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RAPID COMMUNICATION

Design and optimization of a dividing wall column by factorial design

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Abstract−A factorial design methodology was applied to the design of a dividing wall column, solving the complex multivariable problems and simultaneously optimizing the interacting variables to achieve the best design with respect to total annual cost. Column structure was practically optimized with a minimum of simulation runs. The proposed design method was tested in the design and optimization of an NGL recovery system; it allowed interactions between variables to be identified and quantified. The column system designed by the proposed method reduced reboiler energy consumption and total annual cost by 28.23% and 25.49%, respectively, in case 1, and those by 25.63% and 18.85%, respectively, over conventional distillation in case 2.

Key words: Distillation Process, Dividing Wall Column, Factorial Design, Structure Design

INTRODUCTION

Distillation columns are the most widely used separation units in petrochemical and chemical industries [1]. To reduce their energy consumption, several process and energy integration techniques have been developed, such as the fully thermally coupled distillation system (FTCDS or Petlyuk column, Fig. 1), which can significantly reduce energy consumption [2-6]. This column arrangement allows reversible splits with no part of the separation performed twice, the main source of its superior energy efficiency over other column configurations [7].

Petlyuk systems have strong interactions between their columns because of the thermal integration. This can hinder their design and operation. To overcome this, and to reduce capital costs, a vertical wall can be installed in the central section of the column, dividing it into prefractionator and main sections (Fig. 2). The resulting dividing wall column (DWC) is conceptually similar to the Petlyuk column with a thermodynamically equivalent arrangement [8].

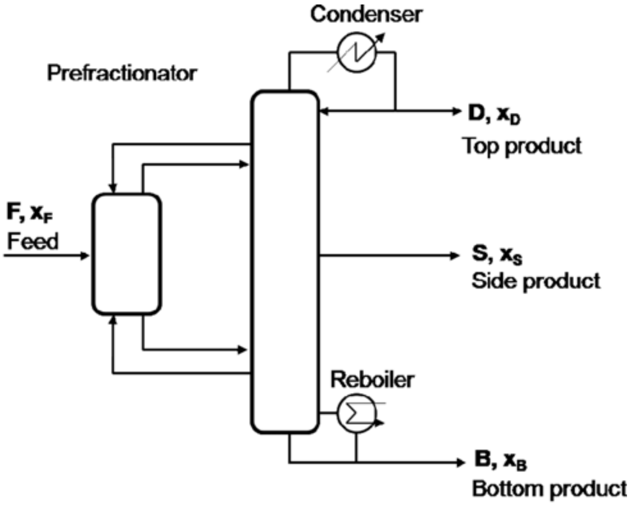

Fig. 1. Petlyuk configuration.

Although DWCs can potentially reduce energy use and investment costs [9-15], their design and optimization is challenging, involving solving multivariable problems with variables that interact with each other and need to be optimized simultaneously. A common difficulty associated with detailed simulation is related to the estimation of the number of stages in each section [16]. Since this is an integer variable, column optimization is a mixed integer nonlinear programming problem (MINLP), which cannot be solved by commercially available process simulators.

DWCs have been optimized through optimizing each variable in succession, keeping the others constant [9,12]. For each chosen number of trays, feed and side tray location, and dividing wall section, internal vapor and liquid flow to the prefractionator were varied to optimize energy consumption. Such a technique does not allow interactions between the variables to be identified or quantified.

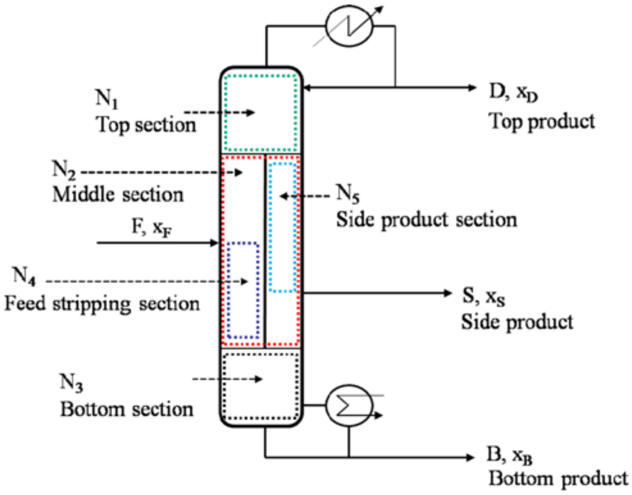

Fig. 2. A dividing wall column.

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The development and application of optimization strategies is an important part of many areas of chemical engineering. Optimization methods can be classified as deterministic or stochastic [15, 17-19]. A rigorous design method has been proposed that is based on detailed column superstructures for a given separation task with subsequent mathematical optimization. A local optimization code, CONOPT, was interfaced to the gPROMS process modeling tool. This method can simultaneously determine design parameters and perform simulations [19]. A genetic algorithm with restrictions coupled to the Aspen Plus™ process simulator is available for the evaluation of the objective function [15]. However, these methods are complex to implement and thus a more practical and simpler optimization method of DWCs would be useful.

Statistical approaches have shown potential for this, with dividing wall columns' structures having been optimized by response surface methodology [20]. This method can be easily and efficiently implemented using HYSYS and MINITAB. Another statistical approach, factorial design, is widely used in experimental investigation [21-25]. It can attain information about each studied factor and the interactions of them from minimal experimental data. Its use is economical through the reduced number of simulations and time saving. This work proposes a simple and efficient approach to the design and optimization of DWCs using factorial design. Two case studies of NGL recovery are performed to demonstrate its application.

DESIGN AND OPTIMIZATION METHODOLOGY

1. Design

Initial DWC structure design involved a shortcut design procedure [8-10] based on a conventional column configuration (Fig. 3), in which the first column corresponds to the prefractionator section of the DWC. The rectifying section of the second column and the stripping section of the third, respectively, represent the top and bottom sections of the DWC. The stripping section of the second column and the rectifying section of the third are equivalent to the dividing wall section of the DWC. 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 structure can be divided into four sections: the prefractionator for feed mixture, the top and bottom sections above and below the dividing wall section, and the dividing wall section.

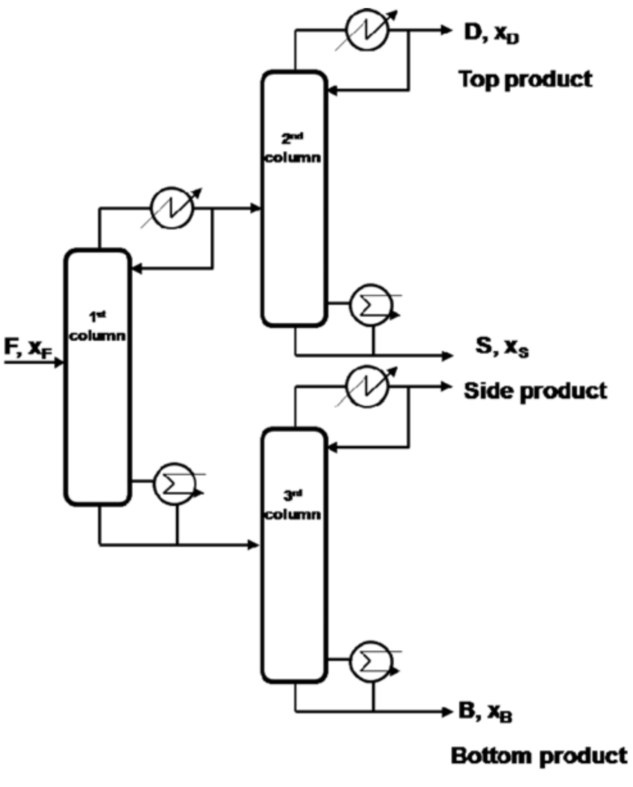

Fig. 3. A three-column distillation system for the initial design of DWC structure.

2. Optimization

After the DWC structure was set, the main design variables including the internal vapor (F_V) and liquid (F_L) flows to the prefractionator, the number of trays in the top (N1), middle (N2), bottom (N3), feed stripping (N4), and side product (N5) sections were optimized. The numbers of trays in the section each side of the dividing wall were both fixed as N2. For processes influenced by multiple variables, statistical experimental design has been shown to be a powerful tool for determining the effects of operational factors and the interactions between them. Factorial design has been used widely in industry; it was employed to analyze factors' interactions and to optimize the column structure through maximizing total annual cost (TAC) saving. Simulation data were fitted to a second-order polynomial model and regression coefficients obtained. A generalized second-order polynomial model was used in the factorial design:

$$Y=\beta_0+\sum_{i=1}^{k}\beta_i X_i+\sum_{i<j}\sum\beta_{ij}X_i X_j+\varepsilon \tag{1}$$

where Y is the predicted response (total annual cost saving), X_i are the uncoded or coded values of the variables, β_0 is a constant, β_i are the main effect coefficients, β_{ij} are the interaction effect coeffi-

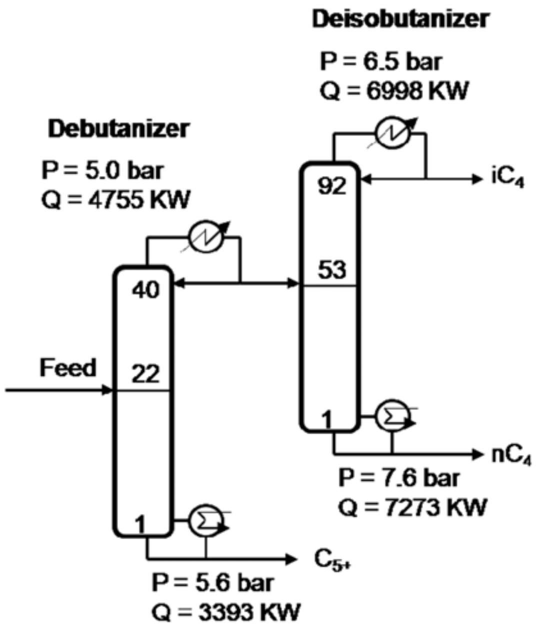

Fig. 4. Simplified flow sheet illustrating the existing separation train of two conventional columns (case 1).

cients, and ε is the error. The coefficients and optimized total annual cost saving were obtained using MINITAB software.

CASE STUDY

1. Case 1 - Debutanizer and Deisobutanizer

1-1. Conventional Distillation Sequence

A debutanizer, with 40 theoretical trays, was designed and operated for 5.0 bar (Fig. 4). Deisobutanizer columns, with 92 trays, were operated at 6.5 bar as commercial isobutane can be condensed with cooling water at this pressure [26,27]. Feed composition, temperature, and pressure are listed in Table 1. Modeled columns' maximum flooding was determined using a rating mode simulated using the columns' internal specifications such as type of trays, column diameter, tray spacing, and number of passes. Simulations were performed using the simulator ASPEN HYSYS V7.1. The Peng-Robinson equation of state was used to predict the vapor-liquid equilibria of these simulations [28]. Table 2 lists the conditions and product specifications of the columns in the existing sequence. The columns were designed with loads of *ca.* 85% of the flooding point load to prevent flooding. The base case simulation model shows that the energy consumption of debutanizer and deisobutanizer was 3,393 and 7,273 KW, respectively.

Table 1. Feed mixture conditions

Component	Mole flow (kgmol/hr)	Mole fractions (%)
	Feed conditions	
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. The existing columns' hydraulics, energy performance, and product specifications (case 1)

	Debutanizer	Deisobutanizer
Number of trays	40	92
Tray type	Sieve	Sieve
Column diameter (m)	2.1	2.9
Number of flow paths	1	1
Tray spacing (mm)	457	457
Max flooding (%)	84.07	83.62
Condenser duty (KW)	4755	6998
Reboiler duty (KW)	3393	7273
Purity of iC_4 (mol%)	99	
Purity of nC_4 (mol%)	95	
Purity of C_{5+} (mol%)	99	

Table 3. Factors' coded levels (case 1)

Factor	Levels	
	Low	High
Top section (N1)	36	44
Middle section (N2)	38	46
Bottom section (N3)	10	14
Feed stripping section (N4)	20	26
Side product section (N5)	28	34

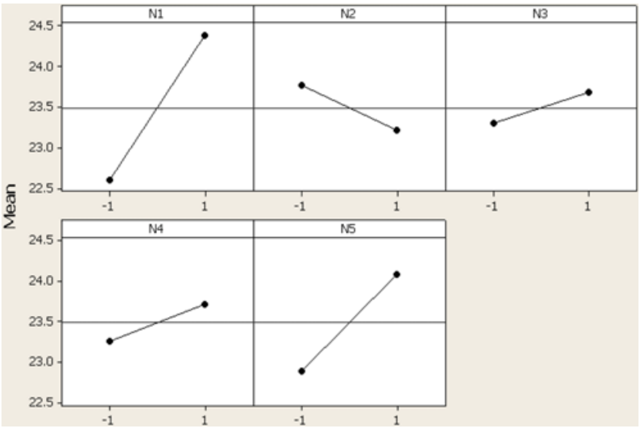

Fig. 5. Main effects of design variables, N1, N2, N3, N4, and N5, on TAC saving.

1-2. Dividing Wall Column

Simulation of DWCs involves significantly more degrees of freedom than modeling conventional distillation columns. A good set of initialization data is essential to ensure convergence of the detailed simulation [13]. The DWC structure was initially estimated by a shortcut design method [10]. It was then optimized by factorial design. Table 3 lists the factors and levels used in this case study. Thirty-two (32) simulations were performed to optimize five parameters of the DWC structure. In each run, internal vapor (F_V) and liquid (F_L) flows to the prefractionator were varied to minimize the total annual cost (TAC), i.e., to maximize the TAC saving over the conventional sequence. Fig. 5 shows main effects of design variables N1, N2, N3, N4, and N5 on TAC saving. In the range of parameters considered, the top section, N1, had the largest influence on TAC saving. Fig. 6 shows the three-dimensional surface plots of interactions between the number of trays in the top (N1), middle (N2), bottom (N3), feed stripping (N4), and side product (N5) sections. Two parameters of each model are plotted on each set of X and Y axes. Total annual cost saving is plotted on the Z axes. The remaining parameters are set at their center point values by the software while the plots are constructed. The resulting second-order polynomial model is as follows:

$$\begin{aligned}Y=&23.496+0.894X_1-0.278X_2+0.193X_3+0.231X_4+0.593X_5\\&-0.148X_1X_2+0.187X_1X_3-0.131X_1X_4-0.209X_1X_5+0.311X_2X_3\\&-0.371X_2X_4+0.437X_2X_5+0.187X_3X_4-0.133X_3X_5+0.153X_4X_5\end{aligned}\quad(2)$$

The greatest total annual cost saving was found at coded levels of the number of trays in the top, middle, bottom, feed stripping, and side product sections of 1, −1, 1, 1, and −1, respectively. The variables' natural values can be derived from their coded levels. F_V and F_L were then optimized to maximize the total annual cost saving, while maintaining sufficient product purity. Fig. 7 shows a simpli-

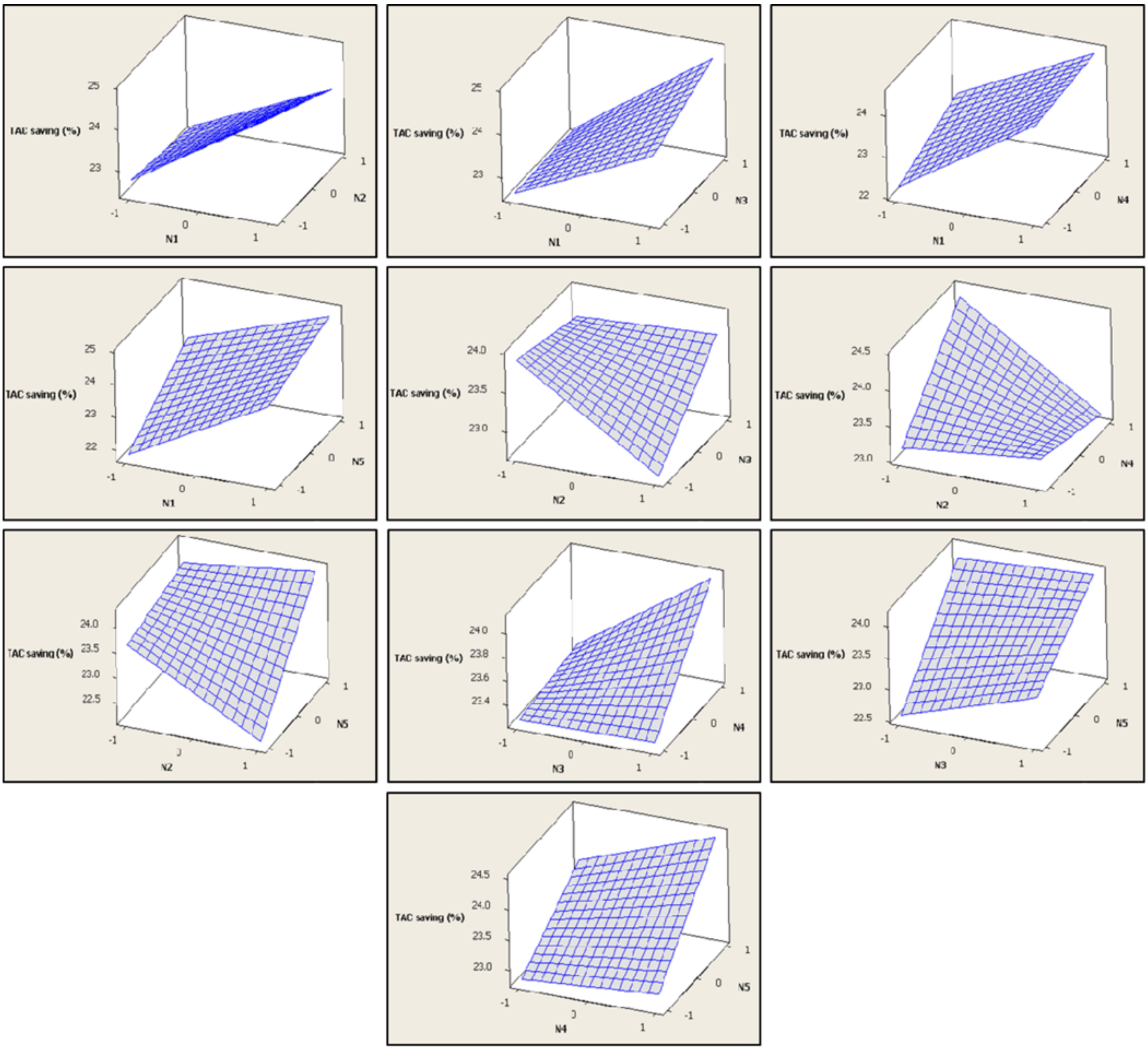

Fig. 6. Three-dimensional surface plots of interactions between main design variables N1, N2, N3, N4, and N5.

fied flow sheet illustrating the resulting DWC system. The result from rigorous simulation also reveals that the DWC can save up to 28.23% and 25.49% in terms of reboiler energy and total annual costs, respectively. A 25.14% improvement of total annual cost was achieved for the same system when the DWC variables were optimized one variable at one time. Furthermore, the factorial design that established this only required 32 simulation runs to optimize the DWC structure, fewer than the 19845 required by brute-force mesh searching.

2. Case 2 - Depropanizer and Debutanizer

2-1. Conventional Distillation Sequence

Fig. 8 illustrates the conventional distillation column sequence, including a depropanizer (diameter of 4.9 m) and a debutanizer (diameter of 3.5 m) [26,27,29]. The depropanizer is designed to operate at 17.5 bar so that cooling water can be used to condense the overhead propane product. Table 4 lists the conditions and product specifications of the columns in the conventional column sequence. The energy consumption of the two columns is 21,540 and 11,550 KW, respectively.

2-2. Dividing Wall Column

In this study, a 2^5 factorial design was employed to fit a second-order polynomial model, which indicated a requirement of 32 experiments for analysis. Some preliminary simulation runs were used to determine variables level. Table 5 shows low and high levels used in this case study. The factorial design can cover the main and interaction effects of the parameters within the whole range of selected parameters. According to the sparsity-of effects principle in factorial design, it is most likely that main (single factor) effects and two-factor interactions are the most significant effects, and the higher order interactions are negligible [30]. In other words, higher order

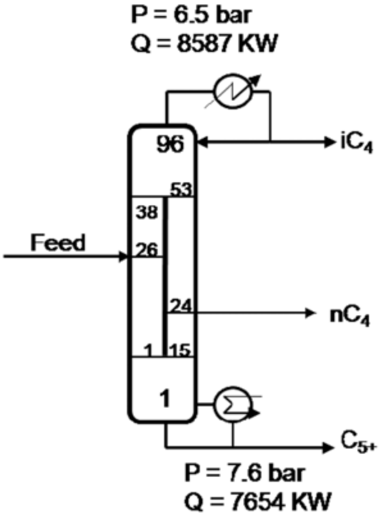

Fig. 7. Simplified flow sheet of the resulting DWC system (case 1).

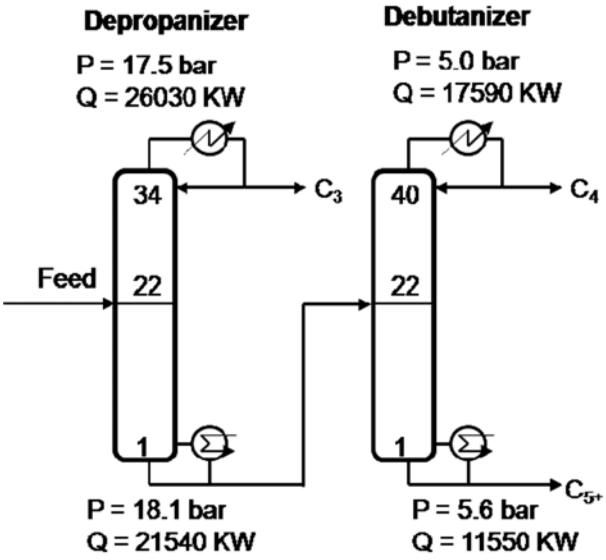

Fig. 8. Simplified flow sheet illustrating the existing separation train of two conventional columns (case 2).

Table 4. The existing columns' hydraulics, energy performance, and product specifications (case 2)

	Depropanizer	Debutanizer
Number of trays	34	40
Tray type	Sieve	Sieve
Column diameter (m)	4.9	3.5
Number of flow paths	1	1
Tray spacing (mm)	609.6	609.6
Max flooding (%)	83.51	84.59
Condenser duty (KW)	26030	17590
Reboiler duty (KW)	21540	11550
Purity of C_3 (mol%)	90	
Purity of C_4 (mol%)	98	
Purity of C_{5+} (mol%)	99	

Table 5. Factors' coded levels (case 2)

Factor	Levels	
	Low	High
Top section (N1)	6	10
Middle section (N2)	36	42
Bottom section (N3)	16	20
Feed stripping section (N4)	14	20
Side product section (N5)	20	24

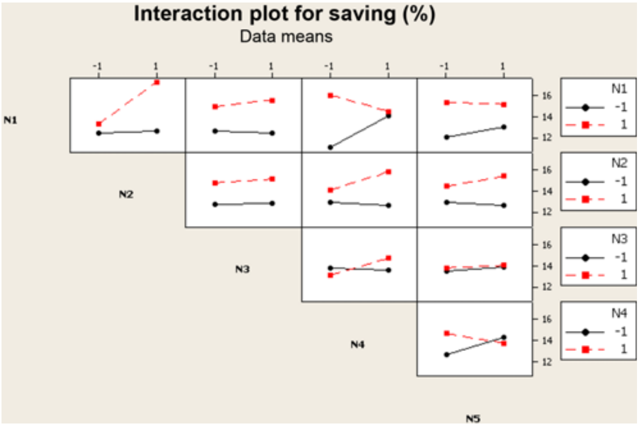

Fig. 9. Effect of main design variables', N1, N2, N3, N4, and N5, interactions on TAC saving.

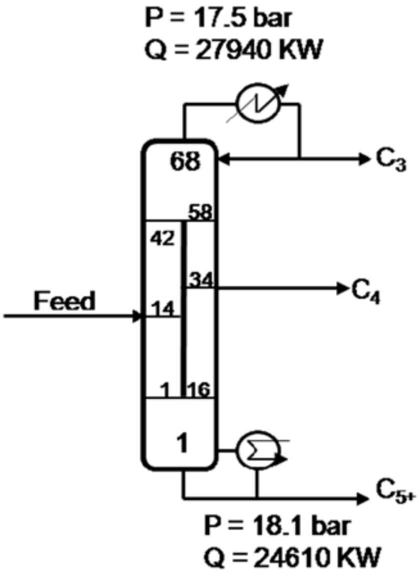

Fig. 10. Simplified flow sheet of the resulting DWC system (case 2).

interactions such as three-factor interactions are very rare and considered as the residual which are dispersed randomly. Fig. 9 shows plots of the effects of interactions between the number of trays in the top (N1), middle (N2), bottom (N3), feed stripping (N4), and side product (N5) sections on TAC saving. It turned out that the interaction effects between N1-N3, N1-N5, N2-N3 and N3-N5 were low. The resulting second-order polynomial model is as follows:

$$\begin{aligned}Y=&13.876+1.379X_1+1.070X_2+0.113X_3+0.355X_4+0.180X_5\\&+0.959X_1X_2+0.188X_1X_3-1.145X_1X_4-0.283X_1X_5+0.053X_2X_3\\&+0.525X_2X_4+0.323X_2X_5+0.456X_3X_4-0.048X_3X_5-0.638X_4X_5\end{aligned}\tag{3}$$

In the range of parameters, the top section, N1, had the largest influence on TAC saving. The greatest total annual cost saving was found at coded levels of the number of trays in the top, middle, bottom, feed stripping, and side product sections of 1, 1, −1, −1, and 1, respectively. As a result, 68 trays were employed in the design of the DWC (Fig. 10). From the simulation results, the liquid split ratio (R_L) and vapor split ratio (R_V) were 0.40 and 0.59, respectively. Note that DWC needs to be operated at high pressure to satisfy condensing top product using cooling water. An increase in the pressure causes an increase in the temperature of the column bottom. Thus, medium pressure steam is required in the DWC, while the conventional column sequence needs low pressure steam. Using the DWC can save up 25.63%, 13.71% and 18.85% in terms of reboiler duty, investment cost and TAC, respectively.

CONCLUSIONS

A practical method of designing and optimizing DWCs was developed based on factorial design. It could easily and efficiently be implemented by HYSYS and MINITAB. Factorial design allowed rapid optimization of DWC structure with little computational effort; it could also identify and quantify interactions between variables. The proposed design technique allowed variables to be optimized simultaneously. A DWC system designed by the proposed method reduced reboiler energy and total annual costs dramatically over conventional distillation.

ACKNOWLEDGEMENTS

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APPENDIX. COLUMN COST CORRELATIONS

α. Sizing the column: Column diameter was determined using a column flooding condition that fixes the upper limit of vapor velocity. Operating velocity is normally between 70 and 90% of the flooding velocity [12,31]; 85% was used here.

β. Capital cost: Guthrie's modular method was applied [32]. The investment cost for conventional distillation is the total cost of the column and auxiliary equipment, such as reboiler and condenser. For the DWC, it included the cost of the additional dividing wall. Cost updating was performed using the Chemical Engineering Plant Cost Index of 575.4.

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

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

$$\text{BC is bare cost: For vessels: } \text{BC}=\text{BC}_0\times\left(\frac{\text{L}}{\text{L}_0}\right)^{\alpha}\times\left(\frac{\text{D}}{\text{D}_0}\right)^{\beta}\tag{6}$$

$$\text{For the heat exchanger: } \text{BC}=\text{BC}_0\times\left(\frac{\text{S}}{\text{S}_0}\right)^{\alpha}\tag{7}$$

$$\text{Area of heat exchanger: } \text{S}=\frac{\text{Q}}{\text{U}\Delta\text{T}}\tag{8}$$

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.

χ. Operating cost (Op):

$$\text{Op}=\text{C}_{steam}+\text{C}_{CW}\tag{9}$$

where C_{stream} is the cost of low and medium pressure steam: 300 and 350 USD/KW·year, respectively [33]

and C_{CW} is the cost of cooling water: 90 USD/KW·year

δ. Total annual cost (TAC) [34]

$$\text{TAC}=\text{capital cos t}\times\frac{\text{i}(1+\text{i})^n}{(1+\text{i})^n-1}+\text{Op}\tag{10}$$

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

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