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Design and optimization of heat integrated dividing wall columns for improved debutanizing and deisobutanizing fractionation of NGL

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Abstract−Dividing wall columns, capable of reducing the energy required for the separation of ternary mixtures, were explored for the energy-efficient integration of debutanization and deisobutanization. A new practical approach to the design and optimization of dividing wall columns was used to optimize dividing wall columns. A conventional dividing wall column and a multi-effect prefractionator arrangement were shown to reduce total annual cost considerably compared with conventional distillation sequence. Various configurations incorporating a heat pump in a bottom diving wall columns were also proposed to enhance energy efficiency further. The result showed that operating cost could be reduced most significantly through novel combinations of internal and external heat integration: bottom dividing wall columns employing either a top vapor recompression heat pump or a partial bottom flashing heat pump.

Key words: Distillation, Dividing Wall Column, DWC, Natural Gas Recovery, Fully Thermally Coupled Distillation Column, Heat Integrating, Process Intensification

INTRODUCTION

Separations by distillation columns account for the largest fraction of energy used in industry, making them a major concern for sustainable development in industrially developed countries. Distillation is the most widely used separation process in industry, and its large-scale equipment makes it one of the most capital-intensive industrial processes. With global industrial growth, distillation is increasing in both variety and size of applications. Hence distillation systems are required that are sustainable and economically feasible, i.e., industrially viable [1-3].

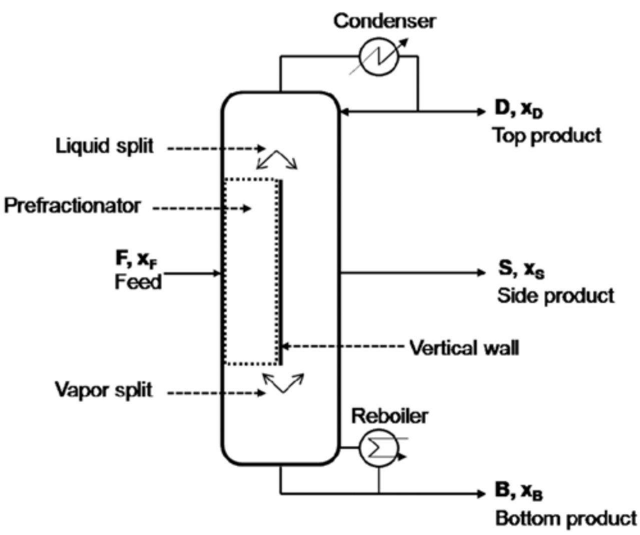

Fig. 1. A dividing wall column.

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There are several reports analyzing the relative advantages of dividing wall columns (DWCs, Fig. 1) for ternary separations that show that DWCs can achieve energy savings of up to 30% over conventional direct and indirect distillation [4-12]. DWCs allow reversible splits with no part of the separation performed twice, the main contributor to their superior energy efficiency over other column configurations [13]. However, their design is more complex than conventional arrangements because of the greater number of degrees of freedom [14], which interact with each other and need to be optimized simultaneously. Since the number of stages is an integer variable, column optimization falls into a class of mixed integer non-linear programming problems (MINLP) [1]. These cannot be solved using commercially available process simulators. This work utilizes a new approach to the design and optimization of dividing wall columns.

Heat pumps in distillation allow the heat of condensation released at the condenser to be used for evaporation in the reboiler [15]. This is an economic way to conserve energy when the temperature difference between the overhead and the bottom of the column is small and the heat load is high. Heat pumps can also be used in grassroots or retrofitting design because they are easy to introduce and plant operation is usually simpler than heat integration [16-20]. However, the high capital expenditure required for compressors make them industrially viable only for high-capacity, end-of-train (practically binary) separations of substances with close boiling points, which require minimal compressor/compression costs. This is the case mainly in the separation of light hydrocarbons, such as C_2, C_3 and C_4 components, where the adiabatic exponents of the substances are large enough to enable significant temperature increases with relatively low compression effort [1,21,22].

Liquid hydrocarbons recovered from NGL are typically separated into relatively pure ethane (C_2), propane (C_3), isobutane (iC_4), normal butane (nC_4), and gasoline (C_{5+}) products. This is conventionally done by the sequential distillation of C_2, C_3 and C_4 from gasoline, followed by further distillation of iC_4 from nC_4 [23]. Because isobutane and normal butane have similar boiling points, their separation requires a large number of trays and a high reflux ratio. E. Díez simulated an isobutane/normal butane distillation process to compare the costs of conventional distillation and heat pump distillation systems [24]. K. A. Amminudin proposed a prefractionator arrangement for retrofitting a debutanizer and a deisobutanizer to achieve the benefits of energy saving and capacity improvement, while fully exploiting existing hardware [25].

Optimization studies rely on statistical approaches, with response surface methodology (RSM) being routinely used in several biotechnological and industrial multivariable processes. In RSM, the Box-Behnken design only has three levels (low, medium, and high, coded as −1, 0, +1) and requires a small number of experiments or simulation runs. A response surface is usually a polynomial whose coefficients are extracted by a simple least-square fit to experimental data. RSM is quite powerful since, in addition to modeling, it can also use the developed model to optimize the conditions of the process under investigation. It is more efficient and easier to arrange and interpret than other methods [26,27]. This work's aim is the maximization of energy efficiency in debutanizing and deisobutanizing NGL recovery using a dividing wall column, a bottom dividing wall column, a heat pump and heat integration. RSM was used to optimize the dividing wall column. Several comparisons of these configurations were analyzed.

DESIGN AND OPTIMIZATION METHODOLOGY

1. Design

Initial DWC design is achieved using a shortcut design procedure [5,14,28,29] based on the conventional column configuration shown in Fig. 2. In this conventional configuration, the first column corresponds to the prefractionator of the DWC. The rectifying section of the second column and the stripping section of the third column represent the top and bottom sections of the DWC, respectively. The stripping section of the second column and the rectifying section of the third column are equivalent to the DWC's dividing wall section. The bottom stream from the second column and the top stream from the third column correspond to the side stream of the DWC. Consequently, the DWC can be divided into four sections: the prefractionator for the feed mixture, the top and bottom sections above and below the dividing wall, and the dividing wall section.

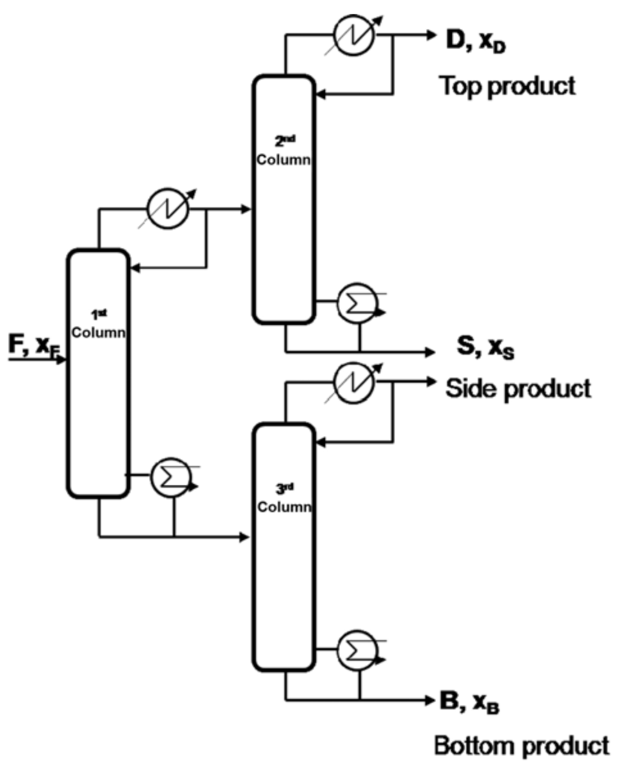

Fig. 2. A three-column distillation system for the initial design of the DWC structure.

2. Optimization

Minimizing reboiler/condenser duties (or equivalently, the reflux ratio) minimizes operating costs and leads to near-optimal column design [30]. This study does not vary the total number of trays, to ensure fair comparison between sequences. Design variables affecting duty are the internal vapor and liquid flows to the prefractionator, the locations of the feed and side trays, and the dividing wall section. After determining the preliminary ranges of the variables through single-factor testing, a Box-Behnken design was employed under the response surface methodology to analyze how the variables interacted and optimize the system in terms of reboiler duty.

Simulation run data were fitted to a second-order polynomial model and regression coefficients were obtained. The generalized second-order polynomial model used in the response surface analysis is as follows:

$$Y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum\sum_{i<j} \beta_{ij} X_i X_j + \varepsilon \quad (1)$$

where Y is the predicted response (reboiler duty), X_i are the uncoded or coded values of the variables, β_0 is a constant, β_i, β_{ii} and β_{ij} are the coefficients of the linear, quadratic and interactive terms, respectively, and ε is the error term.

Simulations were performed using the simulator Aspen HYSYS V7.1. The Peng-Robinson equation of state supporting the widest range of operating conditions and the greatest variety of systems was used to predict the simulations' vapor-liquid equilibriums [31]. MINITAB software was used for response surfaces fitting and optimizing the reboiler duty.

CASE STUDY

1. Conventional Distillation Sequence

The debutanizer, with 40 theoretical trays, was designed for use at 3.5 bar (Fig. 3). The 92-tray deisobutanizer column was designed for use at 4.4 bar, as commercial isobutane can be condensed with cooling water at this pressure [25]. Feed composition, temperature, and pressure conditions are listed in Table 1. To determine each column's maximum flooding, rating modes were simulated using each column's internal specifications, e.g., type of trays, column diameter, tray spacing, and number of passes. Table 2 lists the conditions and product specifications for the columns considered here. The columns were designed with for loads near 85% of the flooding point load to prevent flooding. The base case simulation model shows that energy consumption by the debutanizer and the deisobutanizer

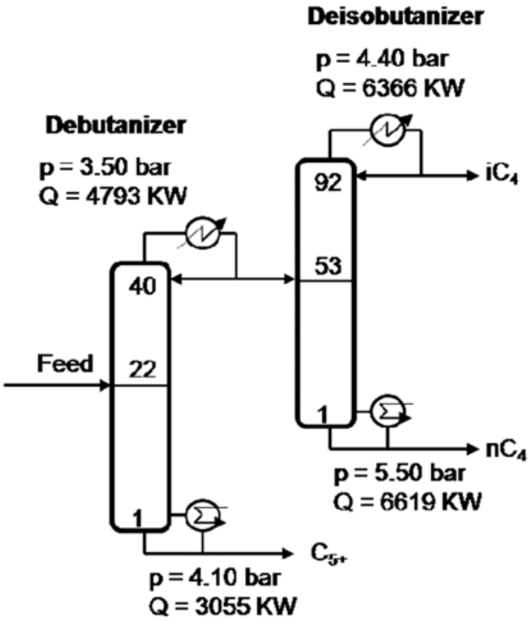

Fig. 3. Simplified flow sheet illustrating the separation train of two conventional columns.

Table 1. Feed mixture conditions

Feed conditions		
Component	Mole flow (kgmol/hr)	Mole fractions (%)
Propane	0.48	0.08
i-Butane	116.58	19.43
n-Butane	290.46	48.41
i-Pentane	50.94	8.49
n-Pentane	58.32	9.72
n-Hexane	83.22	13.87
Temperature (°C)	83.0	
Pressure (bar)	8.0	

Table 2. Column hydraulics, energy performance, and product specifications of the conventional distillation column sequence

	Debutanizer	Deisobutanizer
Number of trays	40	92
Tray type	Sieve	Sieve
Column diameter (m)	2.15	2.75
Number of flow paths	1	1
Tray spacing (mm)	457	457
Max flooding (%)	83.50	84.39
Condenser duty (KW)	4793	6366
Reboiler duty (KW)	3055	6619
Purity of iC_4 (mol%)	99	
Purity of nC_4 (mol%)	95	
Purity of C_{5+} (mol%)	99	

are 3,055 and 6,619 KW, respectively.

2. Conventional Dividing Wall Column (CDWC)

The high efficiency and low energy requirements of dividing wall columns are well reported, but their wider use is prevented by difficulties of their design, optimization, and operation. The initial CDWC structure was estimated using a shortcut design method. It was then optimized using response surface methodology. Some preliminary simulation runs were carried out to determine the main optimizing variables and their level. Corresponding to the changes of factor value, the simulated response values (reboiler duty) was recorded. The presence of curvature indicates that the simulation region is close to the optimum. In this particular work, it was observed that the number of stages of the dividing wall section does not largely affect the reboiler duty when it increases from 42 trays. However, the location of a dividing wall section had a significant effect to reboiler duty. Thus, to simplify the optimization procedure, the location of dividing wall column section was considered as a main variable while the total number of stages of the dividing wall section was fixed by 42 trays. Table 3 lists the factors and levels used in the RSM based optimization. The DWC parameters were optimized over 15 simulation runs. For each run, the internal vapor and liquid flows to the prefractionator were varied to optimize energy consumption and to meet the required product purity and recovery. Fig. 4 shows three-dimensional response surface plots of the interactions between the locations of the feed (N1) and side trays (N3), the feed tray location (N1) and the dividing wall section (N2), and the dividing wall section (N2) and the side stream tray location (N3). A parameter of each model is plotted on each X and Y axis, with reboiler duty on the Z axis. In each case the one remaining parameter was automatically set at its center point value by the software. The resulting second-order polynomial model was as follows:

Table 3. Coded levels of factors

Factor	Levels		
	−1	0	1
Feed tray location (N1)	29	31	33
Dividing wall section (N2)	11-53	13-55	15-57
Side stream tray location (N3)	19	21	23

$$Y=6789.00+181.75X_1-42.63X_2-12.13X_3+157.50X_1^2+106.25X_2^2+142.25X_3^2-7.25X_1X_2-23.25X_1X_3+15.50X_2X_3 \quad (2)$$

Reboiler duty was predicted to be lowest (6733 KW) with coded levels of feed tray location (N1), dividing wall section (N2), and side stream tray location (N3) of −0.5428, 0.1717, and −0.0101, respectively (Fig. 5). The variables' natural values can be derived from the coded levels. Recycling of the vapor and liquid flows was then optimized to minimize reboiler duty and satisfy product purity requirements. A simplified flow sheet illustrating the CDWC system is shown in Fig. 6. The simulation results show that the CDWC can reduce reboiler energy consumption by 29.76% compared with conventional sequences. The simulated value (6794 KW) was in good agreement with the predicted value. Using a CDWC 3.40 m in diameter could reduce energy consumption by 24.68% in terms of TAC compared with using conventional column sequence. Most of the energy savings in the CDWC are attributed to the prefractionator [14]. A major source of separation inefficiency in debutanizer is the remixing effect. As can be seen in Fig. 7, a significant reduction in the remixing inefficiency is provided by a non-sharp split in

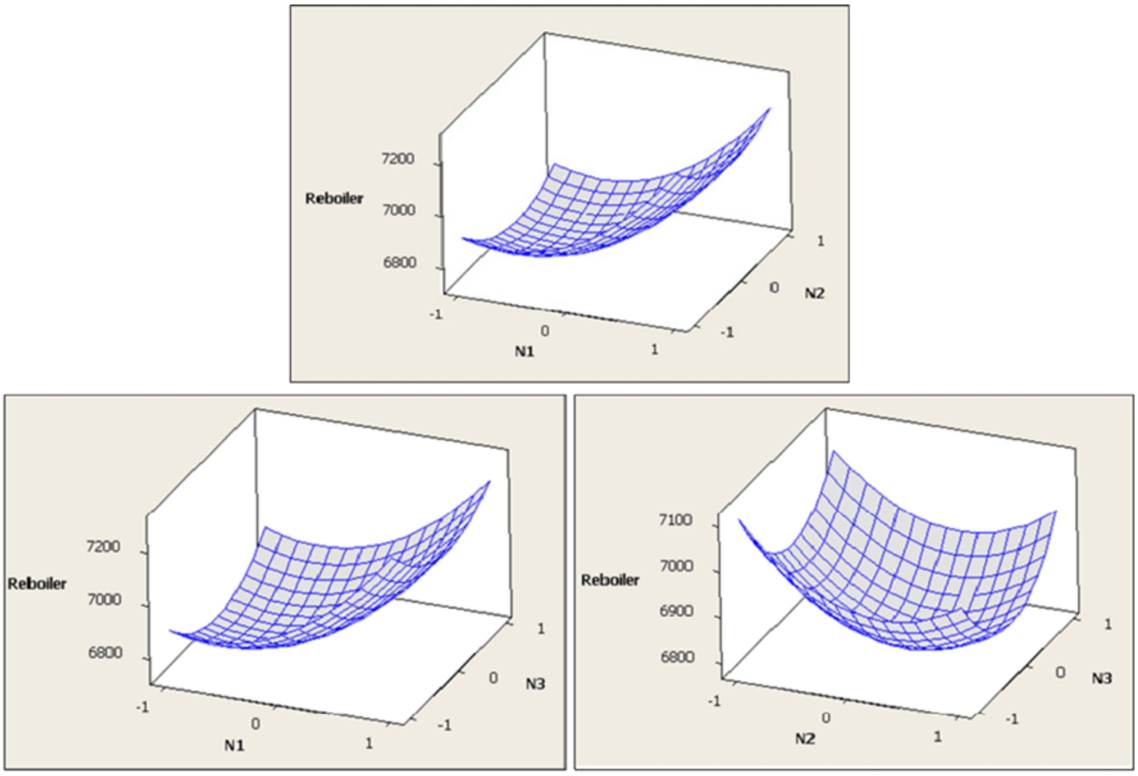

Fig. 4. Three-dimensional response surface plots of interactions between: feed and side tray locations; feed tray location and dividing wall section; and dividing wall section and side stream tray location.

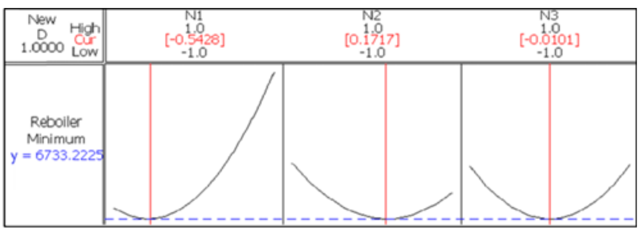

Fig. 5. Optimization plot.

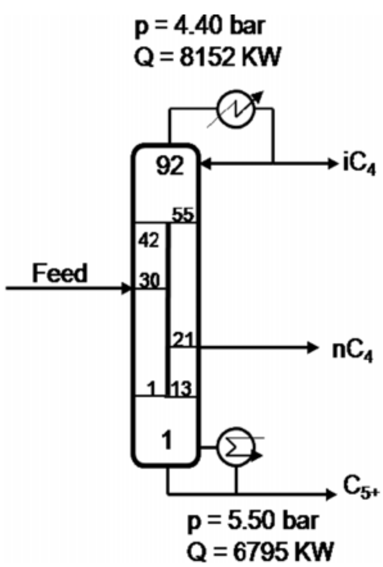

Fig. 6. Simplified flow sheet illustrating the CDWC system.

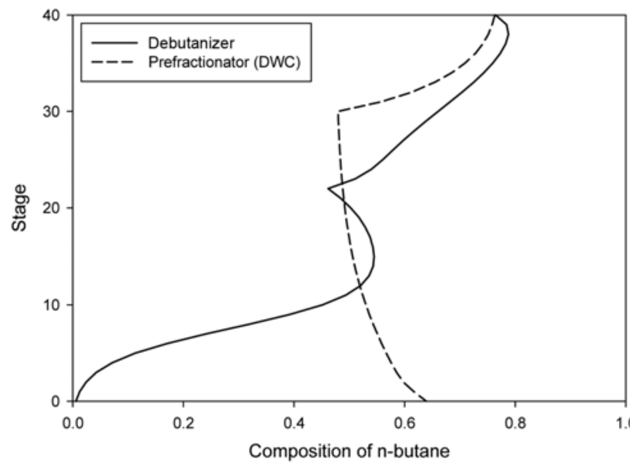

Fig. 7. Composition profile of n-butane.

the prefractionator. In addition, the prefractionator minimizes the mixing losses at the feed tray. The distribution of the middle key component, n-butane, between the top and the bottom of the prefractionator, allows greater freedom to match the column feed composition with the composition on one of the trays in the prefractionator.

Several simulation runs were carried out to validate the three-dimensional response surface plots predicted by the RSM. Fig. 8 compares the three-dimensional response surface plots of interaction between the dividing wall section and side stream tray location evaluated by the RSM and by rigorous simulation. It is apparent from the figure that the three-dimensional response surface plots

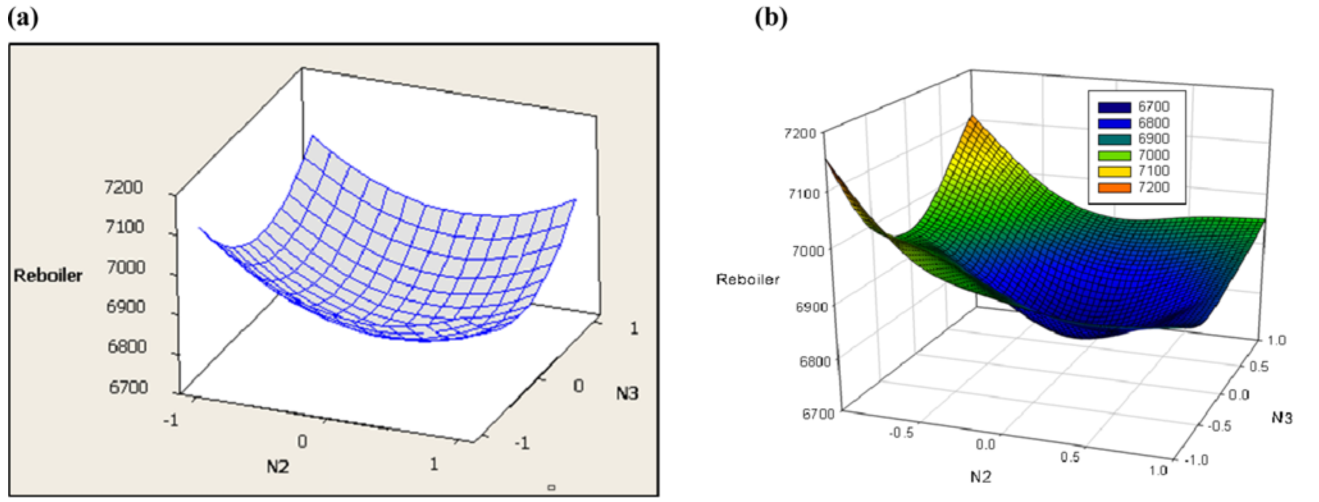

Fig. 8. Three-dimensional response surface plots of interaction between the dividing wall section and side stream tray location predicted by the RSM (a) and by the rigorous simulation (b).

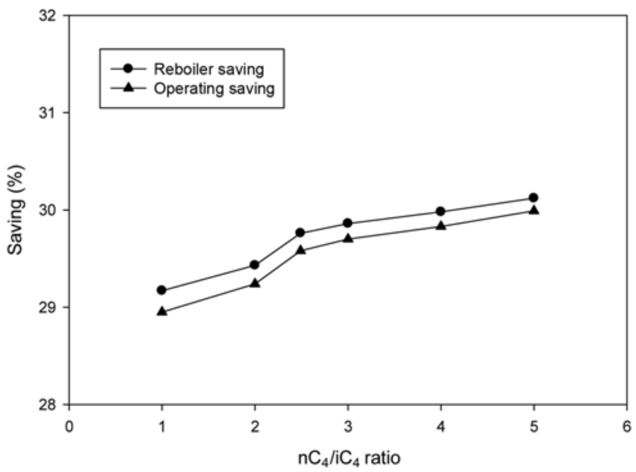

Fig. 9. Effect of nC_4/iC_4 ratio on reboiler energy saving and operating cost saving of the CDWC system.

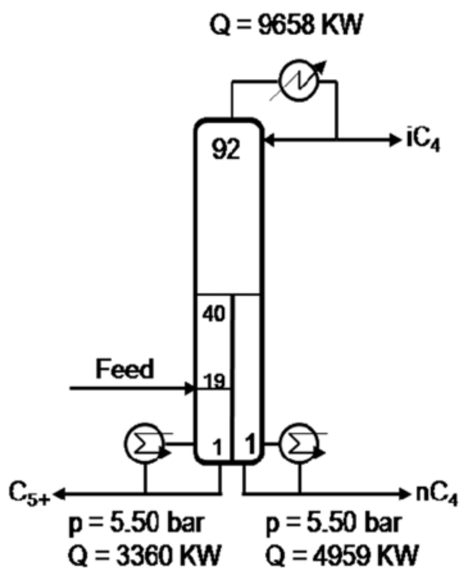

Fig. 10. Simplified flow sheet illustrating the BDWC system.

by the RSM are quite similar to the actual ones.

Increasing nC_4/iC_4 ratio was found to improve DWC performance, reducing reboiler energy use and reducing operating costs over the investigated range (Fig. 9).

3. Bottom Dividing Wall Column (BDWC)

Integrating a debutanizer and a deisobutanizer using a bottom dividing wall column (BDWC), which is equivalent to a side-stripper configuration [4], was also studied (Fig. 10). Rigorous simulation based on the equilibrium-stage model was performed for this arrangement by adjusting the liquid split ratio (R_L), and the locations of the feed and side trays to minimize the size of the column and total energy consumption. The simulation results show that the R_L was 0.39. Energy requirements by the condenser and reboiler were 9658 and 8319 KW, respectively, giving the BDWC system a 13.97% reduction of energy consumption compared with conventional sequences. Note that utility cost data are shown in Table 4 [32].

Table 4. Utilities cost data

Utility	Price ($/GJ)
Refrigerant (moderately low temperature)	4.43
Cooling water	0.35
Steam (LP)	6.08
Steam (MP)	6.87
Electricity	16.80

There are a few reported comparisons of CDWCs and BDWCs [4,33,34]. Table 5 shows that the BDWC gives a smaller energy saving than the CDWC in terms of condenser duty, reboiler duty, and operating cost saving. The BDWC could not be adjusted in terms of vapor split ratio (R_V). It also has one more reboiler, leading to higher investment costs. Nevertheless, such a column with internal integration and external heat integration, via a heat pump, could show improved economy when the temperature difference between the overhead and bottom of the column is small, and the heat load

Table 5. Comparison of different structural alternatives for more efficient debutanization and deisobutanization

Structural alternative	Conventional column sequence		Multi-effect prefractionator arrangement		CDWC	BDWC	BDWC with top vapor recompression heat pump	BDWC with partial bottom flashing heat pump
	Debutanizer	Deisobutanizer	HP	LP				
Tray number	40	92	40	92	92	92	92	92
Column diameter (m)	2.15	2.75	3.40	2.85	3.40	3.70	3.70	3.70
Condenser duty (KW)	4793	6366	0	7284	8152	9658	5762	6120
Compressor duty (KW)	0	0	0	0	0	0	1030	1424
Reboiler duty (KW)	3055	6619	5915	0	6794	8319	3360	3360
Condenser duty saving (%)	0.00		34.73		26.95	13.45	48.36	45.16
Reboiler duty saving (%)	0.00		38.86		29.76	14.01	65.27	65.27
Operating cost saving (%)	0.00		31.02		29.58	13.97	36.65	26.04
TAC saving (%)	0.00		18.24		24.68	11.44	31.68	20.61

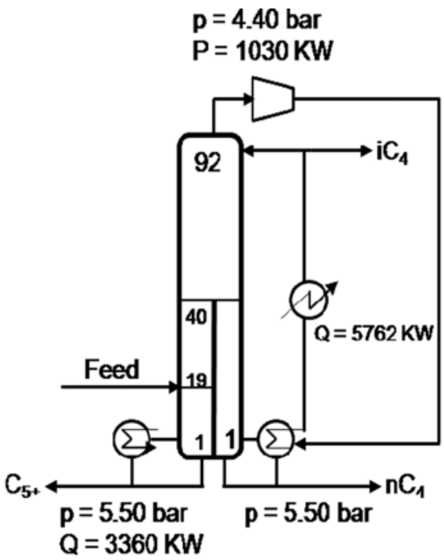

Fig. 11. Simplified flow sheet illustrating the BDWC system with a top vapor recompression heat pump.

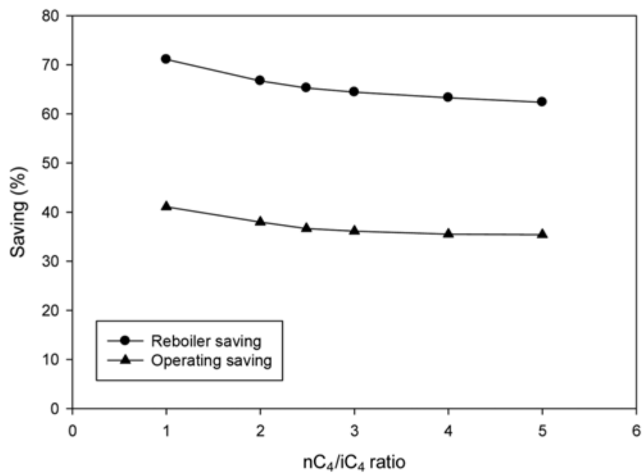

Fig. 12. Effect of nC_4/iC_4 ratio on reboiler energy saving and operating cost saving of the BDWC system with top vapor recompression heat pump.

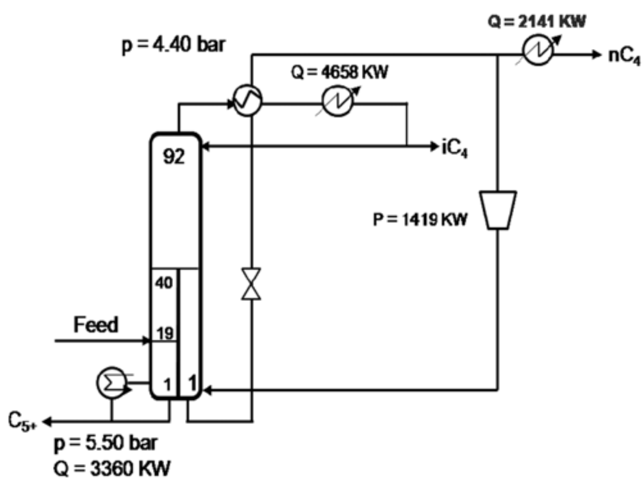

Fig. 13. A BDWC with bottom flashing heat pump.

is high. On the contrary, it is not wise to use a heat pump assisted CDWC due to high temperature difference of about 68 °C.

4. BDWC with Top Vapor Recompression Heat Pump

Vapor from the top of the distillation column can be compressed to a certain pressure (increasing its vapor temperature) and then condensed in the column's reboiler through indirect contact with the liquid in the column's bottom [35]. This allows the heat of the condensing vapor to aid the vaporization at the bottom of the column via a heat exchanger. The top outlet stream must be further cooled before being divided to two streams: one that is recycled back into the column as reflux, and another that is the final top product (Fig. 11). Note that the pressure of the outlet compressor was adjusted to obtain a minimum approach in the heat exchanger of 5 °C. Compared with the conventional column sequence, using a top vapor recompression heat pump can reduce energy consumption by up to 48.36% and 65.27% in the condenser and reboiler duty, respectively, bringing about a 36.65% reduction of operating costs. Thus, this system can be considered for grass-roots or retrofitting design.

Increasing nC_4/iC_4 ratio slightly reduced the performance of the BDWC with a top vapor recompression heat pump over the investigated ratio range, decreasing the reboiler energy saving and the operating cost saving (Fig. 12). Although increasing the nC_4/iC_4

ratio reduced the condenser and compressor duty, it increased the reboiler duty leading to higher operating costs.

5. BDWC with Bottom Flashing Heat Pump

Fig. 13 shows the simplified flow sheet of a BDWC with a bottom flashing heat pump. The column has two bottom streams, one of C_{5+} product, with the remaining flow expanded in the valve to decrease its temperature and to allow heat exchange with the top vapor stream. After heat exchange, depending on each stream's volume and pressure reducing level, a cooler should be added to condense the top vapor stream or a heater is required to boil the bottom stream totally. Here, a cooler was used for total condensing of the top vapor stream before the condensed liquid was recycled back into the column as a reflux stream. The bottom stream was divided into two streams: one that was recompressed to the column pressure and recycled back into the column as a boilup stream, and another that was condensed by refrigeration.

A bottom flashing heat pump in the BDWC involves higher operating costs than using a top vapor recompression heat pump because cooling the final bottom product requires expensive refrigeration to enable an operating cost saving of 11.72% compared with the conventional column sequence. It requires an additional valve and an additional refrigeration system in the bottom flashing heat pump, leading to higher investment costs than the vapor recompression heat pump. Therefore, it is not efficient to flash the entire bottom stream in this case.

6. BDWC with Partial Bottom Flashing Heat Pump

Instead of flashing the entire bottom stream, it can first be divided into two streams: the final product stream, and another that is expanded by a valve to decrease its temperature and to allow heat exchange with the top stream before being recompressed to column pressure. A simplified flow sheet outlining the BDWC with a partial bottom flashing heat pump is shown in Fig. 14. Although this sequence has similar savings of reboiler duty to the sequence with a top vapor recompression heat pump, it has higher condenser and compressor duties (Table 5). This arrangement reduces energy requirement by 26.04% compared with the conventional column sequence.

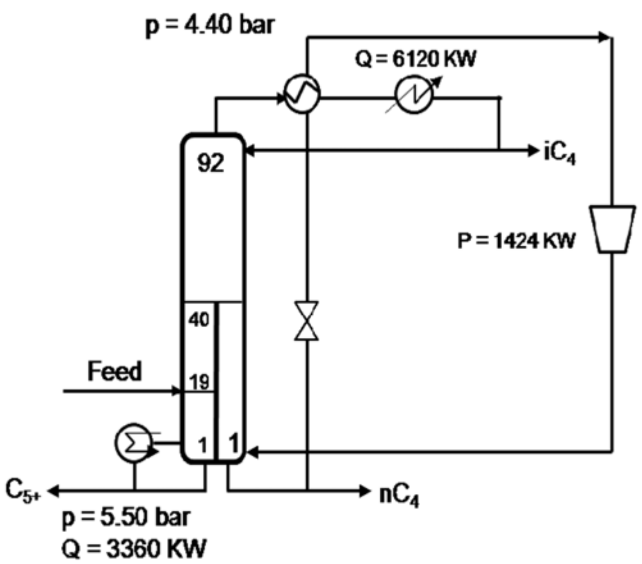

Fig. 14. A BDWC with partial bottom flashing heat pump.

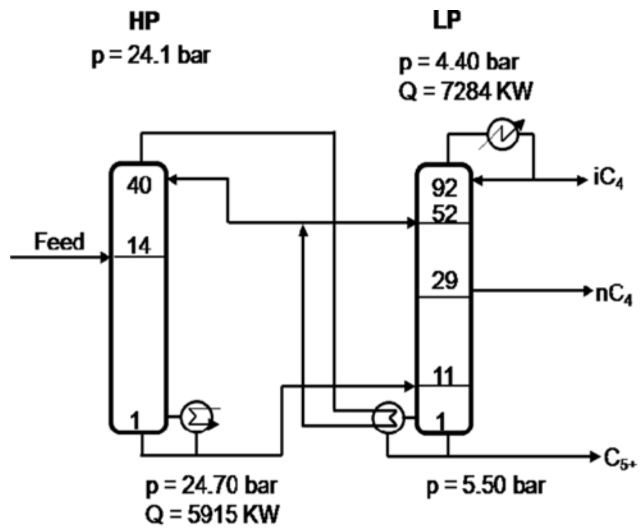

Fig. 15. A multi-effect prefractionator arrangement.

7. Multi-effect Prefractionator Arrangement

Multi-effect (also called pressure-staged) distillation adjusts the column pressures such that the cooling (energy loss) of one column can be used to heat (energy gain) another column [36], giving potential for energy savings. The saving can be enhanced by using a prefractionator arrangement [36-38]. A multi-effect prefractionator arrangement is compared here with other sequences.

Fig. 15 shows a simplified flow sheet of the multi-effect prefractionator arrangement, where the higher pressure of the prefractionator (HP) allows heat from the condensing top to aid the boiling in the main column (LP). This is a forward integration as mass and heat are both integrated in the forward direction, which is easier to initiate and to control than backward integration [36]. One heat exchanger can replace a condenser in the HP column and a reboiler in the LP column. A 5 °C temperature difference was used in the heat exchanger, giving a pressure of 24.1 bar in the top of the HP column and 4.4 bar in the LP column of the multi-effect prefrac-

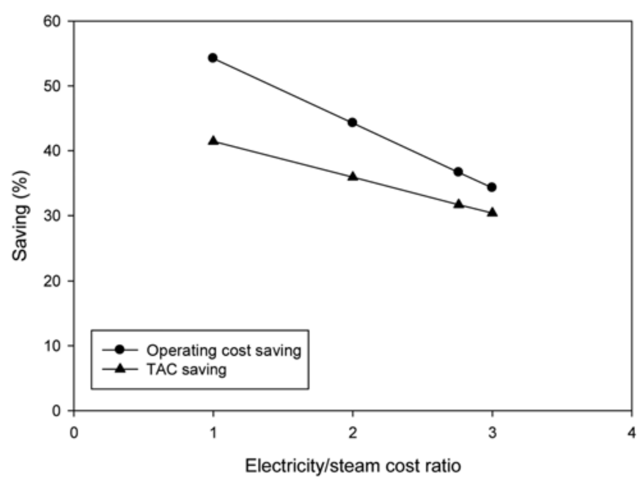

Fig. 16. Effect of electricity/steam cost ratio on operating cost saving and TAC saving of BDWC system with top vapor recompression heat pump.

tionator arrangement. Note that medium pressure steam (MPS) is used in HP column. This arrangement saves 31.02% of the reboiler's energy requirement.

A comparative summary of the key results is listed in Table 5. The BDWC with top vapor recompression heat pump showed the largest TAC saving of the tested sequences. In this study, internal and external heat integration was incorporated for separation of the mixtures of isobutane, *n*-butane and pentane. However, this configuration can also be applied to other mixtures if they satisfy main requirement for heat pump application: heat pump must work across a small temperature difference, which for distillation means close-boiling mixtures [15,39]. Note that the details of economics for each configuration largely depend on the utility costs, which are different country by country, and company by company. Fig. 16 shows the effect of electricity/steam cost ratio on the operating cost and TAC savings of the BDWC system with top vapor recompression heat pump. It is apparent that this configuration takes more advantage when the electricity/steam cost ratio reduces.

CONCLUSIONS

A DWC was designed and optimized for more energy-efficient debutanization and deisobutanization. A shortcut method determined a suitable initial structure for the DWC, which was then optimized by response surface methodology. The proposed method could be simply and efficiently implemented in HYSYS and Minitab. Simulated results were in good agreement with predicted values. Comparisons between various configurations such as a CDWC, a BDWC, a multi-effect prefractionator arrangement, and BDWCs with top vapor recompression and partial bottom flashing heat pump were performed. Incorporating a heat pump into the BDWC, which included internal and external heat integrating, offered a very attractive option to improve energy saving, additionally. BDWCs with top vapor recompression, and partial bottom flashing heat pump showed energy consumptions reduced by 36.65, and 26.04%, respectively, compared with a conventional column sequence. This benefit can increase when the electricity/steam cost ratio reduces or when used in the country/company having cheap electricity cost.

ACKNOWLEDGEMENTS

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APPENDIX. COLUMN COST CORRELATIONS

a. Sizing the column: Column diameter was determined by a column flooding condition that fixed the upper limit of vapor velocity. Operating velocity is normally 70-90% of the flooding velocity [30, 40]. Here, 85% of the flooding velocity was used.

b. Capital cost: Guthrie's modular method was applied [41]. The investment cost for conventional distillation is the total cost of the column and auxiliary equipment, such as reboilers and condensers. For the DWC it includes the additional dividing wall cost. In this study the Chemical Engineering Plant Cost Index of 575.4 was used for cost updating.

$$\text{Tray stack}=(N-1)\times\text{tray spacing} \tag{3}$$

$$\text{Total height}=\text{tray stack}+\text{extra feed space}+\text{Disengagement}+\text{skirt height} \tag{4}$$

$$\text{Updated bare module cost (BMC)}=UF\times BC\times(MPF+MF-1) \tag{5}$$

where UF is the update factor: $$UF=\frac{\text{present cost index}}{\text{base cost index}} \tag{6}$$

BC is bare cost, for vessels: $$BC=BC_0\times\left(\frac{L}{L_0}\right)^{\alpha}\times\left(\frac{D}{D_0}\right)^{\beta} \tag{7}$$

For the heat exchanger: $$BC=BC_0\times\left(\frac{S}{S_0}\right)^{\alpha} \tag{8}$$

Area of heat exchanger, $$S=\frac{Q}{U\Delta T} \tag{9}$$

where MPF is the material and pressure factor; MF is the module factor (a typical value), which is affected by the base cost. D, L, and S are diameter, length and area, respectively.

$$\text{Updated bare module cost for tray stack (BMC)}=UF\times BC\times MPF \tag{10}$$

$$\text{The material and pressure factor: } MPF=F_m+F_s+F_m \tag{11}$$

Compressor cost was interpolated [42].

c. Operating cost (Op):

$$Op=C_{steam}+C_{CW}+C_{refrigerant}+C_{electricity} \tag{12}$$

where C_{stream} is the cost of the steam; C_{CW} is the cost of cooling water; $C_{refrigerant}$ is the cost of refrigerant, and $C_{electricity}$ is the cost of electricity

d. Total annual cost (TAC) [39]

$$TAC=\text{capital cost}\times\frac{i(1+i)^n}{(1+i)^n-1}+Op \tag{13}$$

where i is the fractional interest rate per year and n is the number of years.

NOMENCLATURE

iC_4 : isobutane [_]
nC_4 : normal butane [_]
C_{5+} : gasoline [_]
B : bottom product flow [kg/hr]
BDWC : bottom dividing wall column [_]
CDWC : conventional dividing wall column [_]
D : top product flow [kg/hr]
DWC : dividing wall column [_]
F : feed flow [kg/hr]
R_L : liquid split ratio [_]
R_V : vapor split ratio [_]
S : side product flow [kg/hr]

Subscripts and Superscripts

L : liquid
V : vapor

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