

Novel retrofit designs using a modified coordinate descent methodology for improving energy efficiency of natural gas liquid fractionation process



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ABSTRACT

Tough environmental regulations, intense competition, expensive fossil energy use, and the strong growth predictions of the natural gas market have prompted efforts to retrofit the existing purification processes to reduce their energy requirements. The important goals of retrofit design are to analyze, evaluate and propose suitable technologies to improve the energy efficiency and/or increase the capacity. This paper reports the results of a techno-economic feasibility study to retrofit a natural gas liquid (NGL) fractionation process. A novel hybrid system, side reboiler and heat pump-assisted, thermally-coupled distillation sequence to maximize the energy efficiency, was proposed. Fractional utilization of the area was used as a hydraulic performance indicator to determine if a bottleneck occurs in a retrofit design. A modified coordinate descent methodology was employed to solve the optimization problem. As a result, the modified coordinate descent methodology was successful in finding the optimal proposed sequence structure and the operating variables, which resulted in operating cost savings of 44.55% compared to the representative base case. The short payback period of 14 months and reduced CO₂ emissions of up to 42.05% showed that the proposed sequence is an attractive option for retrofitting in industrial implementation. This sequence can be employed for both grass-root and retrofit designs. This study also showed that even the heat pump can reduce the energy requirements significantly, and may have higher exergy loss than the existing conventional distillation columns.

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1. Introduction

Natural gas (NG) is used primary as a fuel and as an important source of hydrocarbons for petrochemical plants. NG is also a major source of elemental sulfur, which is an important industrial chemical (Long and Lee, 2013a; Kidnay and Parrish, 2006). The continued demand for natural gas can be ensured because of clean burning and satisfying the stringent environment requirements (Elliot et al., 2005). The fractionation of NGL is economically attractive because its products can be sold separately. On the other hand, the large-energy consumption, increasing energy costs and tighter environmental regulations have increased the demand to

maximize the energy efficiency of the separation in this process, which normally accounts for approximately 60% of the total manufacturing costs (Knapp and Doherty, 1990; Malinenand and Tanskanen, 2009; Hamidzadeh and Salehi, 2012). Therefore, several methods have been proposed to improve NGL fractionation from a feed gas (Mak, 2006; Long and Lee, 2012a). Accordingly, studies not only at the grass-root level but also in the retrofit of existing NGL process are needed. In particular, distillation, which has many advantages, has the disadvantage of a large energy requirement (Halvorsen and Skogestad, 2011), and requires retrofitting to increase the efficiency in energy utilization and reducing the operating cost. Several studies have focused on retrofitting the demethanizer to reduce energy or achieve high ethane recovery (Shin et al., 2015; Lynch et al., 2003; Bai et al., 2006; Hernandez-Enriquez and Kim, 2009) while retrofit of the deethanizer, depropanizer, debutanizer, and deisobutanizer is needed.

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A retrofit project of a distillation process is generally considered over a wide range. Simple modification, such as adjusting the operating conditions or replacing a column internal, to significant modifications of the distillation columns or sequence, or adding a new column or equipment can be considered (Liu and Jobson, 2004a; Long and Lee, 2013b). In any case, a successful retrofit project is normally based on the maximum employment of existing equipment to reduce the investment cost (Long et al., 2010). The rearrangement of existing columns to complex column arrangements, such as the Petlyuk column and prefractionator arrangement, have been proposed for retrofitting (Amminudin and Smith, 2001). Similarly, addition of a new column, such as a post-fractionator or prefractionator, could also provide a process debottlenecking option (Liebman, 1991). Adding a new wall to the middle of a column to form a dividing wall column (DWC) might be an attractive option for process debottlenecking (Long et al., 2010, 2013). Several guidelines for retrofit the distillation sequence were proposed (Long and Lee, 2011). To choose the best sequence for retrofit, it is necessary to consider the whole process, including feed conditions, component characteristics, number of trays, column internal, column hydraulics, operating conditions, equipment lifetime, construction material, and feasibility of a combination of columns to make a complex re-arrangement and retrofit to the DWC.

Recently, the relative advantages of the thermally-coupled distillation sequence (TCDS) has highlighted the substantial potential for improving the energy efficiency (Nguyen and Demirel, 2011; Long and Lee, 2013a, 2015). These studies reported that TCDS systems can gain significant energy savings compared to conventional distillation sequences. When the cooling sources in the two columns, including one source coming from refrigeration, are different and the refrigeration cost is quite high, it is not desirable to integrate two columns to one DWC. The TCDS has to be considered (Long and Lee, 2011). Furthermore, retrofit projects using TCDS have attracted considerable attention owing to the easy design, small modification and short time (Long and Lee, 2013c). Note that in many retrofit projects, downtime is the largest economic factor as it leads to a loss of production and an interruption of product supply to customers (Amminudin and Smith, 2001).

On the other hand, a bottleneck can occur in the main column of retrofitted TCDS, which can be removed effectively by using a side reboiler (SR) or a side condenser (SC). One advantage of using a SR is that the difference between the top temperature and that in the SR location is smaller than the difference between the top and bottom temperature, which motivates the use a heat pump (HP) to recover the heat from the overhead to transfer to the SR. Similarly, the temperature difference between SC location and bottom is smaller than that between column top and bottom. This bring a good chance for employing a HP, which allows the recovery of heat released from the SC to be used to boil the liquid in the reboiler. Thus, in general a combination of a SR and HP system with a TCDS is expected to save operating cost significantly and remove bottleneck problem effectively.

In this paper, a sequence was proposed to retrofit the NGL fractionation process using TCDS and HP to improve the energy efficiency. A two-distillation sequence, a novel hybrid system—side reboiler and heat pump-assisted, thermally-coupled distillation sequence (SRHPTCDS), was proposed to reduce the energy requirements significantly. Fractional utilization of the area (FUA) was used as an effective hydraulic performance indicator to illustrate the performance of the hydraulic condition of the distillation column in the retrofit design. The design and optimization procedures using the linking of Hysys and Excel were employed for retrofit design with particular emphasis on simple and efficient efforts. In particular, a modified coordinate descent methodology

(MCD), which can handle both structure and operating variables simultaneously, was used to solve the process optimization problem. Furthermore, exergy loss and carbon dioxide (CO₂) emissions were considered and calculated when retrofitting an existing NGL process to the proposed sequence.

2. Methodologies

2.1. Retrofit assumptions

Because distillation is a separation process requiring large energy consumption and capital investment, distillation retrofit projects are performed more often than the grass-roots projects (Gadalla et al., 2003). In this paper, the retrofit purpose was performed to improve the energy efficiency in the NGL fractionation process with the following assumptions: all columns are already fully used; the highest performance internals are already employed in all existing distillation columns; all products are kept constant in terms of recovery and purity in retrofit design.

2.2. Thermally coupled distillation sequence

Direct and indirect conventional distillation sequences are normally used to separate ternary mixtures into light (A), intermediate (B) and heavy (C) components. These two sequences are well-known, easy to control and operate, and are familiar to the operators. On the other hand, the energy efficiency is low because of the mixing entropy occurring in the first column by the irreversible split (Asprion and Kaibel, 2010). The TCDSs were obtained by implementing the interconnecting vapor and liquid streams with the second column (Fig. 1) (Long and Lee, 2012b). Each interconnection replaces one reboiler and one condenser in the side rectifier and side stripper, respectively. Such systems for saving substantial investment and operating cost compared to conventional distillation sequences have attracted considerable attention from academia and industry.

2.3. Heat pump

Distillation processes, which involve separating liquid mixtures based on the differences in boiling point, are run by supplying heat to a reboiler to generate vapor flow (Kiss, 2014). Mostly, the heat is released from the condenser causing low energy efficiency (Karaca et al., 2002). Using HPs in distillation, the condensation heat can be used for evaporation in the reboiler (Karaca et al., 2002; Díez et al., 2009).

Energy conservation is more attractive when separating close-boiling mixtures or the temperature difference between the top and bottom of the column is small and the heat load is high because of the minimal compressor/compression cost (Kiss et al., 2012; Suphanit, 2011; Bruisma and Spoelstra, 2010). For wide-boiling mixtures, a side heat pump (SHP) or a SR can be considered to overcome the problems related to the high compressor cost. HP can also be in both grass-roots projects and retrofit designs because it is easy to implement and does not affect the traffic of vapor and liquid in the column when it is installed in the top of the column (Long and Lee, 2013d). However, reactions or polymerization can occur with increasing vapor temperature when a HP is employed (Long and Lee, 2014). Therefore, engineers should also be aware of the decomposition or polymerization of components, which are sensitive to temperature when the vapor pressure is increased using a HP.

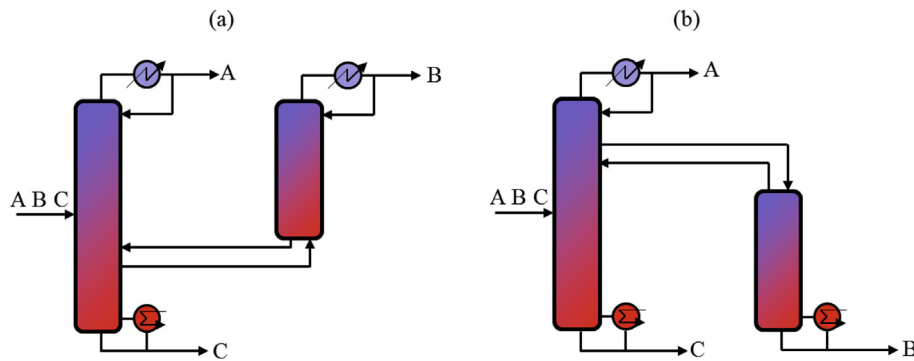


Fig. 1. Schematic diagram of the TCDs: (a) system with a side rectifier and (b) system with a side stripper.

2.4. Fractional utilization of area

In most of retrofit projects, the column diameter is fixed. Information of the hydraulics for each tray, which is primarily influenced by the upper operational limit of the operating column, is necessary for preventing flooding and determining at which stage(s) should the traffic of vapor and liquid flow be decreased, and at which stage(s) can these flows be increased during retrofit design. In this paper, the FUA introduced by Liu and Jonson (Liu and Jobson, 2004a, 2004b), which is associated with the area to handle vapor flow to prevent flooding, was used. The indicator allows the identification of bottlenecks, as well as an evaluation of the modifications proposed to remove these bottlenecks. The FUA is calculated as follows:

$$FUA = \frac{\text{Area required on stage } i \text{ for vapor flow}}{\text{Area available on stage } i \text{ for vapor flow}} \quad (1)$$

where the area required for vapor flow is determined by setting the vapor velocity is 85% of the flooding velocity in a simulator (Long and Lee, 2015).

2.5. Modified coordinate descent methodology

Designing SRHPTCDS is more complex than conventional arrangements because of the greater number of degrees of freedom. These degrees of freedom interact with each other and need to be optimized simultaneously for optimal column design. A common difficulty is estimating the number of stages in each section. Since the number of stages is an integer variable, column optimization is a mixed integer non-linear programming problem (MINLP), which cannot be solved with commercially available process simulators (Dejanović et al., 2010). External optimization routines are therefore required to be coupled with process simulators. Furthermore, solving the MINLP does not guarantee finding the global optimum in a non-convex problem. Furthermore, this method is quite complex and easily causes the unconverged problem in simulation. A more simple, practical and efficient method is needed to solve the optimization problem.

The modified coordinate descent (MCD) methodology is based on the idea that the optimization of any multivariable function is performed by minimizing the objective function along one coordinate at a time (Venkataraman, 2009). This method is different from the CD methodology in obtaining a local optimal solution and randomizing the search after obtaining a local solution. The main advantages of the MCD methodology lie in the simplicity of each iteration, simple implementation and high efficiency. Thus, this methodology can be suitable for the optimization of highly non-linear and complex sequence in the retrofit of the existing NGL

fractionation process. The proposed methodology shown in Fig. 2 begins by choosing a random candidate solution of the decision variables given by Eq. (2) as the initial starting point (Li and Rhinehart, 1998):

$$X_0 = \{x_1^0, x_2^0, \dots, x_n^0\}^T \quad (2)$$

To obtain the search direction within the vicinity of the starting point, a sufficiently small step size, Δx_i , is prescribed in each of the coordinate directions, u_i , $i = 1, 2, \dots, n$. Obtaining an optimal solution depends strongly on step size selection because a small step size can linger in local points, whereas a large step size can miss a potential solution (Srinivasan et al., 2008). Utilizing the provided step size, and a randomly chosen starting point, X_0 , exploratory steps similar to a pattern search are made to find the base point. Once a base point is obtained, cyclical iterations are performed through each coordinate individually, by minimizing the objective function with respect to the individual coordinate direction. If X^k is given, the i th coordinate of x_i^{k+1} is given by Eq. (3).

$$x_i^{k+1} = \operatorname{argmin}_{y \in R} (x_i^{k+1}, \dots, x_{i-1}^{k+1}, y, x_{i+1}^k, \dots, x_n^k) \quad (3)$$

An iteration of all different directions or coordinates is performed cyclically to determine the descent direction, which is equivalent to a gradient descent. After performing a line search on all coordinates, a new candidate solution update from X_0 to X_1 , $F(X_0) \geq F(X_1)$, is obtained. Assuming X_1 as the new starting point, the coordinate descent search is performed over the narrow space or the so-called box space with a smaller step size around X_1 to find more promising solutions in the immediate vicinity of X_1 . An imaginary space of given dimensions is formed around X_1 and is explored in case a previous search had overlooked some of the potential solutions to ensure the optimum within the box space with a given step size. After obtaining the locally optimal solution, $f(X'_1)$, an update from $f(X_1)$, the first coordinate of X'_1 (rand, 2, 3, ..., n), is randomized while fixing the others to their previous obtained optimal values. The coordinate descent search is performed using X'_1 (rand, 2, 3, ..., n) as the new starting value, and the optimal space around X_2 is explored further in box space to obtain a new optimal solution, X'_2 . This time, the second coordinate of X'_2 (1, rand, 3, ..., n) is randomized and search moves are made. Therefore, a number of locally optimal solutions can be obtained in this manner. The search is terminated if the same solutions are obtained repetitively within the function tolerance. The termination criterion is a user defined value. Repetition of the same results requires more computational time, whereas less repetition may overlook some potential solution. Therefore, the stopping criterion can be adjusted based on the objective function. A more detailed

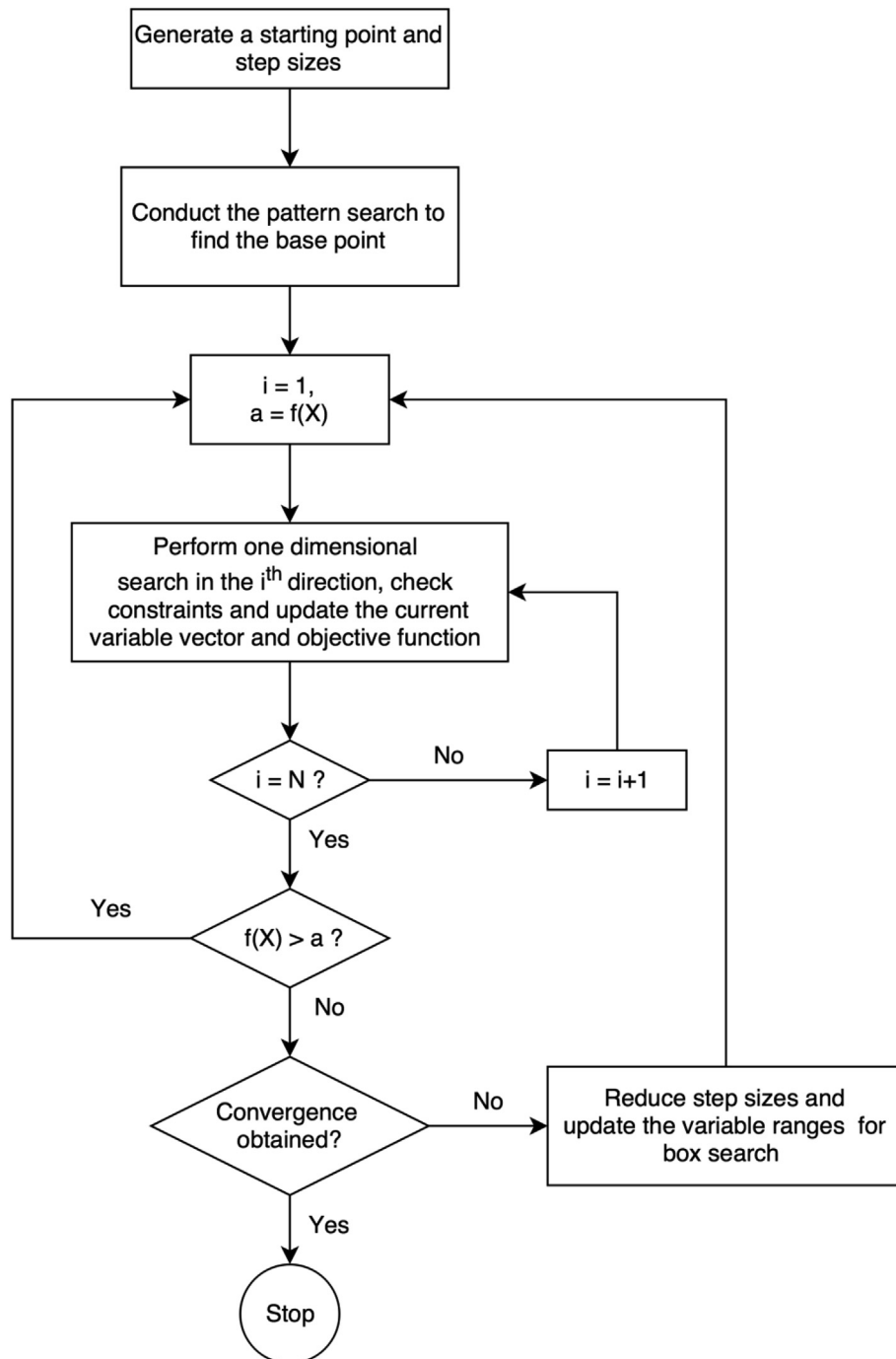


Fig. 2. Optimization algorithm for MCD approach.

description of the MCD methodology can be found elsewhere (Park et al., 2014).

3. Case study

3.1. Existing conventional column sequence

NGL is typically separated and purified into relatively pure products, such as ethane (C_2), propane (C_3), isobutane (iC_4), normal butane (nC_4), and gasoline products (C_{5+}). Normally C_2 , C_3 and C_4 are distilled from gasoline before separating iC_4 and nC_4 in the

distillation sequence. Fig. 3 shows the existing conventional distillation sequence as well as the operating conditions for each column (Amminudin and Smith, 2001; Manley, 1997). A refrigerated condenser is required in the NGL deethanizer column when producing relatively pure ethane. The deethanizer was operated at very high pressures of approximately 31.0 bar to minimize the refrigeration costs, while the depropanizer is designed at 17.50 bar. The debutanizer is designed with 40 trays, whereas the deisobutanizer has 92 trays to separate iC_4 from nC_4 , which is a close-boiling mixture (Amminudin and Smith, 2001; Manley, 1998). Table 1 lists the feed conditions. Aspen HYSYS V8.4 was used to

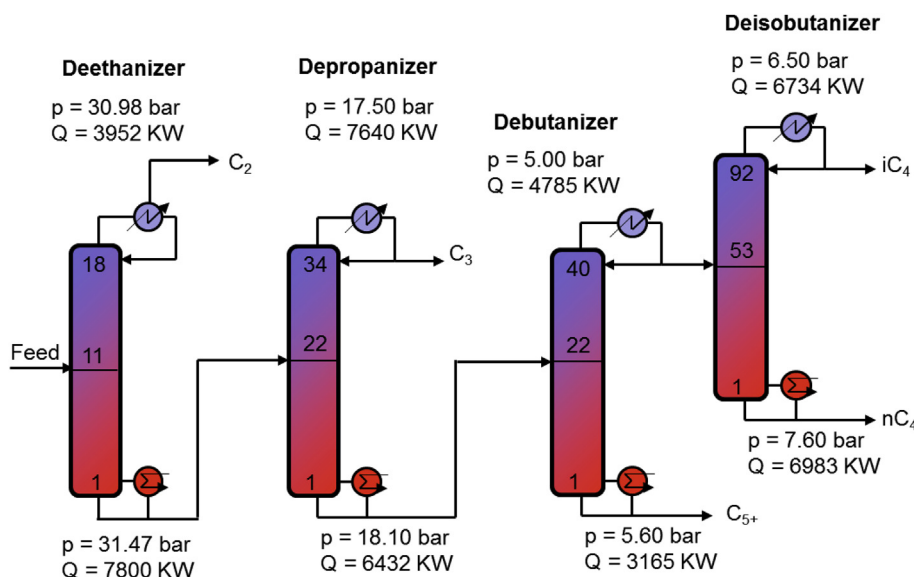


Fig. 3. Simplified flow sheet illustrating the separation train of four conventional columns.

Table 1

Feed conditions of the mixture.

Feed conditions	
Component	Mass flow [kg/hr]
Methane	267.15
Ethane	23485.72
Propane	23509.56
<i>i</i> -Butane	7220.74
<i>n</i> -Butane	15404.07
<i>i</i> -Pentane	5562.95
<i>n</i> -Pentane	3933.33
<i>n</i> -Hexane	4730.34
<i>n</i> -Heptane	2451.37
Temperature (°C)	55.83
Pressure (bar)	31.37

simulate the conventional and proposed process as well as to determine the FUA value, while Aspen Plus was used to obtain exergy loss of distillation. The Peng-Robinson equation of state was used to calculate the vapor-liquid equilibria (Aspen Technology, 2009). Table 2 lists the column conditions, condenser and reboiler

duty as well as the products purity.

3.2. Proposed sequence for retrofit

3.2.1. Integration of the deethanizer and depropanizer

As mentioned above, in general a combination of a SR and HP system with a TCDS is expected to save operating cost significantly and remove bottleneck problem effectively. Fig. 4 presents the general novel retrofitted system – SRHPTCDS, which is constructed by adding the vapor and liquid streams between the two columns. Vapor from the distillation overhead is compressed using a compressor to increase its vapor temperature so that it can transfer the heat to the SR through a heat exchanger. To optimize the structure and operating conditions of the proposed sequence, some variables, such as the vapor flow (FV), liquid flow (FL), feed (N1), vapor (N2), and liquid (N3) stream locations, were varied. The MCD implemented in the MS Visual basic application and connected to the Hysys model via the MS Excel platform was employed to examine their effects on the operating cost of the SRHPTCDS. Excel worksheets and Excel Macro were employed to interface and calculate the objectives as well as implement the optimization

Table 2

Column hydraulics, energy performance and product specifications of the conventional column sequence.

	Deethanizer	Depropanizer	Debutanizer	Deisobutanizer
Number of trays	18	34	40	92
Tray type	Sieve	Sieve	Sieve	Sieve
Column diameter (m)	3.1	2.4	1.8	2.3
Number of flow paths	1	1	1	1
Tray spacing (mm)	609.6	609.6	457.0	457.0
Condenser duty (kW)	3952	7640	4785	6734
Reboiler duty (kW)	7800	6432	3165	6983
Annual operating cost (US \$)	3,766,776	2,740,456	1,359,791	2,958,053
Exergy loss (kW)	853	723	273	231
Annual CO ₂ emission (kg)	14,958,340	12,334,877	6,069,634	13,391,550
Purity (mole %)				
C ₂	94.48			
C ₃	90.30			
<i>i</i> C ₄	99.00			
<i>n</i> C ₄	95.00			
C ₅₊	99.00			

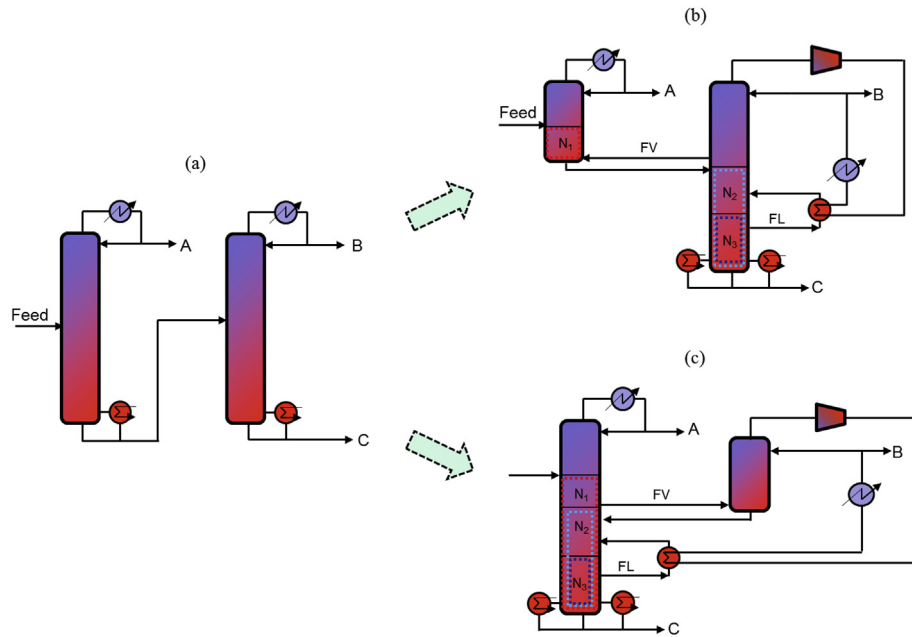


Fig. 4. Simplified flow sheet illustrating the retrofitted hybrid system including TCDS with a top vapor recompression HP and SR.

algorithm. Table 3 provides details of the decision variable bound, constraints and objective.

The lowest operating cost was observed at FV, FL, N1, N2, and N3 values of 55,465, 42,607, 11, 6, and 12, respectively. Fig. 5 presents a simplified flow sheet illustrating the proposed SRHPTCDS. The optimization results from the MCD methodology represent the refrigeration duty (deethanizer), cooling-water condenser duty (depropanizer) and reboiler duty savings of 4.76, 83.04 and 54.08%, respectively, compared to the existing sequence. As a result, an operating cost saving of 39.2% can be obtained, which is much higher than the simulated result estimated from the response surface methodology proposed by Long and Lee (29.7%) (2013a). Table 4 lists the utility cost data (Turton et al., 2012). Fig. 6 shows the FUA curve, as a graphical display of the hydraulic performance. The FUA value at each stage is different and smaller than 1. This suggests that there is no flooding problem in the column when retrofitting the hybrid system.

Fig. 7 presents the composition profiles of ethane and propane in the existing depropanizer and main column of the proposed sequence. In the bottom section, a portion of the liquid stream is vaporized to the vapor phase. This causes an increase in the intermediate component (C_3) composition profile and a decrease in the heavy component (C_{4+}) composition profile. The reverse phenomenon occurs in the top section: a decrease in the intermediate component (C_3) composition profile and an increase in the heavy component (C_{4+}) composition profile. As a result, the temperature profile is increased in the top section while that in the bottom section is reduced compared to that in the existing depropanizer (Fig. 8). This suggests that TCDS offers a preferential profile

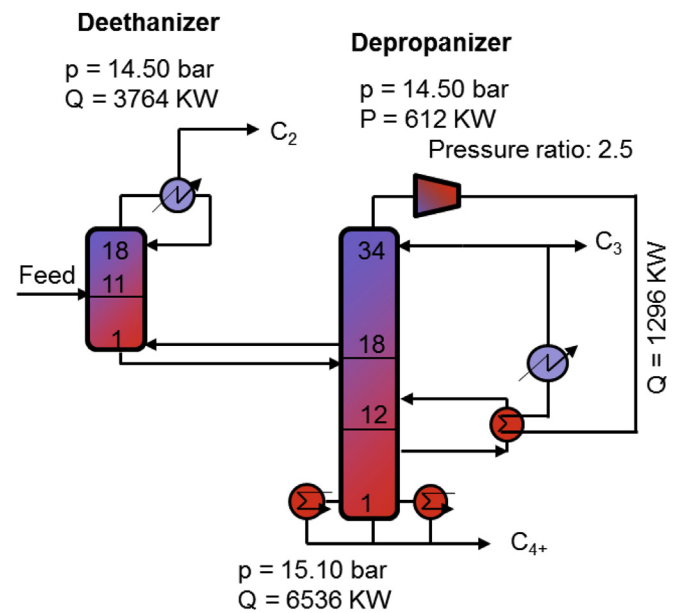


Fig. 5. Simplified flow sheet illustrating the retrofitted hybrid configuration for a deethanizer and depropanizer.

structurally for a HP configuration. In addition, the use of a TCDS can reduce the reboiler duty, which can also reduce the compressor duty. These two synergetic effects by TCDS improve the

Table 3
Optimized variables, constraints and objective details.

Decision variables	Lower bounds	Higher bounds	Constrained values	Optimization objective
FV (kg/hr)	54,000	58,000	Reboiler duty < 8000 KW (to prevent flooding)	Operating cost minimization
FL (kg/hr)	40,000	44,000	C_2 purity $\geq 94.48\%$	
N1	8	12	C_3 purity $\geq 90.30\%$	
N2	15	20		
N3	5	15		

Table 4
Utilities cost data.

Utility	Price (\$/GJ)
Cooling water	0.35
Steam	13.28
Refrigeration (moderately low temperature) (Available at $T = 5\text{ }^{\circ}\text{C}$)	4.43
Refrigeration (low temperature) (Available at $T = -20\text{ }^{\circ}\text{C}$)	7.89
Electricity	16.80

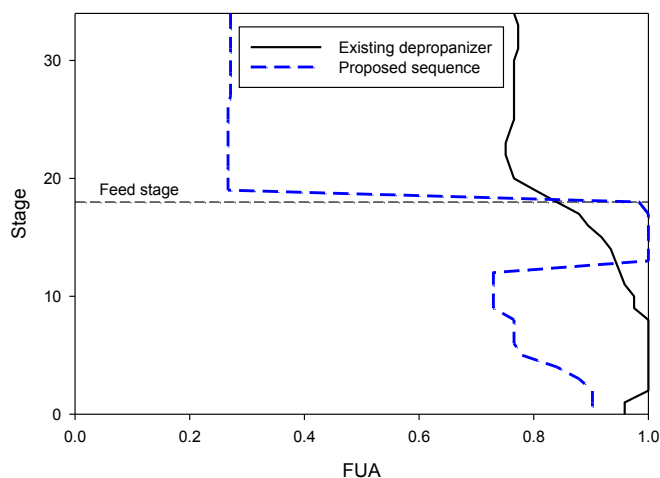


Fig. 6. FUA profiles of the existing depropanizer and main column of the proposed sequence.

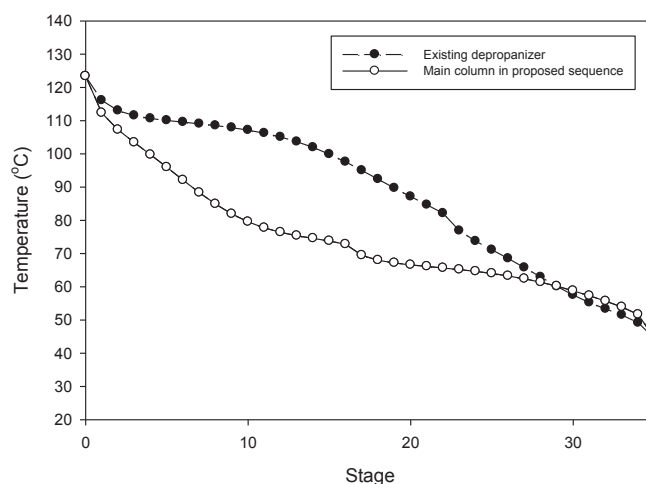


Fig. 8. Temperature profile of the existing depropanizer and the main column of the proposed sequence.

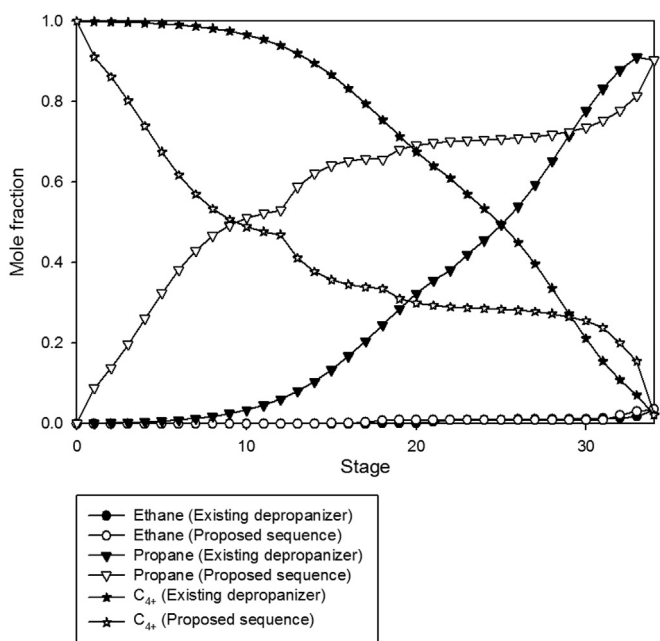


Fig. 7. Composition profiles in the existing depropanizer and main column of the proposed sequence.

performance of the HP dramatically. Note that it is not recommended to use a heat pump system only to recover the heat from top vapor stream to boil the liquid in the reboiler in this case due to large temperature difference.

Exergy loss is also considered when retrofitting the conventional column sequence to the proposed sequence. The

introduction of a thermal link can enhance the second law efficiency in terms of the exergy loss. The HP can upgrade low quality energy to allow the recovery of heat to drive the reboiler of the column. Although it can reduce the energy requirements significantly, it has higher exergy loss in unit operations, such as compressor, heat exchanger, cooler, trays, reboiler instead of condenser, reboiler, and trays in a conventional distillation column. Exergy loss was considered in the entire proposed sequence because the proposed sequence includes both effects from the thermal coupling technique and HP. In particular, the exergy loss reduced from 1576 kW to 1436 kW, which brings a save up to 8.88% when retrofitting the deethanizer and depropanizer to SRHPTCS system.

3.2.2. Integration of debutanizer and deisobutanizer

Because the heat load in the deisobutanizer is high and the difference between the top and bottom temperature ($\sim 19\text{ }^{\circ}\text{C}$) is low, implementing a HP system can be an attractive option for retrofitting a deisobutanizer. The top vapor stream of the deisobutanizer column is compressed with a pressure ratio of 2.0 to drive the reboiler. Note that the minimum approach temperature, ΔT , is chosen at $10\text{ }^{\circ}\text{C}$. This allows the heat to be recovered and used instead of being released to the environment. This can reduce the steam and CO_2 emissions. Furthermore, the top vapor stream of the debutanizer consists of two main components, $i\text{C}_4$ and $n\text{C}_4$, so the temperature of this stream is similar to the vapor from the deisobutanizer. In addition, this stream has a high heat load, which has the potential to employ a HP system. No change was observed in the composition of the produced products. Fig. 9 shows the proposed sequence to retrofit the debutanizer and deisobutanizer. The adiabatic efficiency of 75% was used to simulate and calculate all the compressors. Only 3165 kW steam is used in debutanizer, while 6983 kW in deisobutanizer can be saved by supplying 1306 kW

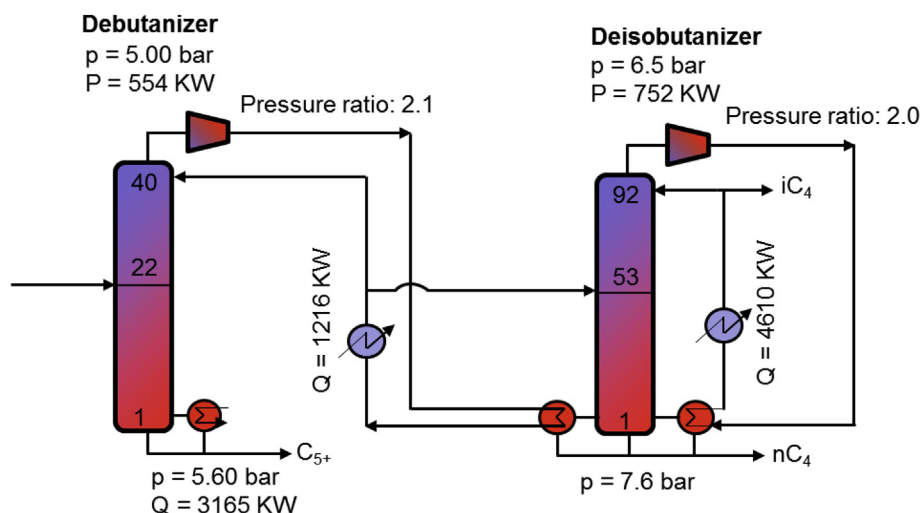


Fig. 9. Simplified flow sheet illustrating the retrofitted sequence of the debutanizer and deisobutanizer.

electricity to run two HP systems. As a result, the proposed configuration containing two top vapor recompression HP systems can save up to 68.80 and 52.58% of the reboiler energy and operating costs, respectively, compared to the existing conventional sequence.

3.2.3. Final proposed sequence for retrofit NGL sequence

Retrofitting the NGL fractionation process (Fig. 10) can improve the plant efficiency and reduce costs substantially. In particular, the annual operating cost of conventional distillation sequence is 10,825,076 US \$ while that of proposed sequence is only 6,002,787 US \$, respectively. As a result, the use of the modified sequence can bring up to 44.55% improvement in operating costs. With the proposed sequence, 5,605,554 USD is needed to invest, which requires simple payback period of 14 months. This payback period is economically attractive because existing equipment is maximally utilized. Note that the economics of each configuration depend largely on the utility costs, which differ according to the country and company. Fig. 11 shows the effect of the electricity/steam cost ratio on the operating cost saving of the proposed sequence. This sequence is more advantageous when the electricity/steam cost ratio decreases.

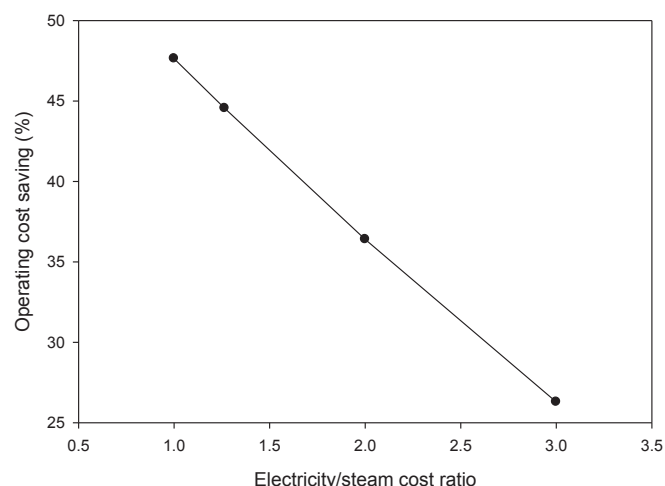


Fig. 11. Effect of the electricity/steam cost ratio on the operating cost saving of the proposed sequence.

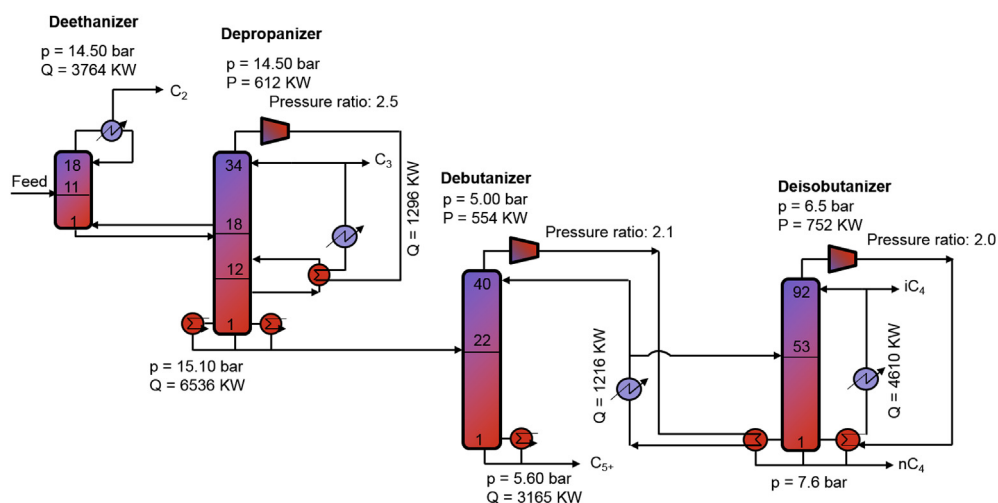


Fig. 10. Simplified flow sheet illustrating the proposed sequence to retrofit the NGL process.

However, due to high exergy loss (2491 kW), the exergy loss is increased by 19.70% as compared to conventional distillation sequence, and even the operating costs are reduced by 44.55%. In particular, instead of considering the exergy loss in a condenser, reboiler and trays in conventional distillation, it should be checked in the compressor, heat exchanger, reboiler or condenser, heater or cooler, and trays. Note that the exergy loss in the trays does not change if only a HP is used in the top of the column. The results show that decreasing energy consumption does not always reduce the exergy loss.

The CO₂ emission reduction associated with the lower energy requirement is another important benefit of using the proposed sequence in the retrofit of a NGL process. The method reported by Gadalla et al. (2005) was used to estimate the CO₂ emissions. The study results showed that CO₂ emissions can be reduced dramatically when distillations are intensified by a thermal coupling technique and a part of the process heat is recovered for use instead of the primary steam. In particular, the annual amount of CO₂ emissions is reduced from 46,754,400 kg to 27,095,052 kg, which brings a reduction of CO₂ emissions of up to 42.05%. Note that the configurations including a HP used to enhance the energy efficiency of a distillation sequence result in smaller CO₂ emission reductions than the operating cost saving. In addition, although the HP is a useful way of conserving energy, it may have higher exergy loss and a lower CO₂ emission value than the operating cost saving.

4. Conclusions

This paper proposed an energy-efficient sequence for retrofitting the NGL fractionation process. A modified coordinate descent methodology was proposed to solve the process optimization problem encountered in a NGL process retrofit. A rigorous simulation was performed in Hysys linked to Excel, which was found to be a simple and effective optimization methodology for a complex system. These attributes make it widely applicable because the MCD was developed considering the process models established in a commercial simulator. The vapor and liquid traffic within the distillation column can be analyzed and redistributed effectively using the FUA curve. These results indicate a substantial energy saving using the proposed compared to the existing conventional configuration. In particular, a 44.55% lower operating cost can be saved. The short payback period and reduced CO₂ emissions show that the proposed sequence is an attractive option for retrofit in industrial implementation. A TCDS can increase the energy efficiency of a HP and reduce its capital cost significantly. Furthermore, this study also showed that even a HP can reduce the energy requirements significantly, and may have higher exergy loss compared to an existing conventional distillation column. In addition, it may have lower CO₂ emissions saving than the operating cost saving.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at <http://dx.doi.org/10.1016/j.jngse.2016.05.038>.

Nomenclature

<i>A</i>	light component
<i>A_r</i>	area [ft ²]
<i>B</i>	intermediate component
<i>BC</i>	bare cost [\$]
<i>BMC</i>	updated bare module cost [\$]
<i>C</i>	heavy component
<i>C₂</i>	ethane
<i>C₃</i>	propane
<i>C₅₊</i>	gasoline
<i>C_{CW}</i>	cost of cooling water [\$]
<i>C_{electricity}</i>	cost of electricity [\$]
<i>C_{steam}</i>	cost of the steam [\$]
<i>C_{refrigeration}</i>	cost of refrigeration [\$]
<i>CO₂</i>	carbon dioxide
<i>DWC</i>	dividing wall column
<i>Ex</i>	exergy [kW]
<i>FUA</i>	fractional utilization of area
<i>FL</i>	liquid flow [kg/hr]
<i>FV</i>	vapor flow [kg/hr]
<i>h_{proc}</i>	enthalpy of steam delivered to the process [kJ/kg]
<i>HP</i>	heat pump
<i>i</i>	fractional interest rate
<i>iC₄</i>	isobutane
<i>MCD</i>	modified coordinate descent method
<i>MF</i>	module factor
<i>MINLP</i>	mixed integer non-linear programming
<i>MPF</i>	material and pressure factor
<i>N₁</i>	feed stream location
<i>N₂</i>	vapor stream location
<i>N₃</i>	liquid stream location
<i>nC₄</i>	normal butane
<i>NG</i>	natural gas
<i>NGL</i>	natural gas liquid
<i>n</i>	number of years [year]
<i>Op</i>	operating cost
<i>Q_{Fuel}</i>	amount of fuel burnt [kW]
<i>S</i>	brake horsepower [hp]
<i>SC</i>	side condenser
<i>SHP</i>	side heat pump
<i>SR</i>	side reboiler
<i>SRHPTCDS</i>	side reboiler and heat pump-assisted, thermally-coupled distillation sequence
<i>T_{FTB}</i>	flame temperature [°C]
<i>T_{stack}</i>	stack temperature [°C]
<i>TAC</i>	total annual cost [\$]
<i>TCDS</i>	thermally coupled distillation sequence
<i>UF</i>	update factor
<i>X_o</i>	starting point
<i>λ_{proc}</i>	latent heat of steam delivered to the process [kJ/kg]

Subscripts and superscripts

<i>in</i>	inlet
<i>out</i>	outlet

Appendix

A. Cost correlations

a. Capital cost: Guthrie's modular method was applied (Biegler et al., 1997). In this study, the Chemical Engineering Plant Cost Index of 585.7 (2011) was used for cost updating.

$$\text{Updated bare module cost (BMC)} = UF \times BC \times (MPF + MF - 1) \quad (4)$$

$$\text{where UF is the update factor : } UF = \frac{\text{present cos t index}}{\text{base cos t index}} \quad (5)$$

BC is the bare cost for the heat exchanger : BC

$$= BC_0 \times \left(\frac{Ar}{Ar_0} \right)^\alpha \quad (6)$$

$$\text{Area of the heat exchanger, } Ar = \frac{Q}{U\Delta T} \quad (7)$$

$$\text{or the compressor : } BC = BC_0 \times \left(\frac{S}{S_0} \right)^\alpha \quad (8)$$

where MPF is the material and pressure factor; MF is the module factor (typical value), which is affected by the base cost. Ar and S are the area and brake horsepower, respectively.

$$\text{The material and pressure factor : } MPF = F_m + F_s \quad (9)$$

b. Operating cost (Op):

$$Op = C_{\text{steam}} + C_{\text{CW}} + C_{\text{electricity}} + C_{\text{refrigeration}} \quad (10)$$

where C_{steam} is the cost of the steam; C_{CW} is the cost of cooling water; $C_{\text{electricity}}$ is the cost of electricity; and $C_{\text{refrigeration}}$ is the cost of refrigeration

$$\text{c. Cost saving} = \text{Operating cos t saving} - \text{modification cos t} \quad (11)$$

$$\text{d. Payback period} = \text{cos t of project/saving per year} \quad (12)$$

B. Estimation of the exergy and exergy loss

Exergy (Ex) is considered the maximum available work destroyed during any real process as a result of the second law, whose destruction is directly proportional to the generation of entropy (Theodore et al., 2009). Exergy includes physical exergy, which accounts for differences in physical conditions with respect to the environment and chemical exergy, which expresses the amount of work available due to the differences in composition with respect to the environment (Sankaranarayanan et al., 2010). The physical exergy of a stream can be calculated as

$$Ex = (h - h_0) - T_0(s - s_0) \quad (13)$$

The calculation of chemical exergy can be divided into four steps with detail description can be found elsewhere (Abdollahi-Demneh et al., 2011). The exergy related to heat transfer (Ex_Q) can be calculated as (Shin et al., 2015)

$$Ex_Q = Q \left(1 - \frac{T_0}{T} \right) \quad (14)$$

The exergy loss in the system can be determined as follows:

$$Ex_{in} + Ex_{Q_{in}} = Ex_{out} + Ex_{Q_{out}} + W + Ex_{loss} \quad (15)$$

where Ex_{in} and Ex_{out} are the inlet and outlet exergy of a system, $Ex_{Q_{in}}$ and $Ex_{Q_{out}}$ are the inlet and outlet thermal exergy of a system,

W is the shaftwork, and Ex_{loss} is the exergy loss of a system (Shin et al., 2015). Exergy loss calculation for the unit operation:

$$\text{Heat exchanger : } Ex_{HE,loss} = \sum Ex_{in} - \sum Ex_{out} \quad (16)$$

The hot and cold utilities used in heat exchangers may be specified by the heat duty only, rather than having all the detailed thermodynamic information for hot and cold streams. Therefore, for heaters or coolers, the calculation of exergy loss cannot be the same as that for heat exchangers, in which the stream conditions are specified.

$$\text{Cooler : } Ex_{c,loss} = Ex_{in} - Ex_{out} + Q_c \left(1 - \frac{T_0}{T_c} \right) \quad (17)$$

$$\text{Heater : } Ex_{h,loss} = Ex_{in} - Ex_{out} - Q_h \left(1 - \frac{T_0}{T_h} \right) \quad (18)$$

$$\text{Compressor : } Ex_{Com,loss} = \sum Ex_{in} - \sum Ex_{out} + W \quad (19)$$

Aspen Plus was used to simulate and obtain exergy loss for the condenser, reboiler and trays of distillation columns (Demirel, 2004, 2006, 2007; Nguyen and Demirel, 2011; Sapali and Raibhole, 2013).

C. Estimation of the CO₂ emission (Gadalla et al., 2005)

In the combustion of fuels, air is assumed to be in excess to ensure complete combustion, so that no carbon monoxide is formed. The amount of CO₂ emitted, $[CO_2]_{\text{Emissions}}$ (kg/s), is related to the amount of fuel burnt, Q_{Fuel} (kW), in the heating device, as follows:

$$[CO_2]_{\text{Emissions}} = \left(\frac{Q_{\text{Fuel}}}{NHV} \right) \left(\frac{C\%}{100} \right)^\alpha \quad (20)$$

where α (=3.67) is the ratio of the molar masses of CO₂ and C, while NHV, which is equal to 47,141 (kJ/kg), represents the net heating value of natural gas with a carbon content of 75%.

The amount of fuel burnt can be calculated using the following equation:

$$Q_{\text{Fuel}} = \frac{Q_{\text{Proc}}}{\lambda_{\text{Proc}}} (h_{\text{Proc}} - 419) \frac{T_{\text{FTB}} - T_0}{T_{\text{FTB}} - T_{\text{stack}}} \quad (21)$$

where λ_{Proc} (kJ/kg) and h_{Proc} (kJ/kg) are the latent heat and enthalpy of steam delivered to the process, respectively, while T_{FTB} (°C) and T_{stack} (°C) are the flame and stack temperatures, respectively.

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