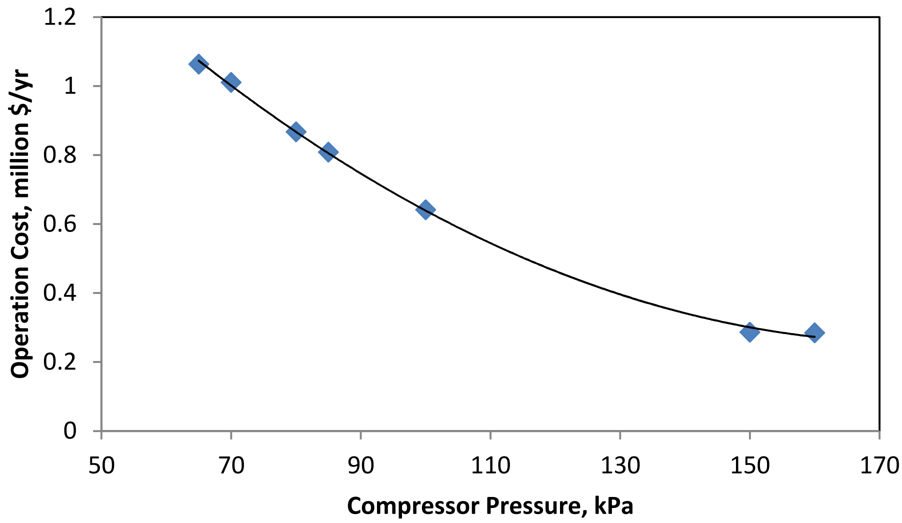

Figure 4.10: Operation Costs with Increasing Compressor Pressures for Column C2

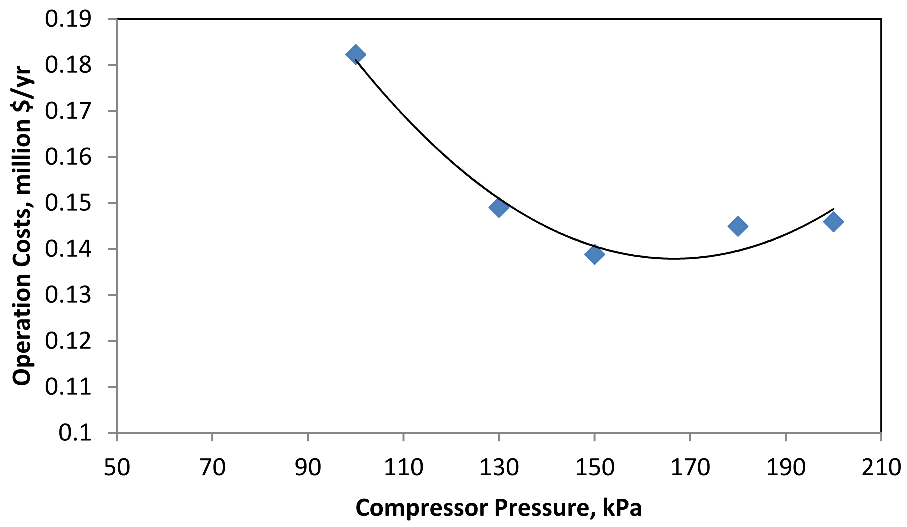

Figure 4.11: Operation Costs with Increasing Compressor Pressures for Column C3

4.3 Conventional Versus i-HIDiC

The conventional column and the i-HIDiC were compared based on their reboiler and condenser duties, and operation and capital costs. As the distillation sequence is already an optimum sequence, the number of stages in the conventional column and the i-HIDiC is assumed to be optimal. The heat panels in the i-HIDiC were assumed to have an efficiency of 100 % and will not degrade the column performance (Olujić, Sun, de Rijke & Jansens, 2006).

4.3.1 Duties

Figures 4.12 and 4.13 show the comparison of reboiler and condenser duties respectively between the conventional column and the i-HIDiC. Significant reduction of both reboiler and condenser duties are observed especially in columns C2 to C4. The lower reduction in reboiler (16.4 %) and condenser (11.3 %) observed for column C1 is due to the low heat transfer area provided by the heat panels compared to the other three columns. Although the reduction of duties can be increased further by increasing the pressure, it is not optimal as the cost of compression will increase much faster than the amount that could be saved from the reduction of duties. Table 4.5 summarises the reduction in duties between the conventional column and the i-HIDiC. The large reduction in duties in columns C2 and C4 is due to the larger surface area available for heat transfer and heat transfer that occur almost along the whole length of the column (Table 4.2). On the other hand, column C3 has a larger temperature difference between the rectifying and stripping sections that provided a larger driving force for heat transfer to occur (Table 4.3).

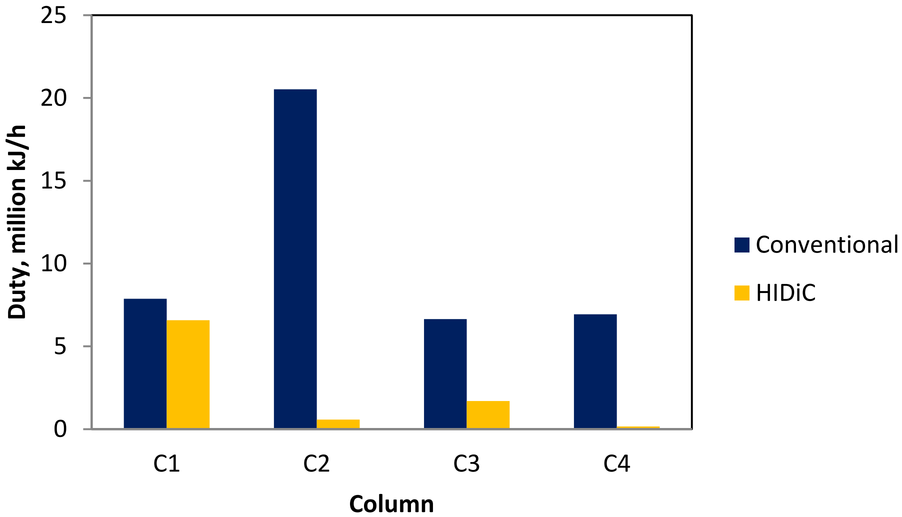

Figure 4.12: Comparison in Reboiler Duty between the Conventional Column and the i-HIDiC

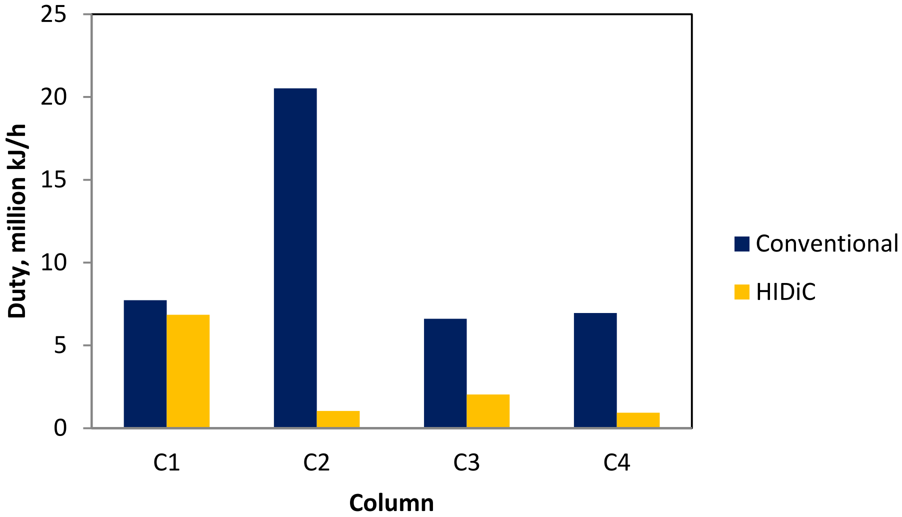

Figure 4.13: Comparison in Condenser Duty between the Conventional Column and the i-HIDiC

Table 4.5: Summary of the Reduction in Duties between the Conventional Column and the i-HIDiC for Reboiler and Condenser

Column	Reboiler Duty (kJ/h)			Condenser Duty (kJ/h)		
	Conventional	HIDiC	%	Conventional	HIDiC	%
C1	7 873 924	6 580 959	16.42	7 725 961	6 852 639	11.30
C2	20 524 299	573 658	97.20	20 524 361	1 040 672	94.93
C3	6 645 763	1 693 081	74.52	6 606 804	2 030 560	69.27
C4	6 934 264	160 382	97.69	6 956 783	932 913	86.59
Total	41 978 251	9 008 080	78.54	41 813 909	10 856 784	74.04

4.3.2 Costs

Figure 4.14 shows the comparison in operation costs. It is observed that operation costs are much lower for columns C2 to C4 while higher for column C1 in the i-HIDiC system. Despite having a lower energy consumption from the reboiler and condenser in column C1 in the i-HIDiC design, the increase in energy costs from compression was much higher than what could be saved from lower steam and cooling water consumption. On the other hand, large amount of savings from the efficient use of energy from the rectifying section resulted in lower steam consumption for heating and lower cooling water consumption for condensing the product for columns C2, C3 and C4. As mentioned in Section 4.2.1, the operation costs for all four columns are optimal with respect to the steam, cooling water and electricity consumption.

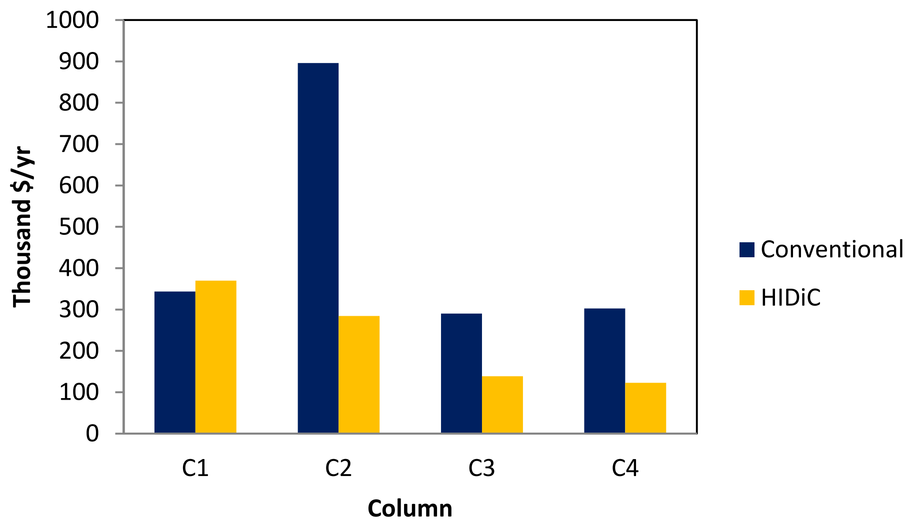

Figure 4.14: Comparison in Operation Costs between the Conventional Column and the i-HIDiC

Table 4.6 summarises some of the parameters used in the determination of capital costs such as column diameter (obtained from Aspen Plus) and heat exchange areas.

Table 4.6: Summary of the Capital Cost Calculation Parameters

Column	Conventional			
	C1	C2	C3	C4
Height, m	21.95	69.50	37.31	26.34
Diameter, m	1.08	1.72	1.04	1.07
Reboiler Area, m²	1 109	19 093	1 780	22 468
Condenser Area, m²	5 983.7	105 575	9 493.8	5 315.6
Column	**i-HIDiC**			
	C1	C2	C3	C4
Height, m*	14.63/7.32	35.15/34.38	24.88/12.44	13.17/13.17
Diameter, m*	1.23/0.97	3.51/1.46	1.67/0.8	2.38/0.8
Reboiler Area, m²	965.7	995.5	605.68	22.57
Condenser Area, m²	5 776	9 838	2 943	797.5
Heat Panel Area, m²	173.6	2 425.6	239.2	371.6

* - (stripping/rectifying)

Figures 4.15 shows the comparison of capital costs for both conventional and i-HIDiC systems. Like Figure 4.14, it is observed that the capital costs are very much lower for columns C2 to C4 in the i-HIDiC system. However, the opposite is true for column C1. The higher capital costs of column C1 is due to the addition of a compressor and heat panels while having only a slightly smaller reboiler and condenser compared to the conventional column. The tower cost only (excluding heat exchangers) is much higher for the i-HIDiCs compared to the conventional column (Appendix A; Table A.5 and A.6). This is due to the use of a larger diameter shell as well as the annular layout of the column (Figure 3.2 & 3.4). As heat exchanger size is highly dependant on the amount of duty required, a reduction in duty will indefinitely reduce its size thus the capital cost. The size of the heat exchangers (reboiler and condenser) are generally smaller in the i-HIDiCs compared to the conventional column (Table 4.6). These smaller heat exchangers provide a large contribution in savings in capital costs despite having additional equipments (i.e. compressor and heat panels).

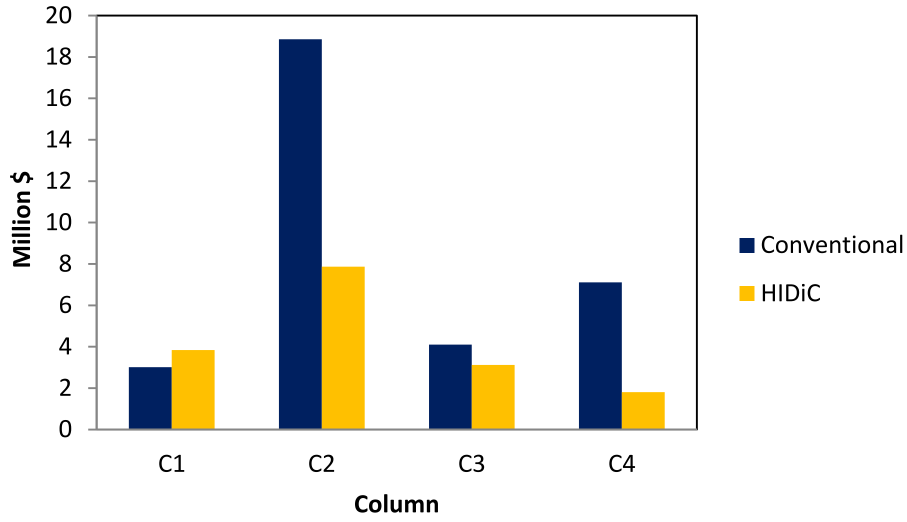

Figure 4.15: Comparison in Capital Costs between the Conventional Column and the i-HIDiC

Other than operation and capital costs, the total annualized cost (TAC) is important in any production plant. Performing internal heat integration on the columns also resulted in overall reduction of TAC of up to 50%. Despite having a higher TAC for column C1, the lower TAC of the other three columns managed to cover the losses. The summary of the operation, capital and total annualized cost (TAC) are shown in Tables 4.7 and 4.8.

Table 4.7: Summary of Cost Comparison between the Conventional Column and the i-HIDiC

Column	Conventional				
	C1	C2	C3	C4	Total
Operation Cost, $/yr	343 349	895 851	289 988	302 720	1 831 909
Capital Cost, $	3 011 872	18 856 589	4 102 004	7 112 514	33 082 979
TAC, $/yr	1 347 306	7 181 382	1 657 323	2 673 558	12 859 569
Column	i-HIDiC				
	C1	C2	C3	C4	Total
Operation Cost, $/yr	369 914	284 194	138 799	122 944	915 853
Capital Cost, $	3 839 023	7 864 792	3 123 941	1 804 222	16 631 978
TAC, $/yr	1 649 589	2 905 792	1 180 113	724 352	6 459 846

Table 4.8: Percentage Reduction in Cost between the Conventional Column and the i-HIDiC

Column	C1	C2	C3	C4	Total
Operation Cost	-7.74	68.28	52.14	59.39	50.01
Capital Cost	-27.46	58.29	23.84	74.63	49.73
TAC	-22.44	59.54	28.79	72.91	49.77

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

The design of the internally heat integrated distillation column (i-HIDiC) system for multicomponent separation was performed on an alcohol feed mixture (ethanol, isopropanol, *n*-propanol, isobutanol and *n*-butanol).

Optimal compressor pressure obtained was 200 kPa for column C1, 160 kPa for column C2, 150 kPa for columns C3 and C4. From the simulation performed, the overall reduction of reboiler and condenser duties for the distillation train when using the i-HIDiC were 78.54 % and 74.04 % respectively. For individual columns, it was found that columns C2 and C4 had the largest reduction in duties. Column C1 was found to have the lowest reduction in duties.

The overall reduction in costs for the whole distillation train was 50.01 % for operation, 49.73 % for capital and 49.77 % for TAC. It was found that cost savings was not be applicable for all columns when i-HIDiC was used. In this study, the costs (operation, capital and TAC) for column C1 increased whereas the other columns decreased. The largest amount of cost savings was contributed by columns C2 and C4.

The main factors that influenced the reduction in duties were the amount of available heat transfer area and the temperature driving force. On the other hand, it was the column, condenser and reboiler sizes, heat panel area and compressor size that influenced the reduction in costs.

5.2 Recommendations

This work only focused on the column thermodynamic and hydraulic feasibility as well as the costs involved. Other aspects of the column should be explored.

a. Column controllability. The increased complexity of the column from the addition of a compressor and a throttling valve may increase the difficulty in proper control of the column. Besides that, the higher vapour flows and the presence of a recycle stream in the column may further increase the control complexity.

b. Mechanical design. So far, there is no known method to properly design the column with heat panels attached to the internal shell and the annular layout of the column with varying diameter of the inner column. Proper mechanical design will allow for more accurate costs estimations.

c. Heat transfer medium. Perhaps there are much more efficient ways to transfer heat from the rectifying to the stripping section other than heat panels. Besides that, a different method or medium for heat transfer may change the column design and have an effect on the column performance.

d. Other multicomponent feed. Other feed options may yield different results from this work. Therefore, a more thorough study should be conducted and compiled to determine which kind of feed type is the most suitable for the i-HIDiC.

e. Other column designs and optimal configuration should be explored together with other aspects highlighted in this section.

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APPENDICES

APPENDIX A: SUMMARY OF DATA

Table A.1: Summary of Column Duties for the Conventional Column

Column	Reboiler Duty (kJ/h)	Condenser Duty (kJ/h)
C1	7 873 924	7 725 961
C2	20 524 299	20 524 361
C3	6 645 763	6 606 804
C4	6 934 264	6 956 783

Note: All values are obtained from Aspen Plus

Table A.2: Summary of Column Duties for the i-HIDiC

Column	Reboiler Duty (kJ/h)	Condenser Duty (kJ/h)	Compressor (kWh)
C1	6 580 959	6 852 639	172.6
C2	573 658	1 040 672	543.1
C3	1 693 081	2 030 560	134.9
C4	160 382	932 913	240.3

Note: All values are obtained from Aspen Plus

Table A.3: Summary of Inlet and Outlet Temperatures for Reboiler and Condenser, Liquid to Reboiler and Vapour to Condenser Flow Rates for the Conventional Column

Column	Reboiler Temperature		Vapour from Reboiler	Condenser Temperature		Liquid from Condenser
	In (°C)	Out (°C)	(kmol/h)	In (°C)	Out (°C)	(kmol/h)
C1	132.5	134.5	204.6	107.9	107.5	208.3
C2	112.2	112.5	553.1	103.2	103.1	554.9
C3	147.2	148.3	172.0	127.0	126.7	178.9
C4	153.9	154.0	185.8	140.6	140.1	180.7

Note: All values are obtained from Aspen Plus

Table A.4: Summary of Inlet and Outlet Temperatures for Reboiler and Condenser, Liquid to Reboiler and Vapour to Condenser Flow Rates for the i-HIDiC

Column	Reboiler Temperature		Vapour from Reboiler	Condenser Temperature		Liquid from Condenser
	In (°C)	Out (°C)	(kmol/h)	In (°C)	Out (°C)	(kmol/h)
C1	132.6	134.5	171.0	125.6	125.2	194.6
C2	129.2	129.3	16.4	132.2	132.1	30.5
C3	147.5	148.3	33.2	141.5	141.3	45.4
C4	132.5	134.5	4.1	151.2	150.8	25.8

Note: All values are obtained from Aspen Plus

Table A.5: Cost Breakdown for the Conventional Column

Column	Cost ($)			
	C1	C2	C3	C4
Reboiler	695 872	4 422 448	946 269	4 915 889
Condenser	2 080 246	13 439 997	2 808 157	1 926 160
Tower	235 753	994 144	347 577	270 465
Total	3 011 872	18 856 589	4 102 004	7 112 514

Table A.6: Cost Breakdown for the i-HIDiC

Column	Cost ($)			
	C1	C2	C3	C4
Reboiler	635 676	648 339	469 399	55 315
Condenser	2 033 053	2 873 991	1 311 863	561 323
Tower	279 769	1 695 291	523 474	477 160
Heat Panels	208 390	1 156 706	256 605	341 666
Compressor	42 297	179 665	41 940	68 052
Total	3 839 023	7 864 792	3 123 941	1 804 222

APPENDIX B: SAMPLE CALCULATIONS

Taking stage 3 in column C1 as an example;

Stripping		Rectifying	
Diameter, m	Temperature, K	Diameter, m	Temperature, K
1.0474	395.5151	0.9480	399.9557

Rectifying tray area,

Rounding up the diameter gives 0.95 m

$$= \frac{\pi(0.95)^2}{4} = 0.7088 \text{ m}^2$$

Stripping tray area,

$$= \frac{\pi(1.0474)^2}{4} = 0.8617 \text{ m}^2$$

Since the rectifying section is nested in the stripping section, a new stripping diameter is required,

$$= \sqrt{\frac{4(0.8617 + 0.7088)}{\pi}} = 1.4141 \text{ m} \approx 1.42 \text{ m}$$

Heat Panel Area Calculations

$$\sigma = \frac{d_{str} - d_{rec}}{2} = \frac{1.42 - 0.95}{2} = 0.235 \text{ m}$$

$$\delta = \frac{0.10\pi d_{str}^2}{2(d_{str} - d_{rec})} = \frac{0.1\pi(1.42^2)}{2(1.42 - 0.95)} = 0.6739 \text{ m}$$

$$L = \sigma - \varepsilon = 0.235 - 0.001 = 0.234 \text{ m}$$

$L1 = \pi d_{rec} - \delta = \pi(0.95) - 0.6739 = 2.3106 \text{ m}$

$L2 = \pi d_{str} - \delta = \pi(1.42) - 0.6739 = 3.7872 \text{ m}$

$A_{HP} = 0.30L = 0.30(0.234) = 0.0936 \text{ m}^2$

$$N_{HP} = \frac{L1}{0.03} = \frac{2.3106}{0.03} = 77.0203$$

$TA_{HP} = N_{HP}A_{HP} = 77.0203(0.0936) = 7.2091 \text{ m}^2$

$$N'_{HP} = \frac{L2 - L1}{2(0.03)} = \frac{3.7872 - 2.3106}{2(0.03)} = 24.6091$$

$TA'_{HP} = N'_{HP}A'_{HP} = 24.6091(0.0936) = 2.3034 \text{ m}^2$

$SA_{HP} = 2(TA_{HP} + TA'_{HP}) = 2(7.2091 + 2.3034) = 19.025 \text{ m}^2$

Heat Transfer Rate,

$U = 1 \text{ kW/m}^2\cdot°\text{C} = 3\ 600 \text{ kJ/m}^2\cdot\text{h}\cdot°\text{C}$

$Q_{stage} = AU\Delta T_{stage} = 19.025(3\ 600)(399.9557 - 395.5151) = 304\ 133.9 \text{ kJ/h}$

Cost Calculations

Using column C1 as an example,

Capital Cost,

Column,

$$H = N \times 2 \times \frac{1.2}{3.281} = \frac{20(2)(1.2)}{3.281} = 14.6297 \text{ m} \approx 14.63 \text{ m}$$

$$H = N \times 2 \times \frac{1.2}{3.281} = \frac{10(2)(1.2)}{3.281} = 7.3148 \text{ m} \approx 7.32 \text{ m}$$

New stripping diameter after heat integration = 1.23 m (largest)

New rectifying diameter after heat integration = 0.97 m (geometric mean)

$$C = \left(C_{shell} + C_{tray}\right)_{stripping} + (C_{shell})_{rectifying}$$

$$C = (17\,640D^{1.066}H^{0.802} + 229D^{1.55}N)_{stripping} + (17\,640D^{1.066}H^{0.802})_{rectifying}$$

$$C = 17\,640((1.23)^{1.066}(14.63)^{0.802} + (0.97)^{1.066}(7.32)^{0.802}) + 229(1.23)^{1.55}(20)$$

$$C = \$\,279\,769.60$$

Heat Exchangers,

$$A_{reb} = \frac{Q_{reb}}{U_{reb} \times \Delta T} = \frac{6\,580\,959}{(3\,600)(134.5089 - 132.6160)} = 965.7118\ \mathrm{m}^2$$

$$A_{cond} = \frac{Q_{cond}}{U_{cond} \times \Delta T} = \frac{6\,852\,639}{(3\,600)(125.5969 - 125.1849)} = 5\,776.126\ \mathrm{m}^2$$

$$A_{HP} = 173.6526\ \mathrm{m}^2$$

$$C_{HE} = 7\,296\left(A_{reb}^{0.65} \times A_{cond}^{0.65} \times A_{HP}^{0.65}\right)$$

$$C_{HE} = 7\,296((965.7118)^{0.65}(5\,776.126)^{0.65}(176.6526)^{0.65}) = \$\,2\,877\,119.05$$

$$C_{compr} = 0.345 \times V^{0.82} \times 10^6 = 0.345(0.07734)^{0.82} \times 10^6 = \$\,42\,297.52$$

$$C_{cap} = 1.2 \times \$\,(42\,297.52 + 2\,877\,119.05 + 279\,769.60) = \$3\,839\,023.00$$

Operation Cost,

$$\dot{m}_{steam} = \frac{Q_{reb}}{L} = \frac{6\,580\,959}{2\,009.4} = 3275.08\ \mathrm{kg/h}$$

$$C_{steam} = 3275.08(7920)\left(\frac{10.50}{1\,000}\right) = \$\,272\,356.20$$

$$\dot{m}_{cw} = \frac{Q_{cond}}{C_p \Delta T} = \frac{6\,852\,639}{(4.2)(16.67)} = 97\,875 \text{ kg/h} = 97.875 \text{ m}^3/\text{h}$$

$$C_{cw} = 97.875(0.02)(7920) = \$\,15\,506.54$$

$$C_{compr,op} = 172.6677(7920)(0.06) = \$\,82\,051.68$$

$$C_{oper} = \$\,(82\,051.68 + 15\,506.54 + 272\,356.20) = \$\,369\,914.40$$

Total Annualized Cost (TAC)

$$C_{TAC} = \frac{3\,839\,023}{3} + 369\,914.40 = \$\,1\,649\,589.00$$