A Comparison of the Exergy Efficiencies of Various Heat-Integrated Distillation Columns

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This thesis is dedicated to

My Parents

(who have been a great source of inspiration and support)

and

My Supervisor, Dr. Muhammad Faheem

(who encouraged and motivated me toward the world of simulation)

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ABSTRACT

Distillation is the most widely used fluid separation and purification process, and accounts for a major share of the total energy consumption of the process industry. However, because of its relatively low thermodynamic efficiency, it is a prime target for process intensification studies. Numerous alternative designs have been explored with the aim to reduce thermodynamic losses in distillation columns and to improve the overall process efficiency. Among non-conventional distillation technologies, heat-integrated distillation processes have received particular attention due to potentially substantial energy savings.

The objective of this research project is to study exergy losses in various heat-integrated distillation columns. A conventional industrial-scale i-butane/n-butane fractionator has been selected as a case study for comparison of the performances of various heat-integrated designs. Aspen Plus® process simulator is used to perform steady-state simulations and exergy analyses of the conventional distillation column (CDC), internally heat-integrated distillation column (iHIDiC), externally heat-integrated double distillation columns (EHIDDiC), and vapor recompression (VRC) system. The results of these exergy analyses show that a modified VRC system $\left(\eta_E = 10.69\% \right)$ is the most efficient design for this separation. Exergy efficiency of the conventional VRC system is same as that of the CDC $\left(\eta_E = 9.27\% \right)$. EHIDDiC system $\left(\eta_E = 9.77\% \right)$ is somewhat better than the CDC, whereas iHIDiC shows poor exergy efficiency $\left(\eta_E = 8.09\% \right)$, even lower than the CDC.

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CHAPTER 1

INTRODUCTION

1.1. Exergy Efficiency of Distillation Columns

Distillation is the most widely used fluid separation and purification technique in the chemical and petrochemical industries. However, the relatively low thermodynamic efficiency (5–20%)[1-2] of conventional distillation columns (CDC) makes them highly energy intensive. For most refining and chemical processes, 40–50% of the total plant operating cost can be attributed to distillation.[3] A small improvement in the thermodynamic efficiency of distillation columns can therefore make a large difference in the overall process efficiency and profitability.

The exergy, also called availability, is the maximum useful work obtained from a system at a given state in a given environment such that the system achieves chemical, mechanical, and thermal equilibrium with the environment.[4] In other words, exergy of a system is a measure of the disequilibrium between its current state and the environment. A system is said to have reached a so-called "dead state" when it achieves thermodynamic equilibrium with its environment. Dead state temperature and pressure are used as reference conditions for exergy analysis.[5] The exergy is conceptually different from Gibbs free energy which requires the process to be isothermal and isobaric and hence involves no interaction with the environment.[5]

The total exergy of a system is the sum of its physical, chemical, kinetic, and potential exergies. The kinetic and potential exergy terms are generally small and can be safely neglected.[6] The physical exergy is the maximum useful work obtained when the system is taken from its actual conditions (T, P) to reference conditions (T_0, P_0) through purely physical
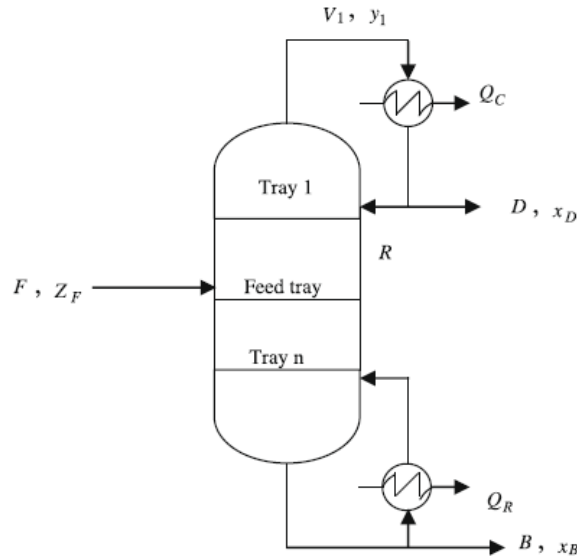
Figure 1.1. Schematic representation of a conventional distillation column[2]

means. The chemical exergy is the maximum useful work obtained while bringing the system in chemical equilibrium with the environment, and accounts for the difference between actual system composition and the composition of the environment.

According to the second law of thermodynamics, irreversibilities in a process lead to a net increase in entropy and degradation in the quality of energy. Exergy analysis thus provides a measure of both the quantity and quality of energy available in a process,[7] evaluates the energy efficiency of the process, and enables identification of the sources of irreversibilities.[8] A reduction in exergy destruction leads to an increase in energy availability, thereby improving the overall process efficiency.

Exergy losses in a distillation column are due to the difference between the exergy entering the column and the exergy leaving the column. In a CDC (Figure 1.1), heat is supplied only through the main reboiler and rejected only through the main condenser, while the column operates adiabatically. Exergy input to a CDC includes exergy of the feed stream plus exergy input to the main reboiler. Similarly, exergy output of a CDC includes exergy of the product streams plus exergy leaving the main condenser. Exergy losses in a CDC are therefore directly associated with the condenser and reboiler duties. In fact, the temperature difference between

the reboiler and the condenser is the main reason for considerable degradation of thermal energy and energy inefficiency of the conventional distillation technique.[9]

1.2.   Non-Conventional Distillation Techniques

The quest for enhanced distillation processes has led to a large number of increasingly complex modifications to, and departures from, conventional distillation processes.[9] Among non-conventional distillation technologies, heat-integrated distillation processes[2] have received particular attention due to potentially substantial energy savings. An important feature of such heat-integrated distillation processes is a net reduction in utility costs, which often results in higher energy efficiency.

A diabatic section of a distillation column allows heat to enter or leave through its stages. As a result, exergy losses from the main condenser or the main reboiler are distributed to other stages of the respective section, hence reducing the main utility load as well as the overall exergy loss of the section.[10] In an internally heat-integrated distillation column (iHIDiC),[11] two diabatic sections with opposite directions of heat transfer are integrated. Thus, the total heat rejection is distributed along the rectifying section, while the total heat absorption is similarly distributed along the stripping section (Figure 1.2). The pressure difference between the two sections, manipulated by a compressor and a throttling valve, results in the temperature driving force necessary for heat transfer between the two sections. Because of relatively small temperature differences between heat-integrated stages, exergy losses linked with heat transfer decrease, resulting in a reduction of net energy requirement for both sections.[10]

In externally heat-integrated double distillation columns (EHIDDiC),[12] the liquid feed is split between two distillation columns operating at different pressures with an integrated condenser–reboiler setup (Figure 1.3). The feed split between the two columns is manipulated to equalize the duties of the condenser of the high-pressure (HP) column and the reboiler of the
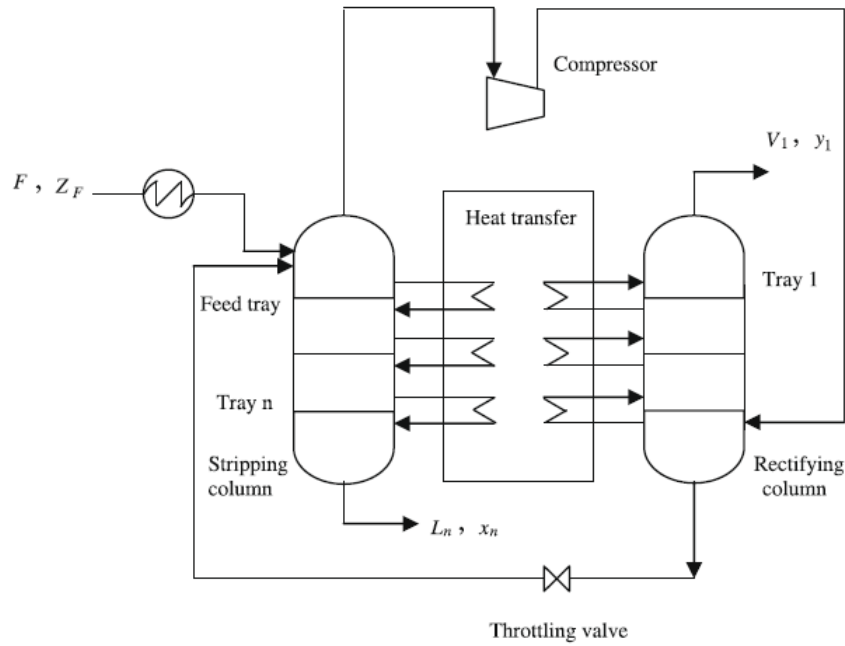
Figure 1.2. Schematic representation of a general iHIDiC system[2]
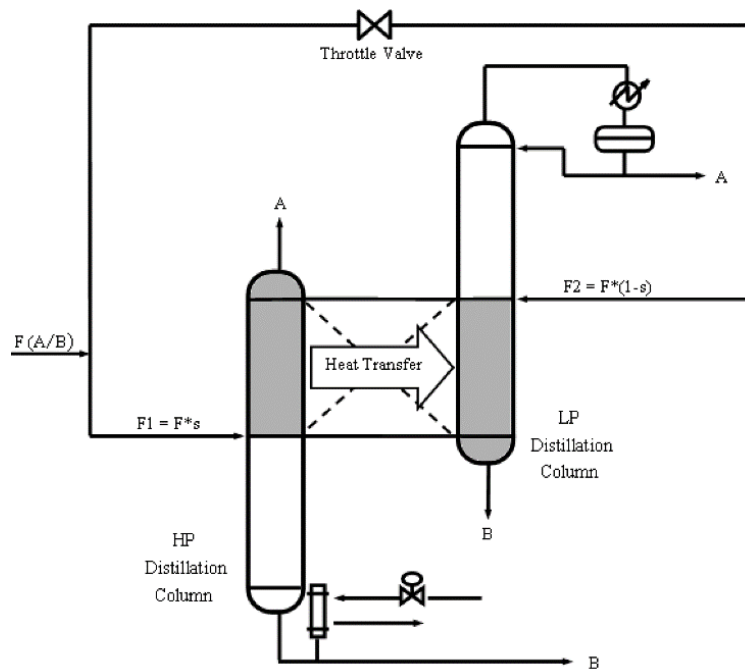
Figure 1.3. Schematic representation of a general EHIDDiC system[13]

low-pressure (LP) column. Because the heat exchange takes place outside the column shells, an EHIDDiC system is, in general, considerably less complicated to design and operate than an iHIDiC system. Furthermore, substitution of compressor with a pump considerably reduces the utility requirements.
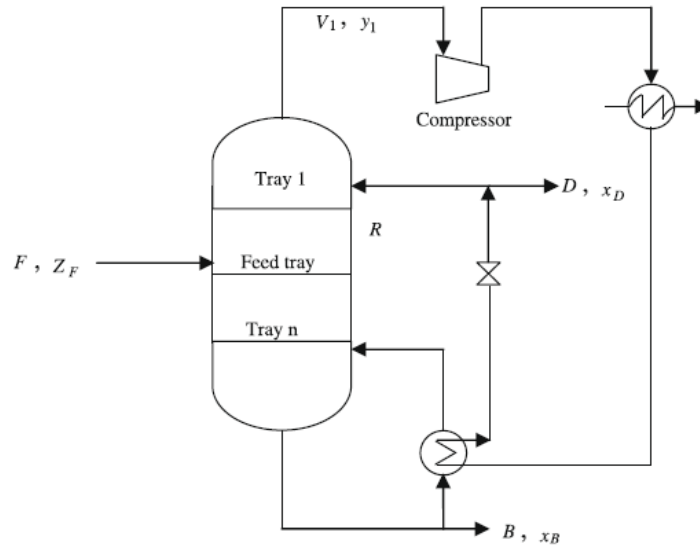
Figure 1.4. Schematic representation of a general VRC system[2]

A vapor recompression (VRC) system[14] utilizes energy from the overhead vapor, with additional mechanical energy from a compressor, to boil the bottoms liquid (Figure 1.4). The compressor duty strongly depends on the pressure ratio required to increase the temperature of the overhead vapor to a level that heat transfer from compressed overhead vapor to the bottom product becomes feasible. VRC designs are more efficient for systems requiring low increase in the energy quality of the overhead vapor (i.e., close boiling systems).[15] Moreover, since a VRC system requires only a single conventional column shell, it is generally the most practical way of implementing heat integration in an existing distillation system through revamping.

1.3. Scope and Objectives of this Project

The principle objective of heat integration in distillation columns is to achieve higher energy efficiency. The fundamental challenge in this respect is to develop a suitable design and a set of optimized operational parameters for a particular application.

Process simulation software allow low-cost yet reliable solution of complex engineering problems by expressing the behavior of the process using fundamental laws of conservation of mass, energy, and phase equilibria. Aspen Plus® has been leading the

development of process simulation models for a diverse range of unit operations. Steady state and dynamic simulations of various conventional and heat-integrated distillation columns using Aspen Plus® have been discussed at length by Luyben.[16]

This research project aims to use process simulation as a tool for a systematic comparison of various heat integration schemes in distillation columns with the objective of identifying the most exergy-efficient configuration. A conventional industrial-scale i-butane/n-butane fractionator has been selected as a case study for comparison of the performances of various heat-integrated designs. Aspen Plus® process simulator is used to perform steady-state simulations and exergy analyses of the CDC,[17-18] iHIDiC,[19] EHIDDiC,[20] and VRC[21] systems. The results of these exergy analyses provide a common basis for comparison of the alternative designs and guide the selection of the most suitable configuration.

1.4.   Organization of this Thesis

Chapter 2, "Literature Review", begins with an introduction to the conventional distillation column selected as case study. This is followed by a description of the salient features of the alternative heat-integrated designs considered in this project.

Chapter 3, "Exergy Analyses" begins with a detailed description of the procedure for calculation of the total exergy of a stream and the exergy efficiency of a system. The procedure is then applied to calculate the exergy efficiencies of the CDC, iHIDiC, EHIDDiC, and VRC systems.

Chapter 4, "Conclusions and Future Research Directions" summarizes important findings of this project and identifies directions for further research on the topic.

CHAPTER 2

LITERATURE REVIEW

2.1. Conventional i-Butane/n-Butane Fractionator

In this project, a conventional industrial-scale i-butane/n-butane fractionator has been selected as a case study for comparison of the performances of various heat-integrated designs. Because of the small relative volatility between the two key components, such columns require a large number of theoretical stages and must be operated at high reflux ratios leading to large column diameters and increased condenser and reboiler duties. These attributes make such separations an excellent target for process intensification studies.

The column under consideration is $51.8 \, \text{m}$ tall with a diameter of $2.9 \, \text{m}$ and contains 74 two-pass valve trays. It operates with a condenser pressure of $658.6 \, \text{kPa}$ and subcooled reflux at $18.5 \, °\text{C}$. Complete column specifications and performance data are listed in Table 2.1 and Table 2.2, respectively. The feed mixture (Table 2.3) contains a total of 8 components with i-butane and n-butane as the light and heavy keys, respectively.

Table 2.1. Column specifications[17-18]

Column height, m	51.8	Active area, m^2	4.9
Column diameter, m	2.900	Downcomer area (side), m^2	0.86
Number of trays	74	Downcomer area (center), m^2	0.86
Type of trays	Two-pass Ballast V-1 valve	Hole diameter, mm	39
Tray spacing, m	0.600	Total hole area, m^2	0.922
Tray thickness, mm	2	Outlet weir height, mm	51
Weir length (side), m	1.859	Number of valves per tray	772
Weir length (center), m	2.885	Free fractional hole area, %	18.82
Liquid flow length, m	0.967 per pass		

Table 2.2. Column performance data[17-18]

Feed tray	37th tray from top	Reboiler duty, MW	10.240
Column top pressure, kPa	658.6	Tray 01 temperature, °C	45.1
Feed pressure, kPa	892.67	Tray 09 temperature, °C	47.5
Pressure drop, kPa	0.47 per tray	Tray 65 temperature, °C	62.2
Reflux ratio	11.43	Tray 74 temperature, °C	63.2
Reflux temperature, °C	18.5		

Table 2.3. Reconciled data of stream compositions and flows[17-18]

	Feed	Distillate	Bottoms
Propane, wt. fraction	0.0154	0.0494	0.0000
i-Butane, wt. fraction	0.2950	0.9420	0.0300
n-Butane, wt. fraction	0.6770	0.0020	0.9810
i-Butene, wt. fraction	0.0013	0.0023	0.0008
1-Butene, wt. fraction	0.0020	0.0041	0.0010
neo-Pentane, wt. fraction	0.0011	0.0000	0.0017
i-Pentane, wt. fraction	0.0077	0.0000	0.0112
n-Pentane, wt. fraction	0.0008	0.0000	0.0011
Total flow, kg/h	26,122	8,123	17,999

2.2.   Internally Heat-Integrated Distillation Column (iHIDiC)

An iHIDiC (Figure 1.2) is a combination of direct vapor recompression and heat integration between two diabatic sections. Heat is transferred from the rectifying section to the stripping section through heat integration of one or more stages, which can be performed at any stage location along the column sections.[22] In addition, it is not necessary for rectifying and stripping sections to contain an equal number of stages.[23] The temperature driving force necessary for heat transfer between the two sections is created by manipulation of the compression ratio. The rectifying section thus operates at a considerably higher pressure than the stripping section. The iHIDiC is effectively a self-heat recovery system where heat-

integrated stages act as mid-way condensers and reboilers. This arrangement reduces the direct utility requirements of the main condenser and the main reboiler.

Because of the progressive evaporation of the descending liquid on heat-integrated stages, the vapor flow typically increases along the stripping section of an iHIDiC. On the other hand, progressive condensation of ascending vapor reduces the overall vapor flow in the rectifying section. In order to accommodate significantly varying vapor flows, the vapor flow area is often flexible along the length of an iHIDiC.[24]

Several heat transfer arrangements have been proposed for implementing heat integration in iHIDiC systems. These include inter-coupled distillation columns,[23] columns with side heat exchangers,[25] columns with partition walls,[26] concentric columns,[27] shell-and-tube exchanger columns,[28] plate–fin exchanger columns,[29] and SuperHIDiC.[30] In addition, heat integration can be distributed using uniform heat transfer area approach or uniform heat distribution approach.[10,31]

2.3. Externally Heat-Integrated Double Distillation Columns (EHIDDiC)

An EHIDDiC system (Figure 1.3) is essentially a modified iHIDiC system. In the iHIDiC, heat integration is arranged between the rectifying and the stripping sections of the same distillation column. On the other hand, in an EHIDDiC system, heat integration is arranged between the rectifying section of one distillation column and the stripping section of another distillation column.[12] This allows the two columns to operate at different pressures while simultaneously replacing the expensive vapor compression process with significantly cheaper liquid pumping operation.

The temperature driving force necessary for heat transfer is created by manipulation of the column pressures. In the so-called "neat mode", the feed split is manipulated to equalize the condenser duty of the HP column and the reboiler duty of the LP column. This arrangement combines the two operations and results in complete elimination of one heat exchanger. Heat

integration between the heat-integrated sections can also be achieved through strategically located external heat exchangers.[13] When the number of stages in the rectifying section of the rectifying section of the HP column and the stripping section of the LP column are equal, the configuration is known as symmetrical EHIDDiC.[13] The more flexible asymmetrical EHIDDiC configuration has unequal number of stages in the heat-integrated sections.

2.4. Vapor Recompression (VRC) System

In a VRC system (Figure 1.4), the overhead vapor is compressed to increase its temperature sufficiently above the bottoms liquid. The compressed superheated vapor is then used to boil the bottoms liquid in an integrated condenser–reboiler setup. The condensate is throttled to the column top pressure and provides necessary liquid reflux. The bottoms liquid is vaporized and provides necessary vapor boil-up.[14] VRC systems are well-suited for separation of close-boiling mixtures, where the difference between the condenser and reboiler temperatures is small, and small compression ratios are sufficient to heat the overhead vapor and create necessary temperature driving force for heat transfer.

CHAPTER 3

EXERGY ANALYSES

3.1. Methodology for Exergy Analysis

The total exergy of a material stream, $E[kW]$, is a product of its molar exergy, $e[kJ/mol]$, and molar flow rate, $\dot{m}[mol/s]$.

$$E[kW] = \dot{m}[mol/s] \cdot e[kJ/mol] \qquad \text{...(3.1)}$$

When kinetic and potential exergy terms are neglected, the molar exergy of a material stream includes only physical and chemical exergies.

$$e = e^{ph} + e^{ch} \qquad \text{...(3.2)}$$

The molar physical exergy, $e^{ph}[kJ/mol]$, of a material stream is calculated using its molar enthalpy and molar entropy relative to a reference environment.

$$e^{ph} = (h - h_0) - T_0(s - s_0) \qquad \text{...(3.3)}$$

where $T_0[K]$ is the reference temperature, and $P_0[Pa]$ is the reference pressure. $h[kJ/mol]$ and $h_0[kJ/mol]$ are molar enthalpies of the stream at actual conditions (T, P) and reference conditions (T_0, P_0), respectively. Similarly, $s[kJ/(mol \cdot K)]$ and $s_0[kJ/(mol \cdot K)]$ are molar entropies of the stream at actual and reference conditions, respectively. In this work, $T_0 = 298.15 \text{ K}$ and $P_0 = 101,325 \text{ Pa}$ have been selected as reference conditions.

The values of molar enthalpy and molar entropy at actual conditions are obtained from the converged steady-state simulation model. The corresponding values at reference conditions are determined by changing the temperature and pressure of the stream to reference conditions using a duplicator block coupled with a simple heater/cooler model.

Table 3.1. Standard chemical exergies of gas-phase components at
298.15 K and 101,325 Pa [32-33]

Component	$e^{ch} \, (kJ/mol)$	Component	$e^{ch} \, (kJ/mol)$
Propane	2154.00	1-Butene	2659.70
i-Butane	2803.41	neo-Pentane	3452.49
n-Butane	2805.80	i-Pentane	3452.70
i-Butene	2646.28	n-Pentane	3463.30

The molar chemical exergy, $e^{ch} \, [kJ/mol]$, of a material stream is a function of its composition.

$$e^{ch} = \sum x_i e_i^{ch} + RT_0 \sum x_i \cdot \ln x_i \qquad \ldots(3.4)$$

where x_i is the mole fraction of component i in the stream, $e_i^{ch} \, [kJ/mol]$ is the standard molar chemical exergy of component i, and R is the gas constant in appropriate units. The values of standard molar chemical exergies of all components in the system are listed in Table 3.1.

The total exergy of a thermal energy stream is calculated as

$$E_q \, [kW] = \left(1 - \frac{T}{T_0} \right) \cdot Q \, [kW] \qquad \ldots(3.5)$$

where heat load, Q, is positive when heat is added to the system (i.e., reboiler duty) and negative when heat is removed from the system (i.e., condenser duty).

The total exergy of a mechanical work stream is equal to the net shaft work.

$$E_w \, [kW] = W \, [kW] \qquad \ldots(3.6)$$

For a distillation column, the minimum amount of work, $\Delta E_{min} \, [kW]$, required for the separation is equal to the total exergy of product streams minus the total exergy of feed streams.[34]

$$\Delta E_{min} \, [kW] = \sum_{products} E_j - \sum_{feeds} E_i \qquad \ldots(3.7)$$

On the other hand, the actual work, $E_{act}[kW]$, consumed to achieve the same separation is the sum of exergies of utility loads.

$$E_{act}[kW] = \sum_{utilities} E_k \qquad \qquad \dots(3.8)$$

Exergy efficiency of a distillation column, η_E, is then calculated as

$$\eta_E[\%] = \frac{\Delta E_{min}}{E_{act}} \times 100 \qquad \qquad \dots(3.9)$$

3.2. Exergy Analysis of the Conventional Distillation Column

The simulation model of the CDC system has been adopted from the work of Kanwal.[19] In this model, the CDC system is simulated as an equilibrium-based RadFrac® column with Soave–Redlich–Kwong (SRK) property package using Aspen Plus® (Version 9.0). Stage efficiencies are adjusted to reproduce the reported data of column duties and stage temperatures (Table 2.2) and product compositions and flow rates (Table 2.3). Using the predicted stage efficiency of 137.9%, the number of theoretical stages in the conventional column is calculated to be 104. A new simulation model (Figure 3.1) is then developed containing 104 theoretical stages with 100% stage efficiency.

Table 3.2 summarizes the results of exergy analysis of the CDC system. As expected for a close-boiling mixture, the exergy efficiency of the CDC is very low (9.27%). This is due to large reflux ratio required to achieve this separation, which results in large condenser and reboiler duties.

3.3. Exergy Analysis of the Internally Heat-Integrated Distillation Column

The simulation model of the iHIDiC system has been adopted from the work of Kanwal.[19] In this model, the iHIDiC system is simulated using two equilibrium-based RadFrac® columns with Soave–Redlich–Kwong (SRK) property package using Aspen Plus® (Version 9.0). Each column contains 76 theoretical stages. A compression ratio of 1.60 is
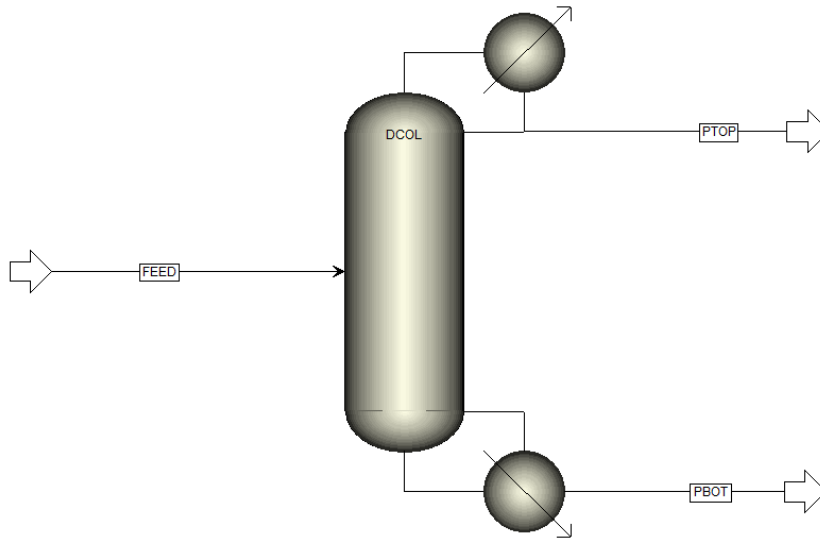
Figure 3.1. Schematic representation of the CDC model in Aspen Plus®[19]

Table 3.2. Exergy analysis of the CDC system

ID	$E(kW)$	ID	$E(kW)$
FEED	350,324	Exergy minimum	165
PTOP	108,979	Exergy actual	1,779
PBOT	241,510	Exergy efficiency (%)	9.27
QREB	1,193		
QCOND	–548		
QSUBC	–39		

maintained in the compressor. The columns are heat-integrated using uniform heat transfer area approach with three side heat exchangers. For simplicity, these side heat exchangers are modeled as side heat streams to the two columns (Figure 3.2). To make a fair comparison with the CDC system, all products are brought to the same thermodynamic conditions as obtained in the reference CDC simulation.

Table 3.3 summarizes the results of exergy analysis of the iHIDiC system. Surprisingly, the exergy efficiency of the iHIDiC system is very low (8.09%). In fact, it is even lower than the existing CDC system. A closer look at the results reveals that the heat integration indeed reduces both the condenser and the reboiler duties. However, the reduction in thermal energy
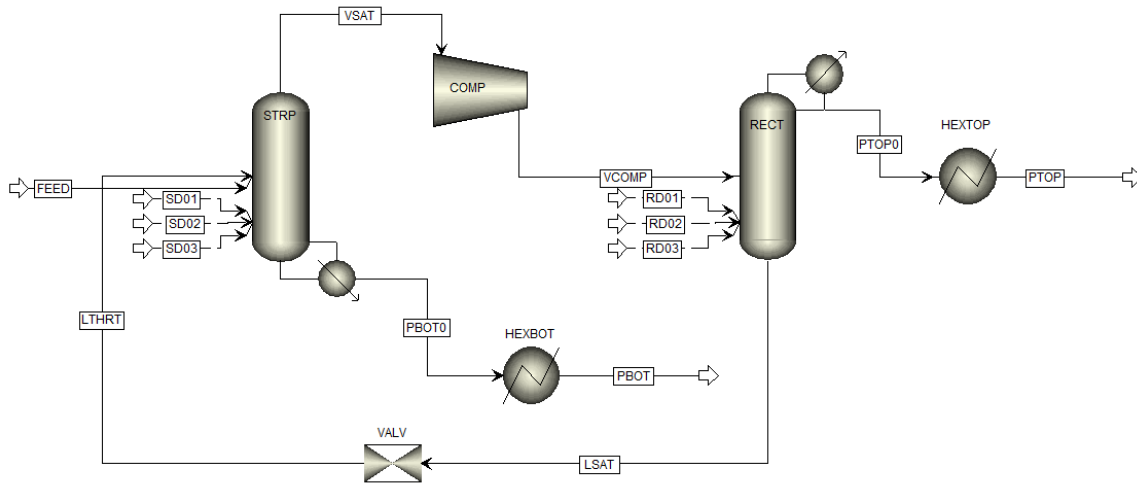
Figure 3.2. Schematic representation of the iHIDiC model in Aspen Plus®[19]

Table 3.3. Exergy analysis of the iHIDiC system

Stream	$E(kW)$	Summary	$E(kW)$
FEED	350,324	RD01	–311
PTOP	108,685	RD02	–306
PBOT	241,822	RD03	–578
QREB	466	SD01	247
QCOND	–461	SD02	253
QSUBC	–31	SD03	435
QHEXTOP	–7	Exergy min.	183
QHEXBOT	21	Exergy act.	2,269
WCOMP	1,283	Exergy efficiency (%)	8.09

duties is much smaller than the mechanical work of compression required to achieve this reduction. Since mechanical energy is a more refined form of energy as compared to thermal energy, the total utility requirements to achieve the same degree of separation are significantly higher, resulting in lower overall exergy efficiency.

3.4. Exergy Analysis of the Externally Heat-Integrated Double Distillation Columns

The simulation model of the EHIDDiC system has been adopted from the work of Sadaf.[20] In this model, the EHIDDiC system is simulated using two equilibrium-based
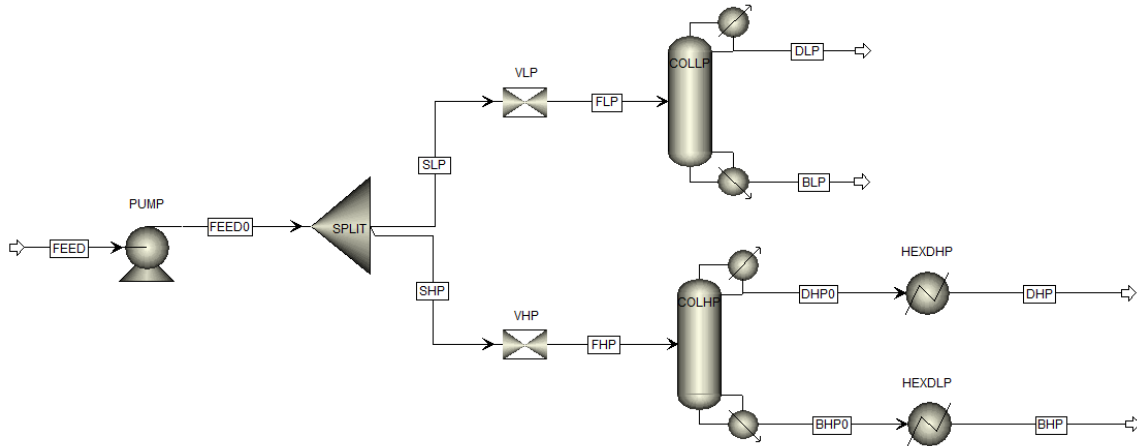
Figure 3.3. Schematic representation of the EHIDDiC model in Aspen Plus®[20]

RadFrac® columns with Soave–Redlich–Kwong (SRK) property package using Aspen Plus® (Version 9.0). The LP and the HP columns contain 119 and 173 theoretical stages, respectively. The LP column operates at the same conditions as the CDC, whereas the HP column operates at 2.5 times higher pressure to ensure a temperature driving force of $\geq 20\,°C$ between the condenser of HP column and the reboiler of LP column.

The feed is pumped to the pressure of the HP column before being split between the two columns (Figure 3.3). The feed split ratio is manipulated to operate the system in "neat mode" such that the duties of HP condenser and LP reboiler are equalized. Top and bottom product purities of both columns are constrained to match those obtained from the CDC system. In addition, to make a fair comparison with the CDC system, products from the HP column are brought to the same thermodynamic conditions as obtained in the reference CDC simulation.

Table 3.4 summarizes the results of exergy analysis of the EHIDDiC system. The overall exergy efficiency of the EHIDDiC system (9.77%) is considerably better than that of the existing CDC system. A comparison with the iHIDiC system reveals that the reduction in thermal energy duties is similar in both systems. However, the replacement of compressor (iHIDiC system) with pump (EHIDDiC system) considerably reduces the mechanical work requirements, leading to higher overall exergy efficiency.

Table 3.4. Exergy analysis of the EHIDDiC system

ID	E(kW)	ID	E(kW)
FEED	350,324	QCONDHP	638
DLP	44,805	QREBLP	443
DHP	63,961	Exergy minimum	174
BLP	99,551	Exergy actual	1,783
BHP	142,181	Exergy efficiency (%)	9.77
QREBHP	1,447		
QCONDLP	203		
QSUBCLP	14		
QSUBCHP	59		
QHEXDHP	10		
QHEXBHP	32		
WPUMP	19		

3.5. Exergy Analysis of the Conventional Vapor Recompression System

The simulation model of the conventional VRC system has been adopted from the work of Maria.[21] In this model, the VRC system is simulated using an equilibrium-based RadFrac® column with Soave–Redlich–Kwong (SRK) property package using Aspen Plus® (Version 9.0). The column specifications are same as the CDC system. The vapor stream leaving the top of the column is compressed and used to boil the liquid stream leaving the bottom of the column (Figure 3.4). A compression ratio of 2.0 is maintained in the compressor to ensure sufficient temperature driving force for heat transfer. A fraction of the partially-vaporized liquid stream leaving the integrated heat exchanger is drawn as bottom product, while the remainder is vaporized and fed to the column as vapor boil-up. The partially-condensed vapor stream leaving the integrated heat exchanger is throttled and completely condensed. A fraction is drawn as top product, while the remainder is subcooled and fed to the column as liquid reflux.
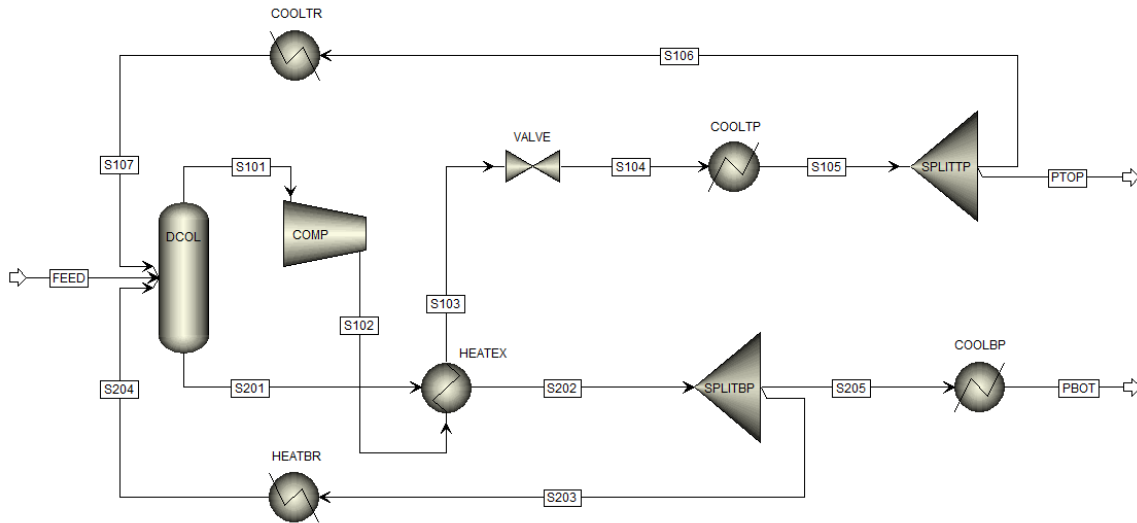
Figure 3.4. Schematic representation of the conventional VRC model in Aspen Plus®[21]

Table 3.5. Exergy analysis of the conventional VRC system

Stream	$E(kW)$	Summary	$E(kW)$
FEED	350,324	HEXVAP	1089
PTOP	108,705	HEXLIQ	851
PBOT	241,782	Exergy min.	164
QHEATBR	436	Exergy act.	1,765
QCOOLTP	143	Exergy efficiency (%)	9.27
QCOOLTR	38		
QCOOLBP	117		
WCOMP	1,031		

Table 3.5 summarizes the results of exergy analysis of the conventional VRC system. The overall exergy efficiency of the conventional VRC system (9.27%) is same as the existing CDC system. A closer look at the results reveals that the heat integration considerably reduces the thermal energy duties. In fact, this reduction in exchanger duties is even more pronounced than the iHIDiC system. However, the mechanical work of compression required to achieve this reduction in thermal energy duties is rather high, resulting in cancellation of the gains in exergy efficiency.
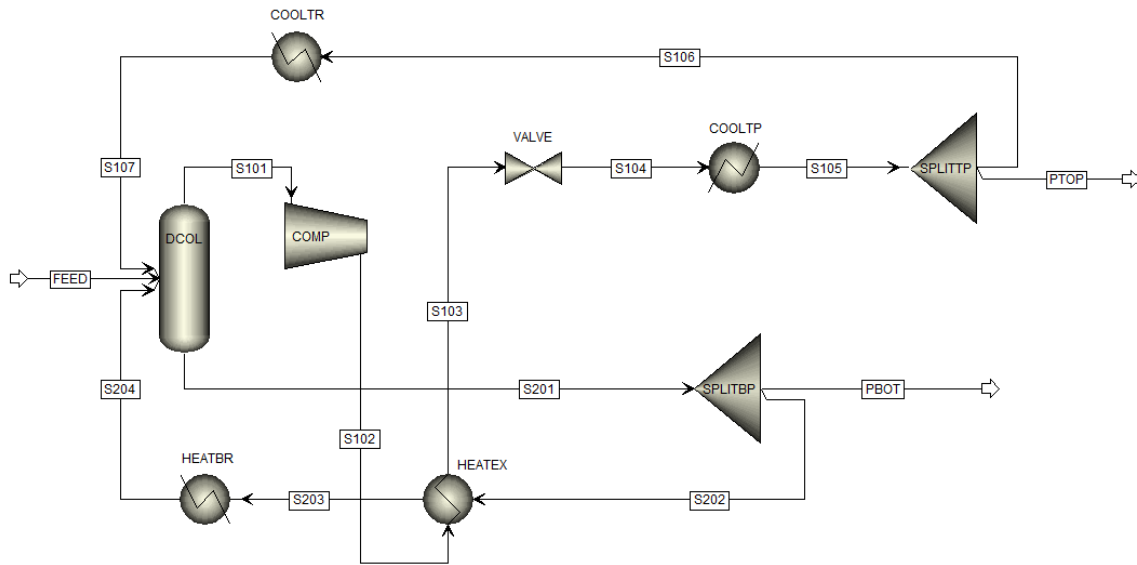
Figure 3.5. Schematic representation of the modified VRC model in Aspen Plus®[21]

3.6. Exergy Analysis of the Modified Vapor Recompression System

A closer look at the conventional VRC system (Figure 3.4) reveals poor heat transfer arrangement in the bottom loop. The whole liquid stream leaving the bottom of the column is boiled using compressed vapor, while only a fraction of it is to be sent back to the column. In other words, in the conventional VRC system, a fraction of the bottom liquid is first heated in the integrated heat exchanger, only to be cooled later as bottom product. A simple rearrangement in the bottom loop can fix this issue.

Figure 3.5 shows a schematic representation of the modified VRC system. Since the liquid stream leaving the bottom of the column is already at desired conditions, a fraction of it can be drawn as bottom product. The remaining fraction is first heated in the integrated heat exchanger using compressed vapor and then completely vaporized before being fed to the column as vapor boil-up. This arrangement not only eliminates one heat exchanger but also further reduces the thermal energy duties.

Table 3.6 summarizes the results of exergy analysis of the modified VRC system. As expected, pre-splitting of bottom liquid before integrated heat exchanger reduces the reboiler

Table 3.6. Exergy analysis of the modified VRC system

Stream	$E(kW)$	Summary	$E(kW)$
FEED	350,324	HEXVAP	1089
PTOP	108,705	HEXLIQ	851
PBOT	241,782	Exergy min.	164
QHEATBR	319	Exergy act.	1,531
QCOOLTP	143	Exergy efficiency (%)	10.69
QCOOLTR	38		
WCOMP	1,031		

Table 3.7. A comparison of the exergy efficiencies of various heat-integrated designs

System	Overall Exergy Efficiency	Improvement over CDC (Absolute)	Improvement over CDC (Relative)
CDC	9.27%	---	---
iHIDiC	8.09%	–1.18%	–12.76%
EHIDDiC	9.77%	0.51%	5.47%
VRC (conventional)	9.27%	0.00%	0.02%
VRC (modified)	10.69%	1.42%	15.32%

duty by the same amount as previously required to cool the bottom product. All other thermal and mechanical utility requirements remain the same as observed in the conventional VRC system. As the total utility requirements decrease, the overall exergy efficiency of the system increases to 10.69%.

3.7. Results and Discussion

Table 3.7 summarizes the results of exergy analyses of alternative heat-integrated designs for the i-butane/n-butane fractionator. It is obvious that selection of an appropriate heat integration scheme is critical for improving the overall exergy efficiency of the separation system. While all heat integration schemes explored in this project show an apparent reduction in total utility requirements, a proportional increase in overall exergy efficiency is not observed

in all cases. It is therefore important to account for both the magnitude as well as the quality of energy required for a given separation. For example, expending $1\,\text{MW}$ of mechanical energy in compression to achieve $1\,\text{MW}$ reduction in reboiler duty is impractical. Similarly, $1\,\text{MW}$ reduction in the duty of a water-cooled condenser at the expense of $1\,\text{MW}$ increase in the duty of a refrigerated condenser is impractical. Moreover, appropriate matching of hot and cold streams when implementing heat integration in a system is also critical. For example, a simple rearrangement of bottom loop in the VRC system not only eliminates one heat exchanger but also improves the overall exergy efficiency of the system by over 15% relative to the conventional distillation column.

CHAPTER 4

CONCLUSIONS AND FUTURE RESEARCH DIRECTIONS

4.1.   Conclusions

Simulation studies have shown that heat integration in distillation processes is a promising technology with potential for significant energy and cost savings. However, most studies have directly compared the total utility requirements for alternative designs without consideration for the quality of energy involved. Since exergy provides a measure of both the quantity and quality of energy available in a process, exergy efficiency is a more suitable measure for comparison of alternative designs.

In this study, a conventional industrial-scale i-butane/n-butane fractionator has been selected as a case study for comparison of the exergy efficiencies of various heat-integrated designs. While all heat integration schemes explored in this project show an apparent reduction in total utility requirements, a proportional increase in overall exergy efficiency is not observed in all cases. These results show that when comparing alternative designs, the type of energy (e.g., thermal or mechanical) as well as the temperature at which a utility is required must be taken into consideration. Moreover, appropriate matching of hot and cold streams when implementing heat integration in a system is also critical.

Based on overall exergy efficiency, a modified VRC system $\left(\eta_E = 10.69\%\right)$ is the most efficient design for this separation, achieving almost 15% higher exergy efficiency relative to the existing CDC system. Exergy efficiency of the conventional VRC system is same as that of the CDC $\left(\eta_E = 9.27\%\right)$. EHIDDiC system $\left(\eta_E = 9.77\%\right)$ is somewhat better than the CDC, whereas iHIDiC shows poor exergy efficiency $\left(\eta_E = 8.09\%\right)$, even lower than the CDC.

4.2. Future Research Directions

Thermodynamic performance evaluation of various heat-integrated distillation designs has been the primary focus of this project. Other areas of interest identified during this project include:

1. Effect of operational parameters (e.g., compression ratio) on overall exergy efficiency may be explored.

2. Topological changes in the flowsheet (e.g., number and location of heat-integrated stages in the iHIDiC system) remain to be studied.

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