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Response surface methodology in optimization of a divided wall column

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Abstract−A dividing wall column (DWC) is a thermally coupled distillation system with a high energy efficiency that requires lower space and investment compared to the conventional column system. The design of a DWC involves a number of structural and process parameters that need to be optimized simultaneously to improve energetic and economic potential and reduce space requirement. We used response surface methodology (RSM) to optimize DWC nonlinearly and to figure out the effect of parameters and their interactions on energy consumption, product quality, and dimensions of a DWC. Results demonstrate that process variables have significant effects on the energy efficiency of a DWC as compared to the effect of structural variables. The optimum DWC parameters can be found by RSM with minimal simulation runs and the prediction results of RSM agree well with the rigorous simulation results.

Keywords: Distillation Process, Divided Wall Column, Optimization, Response Surface Methodology, Energy Efficiency

INTRODUCTION

Distillation is the most common process for material separation, which is performed based on the difference in boiling temperature. Heat is used as a separating agent and approximately 95% of liquid separations are carried out by distillation process [1]. This process accounts for about 3% of total world energy [2]. With the increase in the price of energy and its impact on economic growth, the chemical and petrochemical industry efforts aim to develop an appropriate design method to enhance the thermodynamic efficiency of the process and thus reduce its operating cost. To reduce the energy consumption of distillation, the improvement of distillation systems is important [3,4]. Fig. 1 shows typical arrangements for separation of a ternary mixture in the direct and indirect sequences. Their energy separation demands for the products with same specifications are not equal. A non-optimal choice of the separation sequence can lead to additional cost during the operation [5]. Moreover, heat integration techniques can be applied to make the distillation process more energy-efficient. Petlyuk is one of integrated configurations (Fig. 1(c)) for distillation process, which includes a prefractionator joint to the main distillation column. It requires only one reboiler and one condenser attached to the main column, while one condenser and reboiler are replaced by thermal coupling streams between the prefractionator and the main column [6-8]. By integrating two columns of the Petlyuk configuration into one shell and positioning one (or more) vertical wall(s)

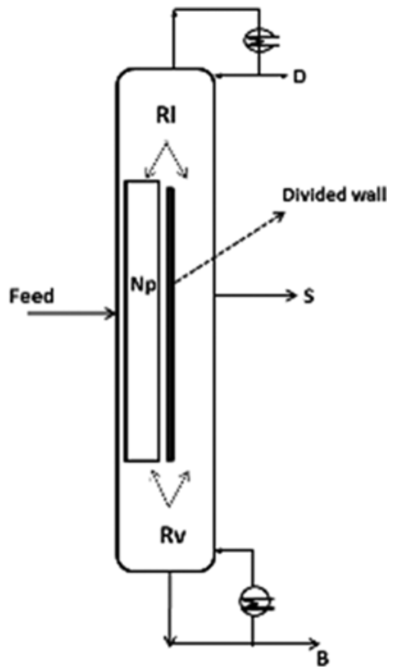

Fig. 1. Column arrangements for separation of a three component mixture; (a) direct sequence, (b) indirect sequence, (c) petlyuk configuration.

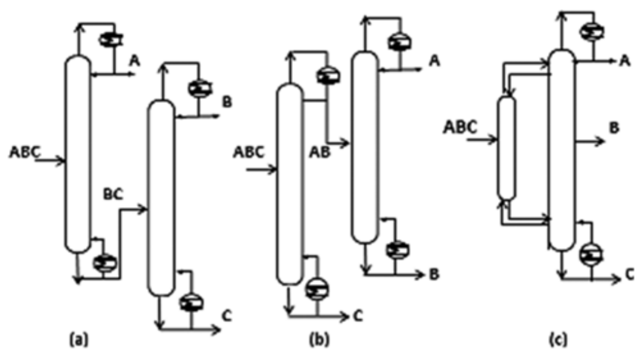

Fig. 2. Schematic of a dividing wall column.

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in the axial section, a dividing wall column (DWC) is constructed. The DWC shown in Fig. 2 has only one reboiler and one condenser [9]. According to Schultz et al. [10], the DWC will become a standard distillation method in the next 50 years. The energy saving and cost reduction in investment and operation of DWC is about 20% to 30% compared to conventional sequences. The main reason for reducing the energy consumption in a DWC configuration is the avoidance of remixing of internal streams, which happens usually in conventional arrangements of two columns [11,12].

The design of divided wall columns or Petlyuk distillations is more complex than traditional distillation because it has more degrees of freedom, such as the number of trays in each section of the column, liquid and vapor splits ratio, the feed tray location, and the side product location. These parameters interact with each other and need to be optimized simultaneously for an economical design of the column [13,14]. During the past decade, a number of papers have been published about the design and modeling (steady state and dynamics), control, and operation of DWCs [15-20]. The design of DWC is solved by a shortcut method, based on the Fenske-Underwood-Gilliland-Kirkbride model (FUGK) [14]. The methods are limited in their applications by certain assumptions, such as constant molar overflow and constant relative volatility [13]. Halvorsen and Skogestad [21] proposed the application of a V_{min} diagram method to determine the minimum energy. In their method, a constant molar flow rate, constant relative volatility, and constant pressure and an infinite number of stages were assumed. Fidkowski and Krolikowski [22] and Carlberg and Westerberg [23,24] introduced the minimum-energy phrases based on Underwood's equations for three components Petlyuk arrangements. Later, Halvorsen and Skogestad [21] expanded the minimum-energy method for the general multicomponent case. Ramirez-Corona et al. [25] presented a procedure for optimization of Petlyuk column. FUGK model was used to determine the structural design parameters of the divided wall column such as the mass and energy balances, the thermodynamic relationships, and cost evaluation.

Although DWCs can potentially reduce energy consumption and investment costs [26-30], their optimization is more complex than conventional arrangements. A common difficulty associated with the design of DWC is determining the number of trays in each section [11]. Rangaiah et al. [30] reported that the vapor and liquid splits in the column have an important effect on the energy demand of a DWC. Moreover, they reported that the positions of the feed tray, side product, and dividing wall must be optimized due to the effect of these parameters on energy requirement. Furthermore, the energy consumption in reboiler depends strongly on the flow rate of the interconnecting stream of a DWC [31,32]. Hernandez and Mendez [33] noted that the energy requirement depends strongly on the values of the vapor recycle stream. Since optimization of a DWC is a mixed integer nonlinear programming problem (MINLP), which cannot be solved by commercially available process simulators, various methods have been suggested for optimizing DWCs; e.g., a method which Aspen Plus software is linked with an external optimization algorithm [34], a sequential quadratic method implemented in Aspen Plus [35], and a MILP approach [36]. Guitérrez-Antonio and Briones-Ramirez [37] estimated the set of optimal solutions between minimum reflux and the minimum number of trays using a genetic algorithm. In this regard, most of the available optimization codes are the local optimal solutions [25] that do not allow interactions between the variables to be identified and analyzed, whilst DWC has various parameters that affect on each other and need to be optimized simultaneously. Thus, a practical and global optimization method should be used for a DWC.

A large number of structural and process variables are used in the rigorous simulation for optimization of a DWC. These variables interact with each other and need to be optimized simultaneously to obtain the optimal design. Most of the reports in the literature optimized the structural and process parameters of a DWC separately. The optimization of a DWC is a mixed integer nonlinear programming problem, which cannot be solved with the existing process simulators. The design of experiments such as central composite design (CCD) technique under response surface methodology (RSM) coupled with Aspen software can be employed to optimize the structural and process parameters of a DWC simultaneously.

RSM is useful in process optimization studies. The design of experiments is a statistical technique for building regression models, optimizing a response, and for identifying the effects of several variables and their interactions on the process. Some researchers applied a method based on the shortcut and RSM to design and optimize the structural or process parameters of DWCs either sin-

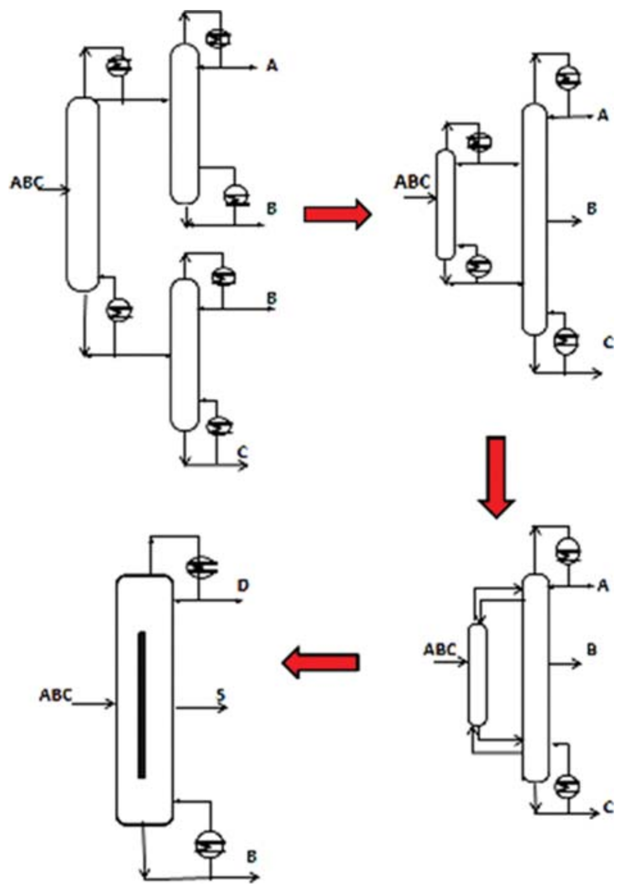

Fig. 3. Procedure of simulating a DWC.

gly or simultaneously [26,27,38,39].

In the present study, the processes of DWCs for a ternary mixture of methanol, 1-propanol, and 1-butanol were simulated with Aspen Plus, followed by applying RSM for optimization to find the optimum operating conditions in terms of product quality and energy consumption. Next, the diameter of the column was optimized as an indispensable parameter in the optimal design of the column.

SIMULATION MODEL

Simulation of a DWC has a difficult procedure because in a commercial process simulator packages such as Aspen plus, Chemcad, and Prosim, DWC is not established as a standard model. However, as shown in Fig. 3, the initial step for designing a DWC is converting two conventional columns to three traditional distillation columns. Then, the prefractionator model is simulated by coupling the last two columns and removing one condenser and one reboiler. At the next step, the Petlyuk configuration is created by excluding condenser and reboiler of the first column. The divided wall column is thermodynamically equivalent to the Petlyuk column by neglecting heat transfer across the dividing wall [14,40].

Nguyen [41] used a ternary mixture of methanol; 1-propanol, and 1-butanol with mass fraction composition 0.22/0.53/0.23 are used for simulation runs with a rigorous Multifrac model of Aspen plus. He assumed that the upper, lower, feed, and side elements of each unit have an equal number of 15 stages, while the number of stages of feed section and side section is ten stages. The parameters required to be specified to operate a DWC as initial condition and their results are listed in Table 1. In the first step, the structural parameters are optimized. Next, keeping the structural parameters constant, the process parameters are varied to achieve the optimum operating conditions. The aim of optimization is to optimize the structural and process parameters for modifying energy efficiency and reducing cost of the DWC. In this work, tray sizing feature of Aspen plus was used to calculate the diameter of prefractionator and the main section of DWC.

RESPONSE SURFACE METHODOLOGY

RSM is a statistical method that is beneficial for optimizing processes. This method is applied to predict the relative significance of several affecting variables even in the presence of complex interactions [42]. In this study, a standard RSM design, called central composite design (CCD) by design expert software, was used to optimize a DWC. Through using the RSM and applying regression analysis, the modeling of the desired response to the several independent variables was obtained. In the following parts of the paper, each quadratic response surface, that predict the optimal condition will be represented by using Eq. (1)

$$Y=\beta_0+\sum_{i=1}^{k}\beta_i\cdot X_i+\sum_{i=1}^{k}\beta_{ii}\cdot X_i^2+\sum_{i\le j}^{k}\sum_{j}^{k}\beta_{ij}\cdot X_i\cdot X_j+e \tag{1}$$

where Y is the predicted response, X_i is the levels of the independent variables, i is the linear coefficient, j is the quadratic coefficient, ij is the interaction effect, ii is the squared effect, e is the random error, and β is the regression coefficients of the independent variables [43].

Analysis of variance (ANOVA) was used to investigate the interaction between the process parameters and the responses. The quality of the fit polynomial model was checked by the coefficient of determination R^2 and its statistical significance were evaluated by the P-value. Furthermore, different operational conditions were tested by three-dimensional plots to deduce the optimal operating conditions.

First, the total number of trays, number of trays in prefractionator, a tray of the feed, the location of the side product tray, and the vertical position of the dividing wall were used to optimize reboiler duty and to investigate the effect of these parameters on product purity. The range of variables is given in Table 2. Central points were selected based on the preliminary simulation (Table 1). The dividing wall was placed between stages 17-26. In the negative range, the vertical position of the dividing wall is lower than the initial position, and in the positive range, the vertical position of the dividing wall is higher than the initial position. The num-

Table 2. Simulation range

Process factor	Simulation range	
	Lower level	Upper level
A: N_t	−6	6
B: N_p	−3	3
C: N_f	−2	2
D: N_s	−2	−2
E: N_w	−3	3

Table 1. Specification of a dwc

Parameters		Results	
No of stages	42	Reboiler duty (kw)	7.2
No of stage of prefractionator	10	Distillate	0.995
feed stage	5	Side stream	0.991
Side product stage	21	Bottom	0.95
Reflux ratio	17	Diameter of prefractionator (cm)	6.95
Vertical position of divided wall	Between tray No of 17-26	Diameter of main column (cm)	6.87
Liquid split	0.5		
Vapor split	0.5		

Table 3. Quadratic model of responses

Response	Final equation in term of code factors	P	R^2	Adj. R^2	F value
D	0.99+2.559B−2.68C+0.98D−0.112E+3.228BC+0.06BE+0.0621DE	<0.0001	0.964	0.98	70.63
S	0.99+0.4A+5.2B−2.724C−2.688E+0.0568AD+0.074AE+1.83BC +2.683BD+2.381BE−2.775DE+2.43A2−8.96B2+1.563D2	<0.0001	0.991	0.97	116.77
B	0.93+0.147A+9.525B+9.985C−7.524D−4.42E+2.16AD+1.775AE+8.31BD	<0.0001	0.98	0.951	35.14
QR	6.66+1.19A+6.479B−5.894C+2.847D+0.0349E+6.644BC+0.0587BE +0.055CD−0.0531CE−1.841B2−1.591D2	<0.0001	0.996	0.960	241.85

ber of trays is decreased in the negative range, while the number of trays is increased in the positive range. The range for each parameter is chosen from the extreme values of these parameters, below and above these values simulations do not converge and the purity of components become so low.

The obtained results were analyzed using ANOVA to select the best model. A quadratic model of RSM was applied to the simulated data followed by modifying them by eliminating the term found statistically insignificant. The model summary statistic demonstrates the high coefficient of determination R^2 (>0.9) and a P-value lower than 0.05, suggesting that the models for product quality and energy consumption of the DWC have been chosen correctly.

RESULTS AND DISCUSSION

1. Structural Parameters Optimization

In this section, the results from the design and optimization of the numbers and locations of the trays of the column are discussed, process variables are optimized, and optimal column dimensions are reported. The data obtained from simulations were investigated for reboiler duty and product quality using the reduced quadratic model. The results of ANOVA analysis for all responses are shown in Table 3. A high R^2 coefficient confirms that a satisfactory match of the quadratic model to the simulated data. In our case, only 0.04% of the variation in the responses was not explained by the model. Furthermore, the F-values are much larger than 5 and P-value for the models is less than 0.05, implying that the model terms are statistically significant [44].

Independent terms and the interactions are statistically significant if the prob>F value is lower than 0.05. According to Table 4, ANOVA analysis result showed that for distillate product, prefractionator's tray number (B) and the location of feed tray (C) and their interaction are significant parameters. The location of side stream (D), number of trays in prefractionator (B), their interaction, and the location of feed tray (C) affect the purity of bottom product. The results indicate a relationship between the purity of side product and the location of dividing wall (E), tray of side stream (D) and B, C and interaction between D and E and BE. The reboiler duty of a DWC was directly related to the stage location of feed and side stream tray numbers of prefractionator and interaction term BC.

The 3D response surface plots for further investigation of the effects of parameters are illustrated in Fig. 4. As shown in Fig. 4(a), to enhance the quality of distillate it is necessary to increase the trays of prefractionator. Importantly, by increasing the number of trays, the capital cost of the system will increase. Furthermore, it can be concluded that the number of stages in section 1 (Fig. 4(a)) has a significant effect on the purity of distillate product. The 3D diagrams of the interaction between parameters that affect the duty of reboiler and purity of sidestream are presented in Fig. 4(b)-(d). As can be seen in Fig. 4(c), the term DE is more effective on the side stream purity than the other interactions.

Table 4. ANOVA analysis for responses (p-value)

Source	D	S	B	Q_R
Model	<0.0001	<0.0001	<0.0001	<0.0001
A-Nt	0.3496	0.4865	0.9442	0.0524
B-Np	<0.0001	<0.0001	<0.0001	<0.0001
C-Nf	<0.0001	0.0002	<0.0001	<0.0001
D-Ns	0.0175	0.0001	0.0001	<0.0001
E-Nw	0.0078	0.0003	0.0122	0.5214
AB	0.6136	0.7354	0.9116	0.8773
AC	0.2123	0.8867	0.8273	0.7267
AD	0.3506	0.4212	0.2087	0.7577
AE	0.2123	0.2954	0.2993	0.8611
BC	<0.0001	0.0141	0.9087	<0.0001
BD	0.4808	0.0008	<0.0001	0.6149
BE	0.1386	0.0002	0.0684	0.3383
CD	0.2348	0.8517	0.4867	0.3694
CE	0.2784	0.8797	0.7311	0.3856
DE	0.1311	<0.0001	0.0066	0.1737
A2	0.9627	0.3493	0.4386	0.9173
B2	0.7919	0.0001	0.0033	0.4470
C2	0.9902	0.7840	0.8626	0.8812
D2	0.6881	0.5567	0.5890	0.5168
E2	0.1175	0.8267	0.9601	0.0191

Results demonstrate that for each response, different parameters and interactions are important; so for optimization of a DWC, all parameters should be considered simultaneously. The optimum condition of all factors was found for simultaneous optimization of energy consumption and product quality using the point prediction option of RSM. The optimum values of parameters are given in Table 5.

Clearly, optimization of the structural parameters of a DWC can be achieved using the RSM. The optimized number of total trays was found to be 36, which is less than that found earlier (i.e., 42) without optimization. Knowledge of the optimum number of stages results in capital cost reduction and also achieving a higher prod-

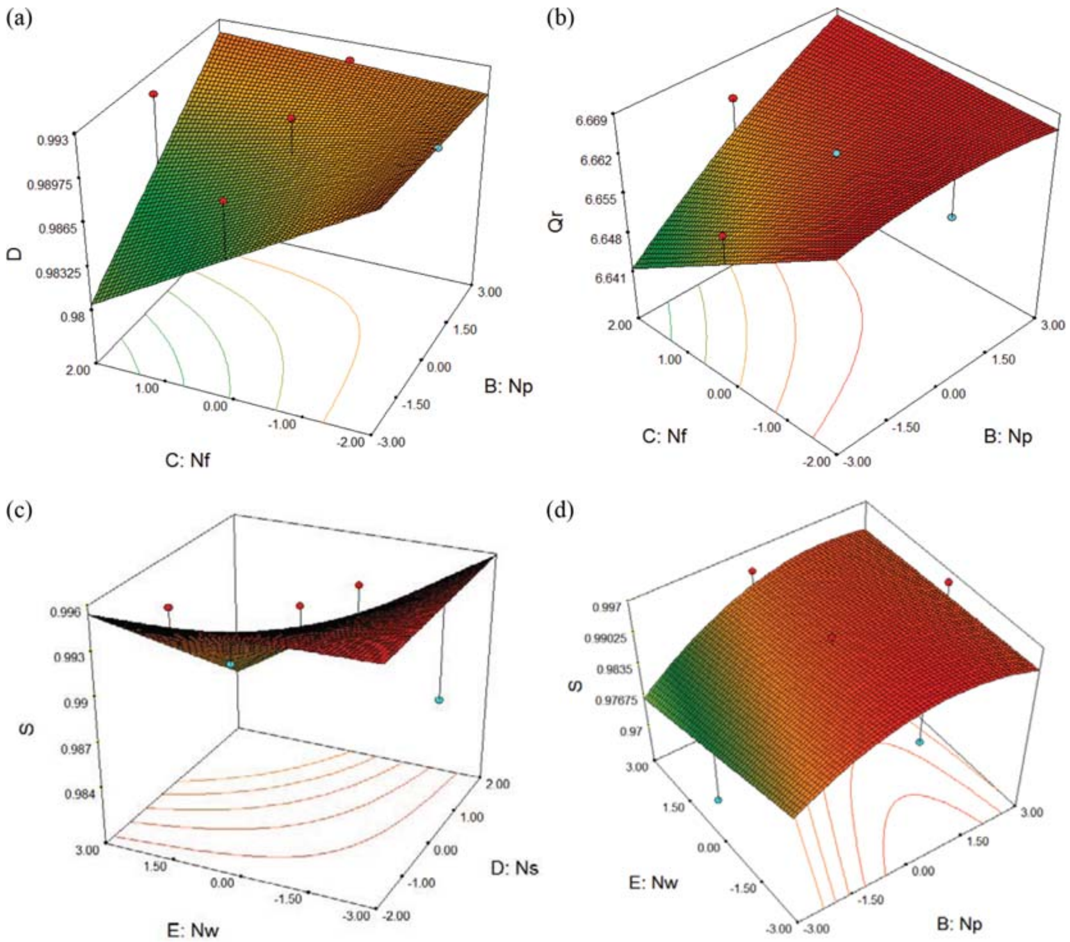

Fig. 4. Three-dimensional response surface plot for the interactive effect of structural parameters.

Table 5. Optimum structural parameters of DWC

N_t	N_P	N_f	N_s	N_w
36	10	7	21	17-26

Table 6. Simulation range

Process factor	Simulation range	
	Lower level	Upper level
A: RR	15	20
B: Rv	0.25	0.75
C: R_l	0.2	0.7

uct quality.

2. Optimization of Process Variables

After optimizing the number of trays and the location of them, the effect of process variables on product quality, reboiler duty, and diameter of a DWC was investigated. Process parameters (reflux ratio, vapor split ratio (R_V), the liquid split ratio (R_l)) were used for optimization of a three-factor three-level CCD design. Levels of parameters are listed in Table 6. The range of process parameters was chosen from the extreme values that out of this range, simulation does not converge. To obtain an optimal DWC, six dependent parameters were analyzed as responses: quality of three products, the duty of reboiler, the diameter of the main column, prefractionator, and total diameter. Any change in the process parameters causes changes in the responses. Table 7 shows the results for all operational conditions proposed by the RSM design.

Normal distribution tests are required to ensure the errors are normally distributed and presumptions of the analysis are satisfied. Several tools are available to assess the normality of data, including producing a normal probability plot, and carrying out an Anderson-Darling normality test. Normal probability plot assays the assumption of normality. This provides a more decisive approach for deciding if a data set is normally distributed. The normal distribution is a good fit if the data points nearly pursue a straight line. The Anderson-Darling Normality Test measures how well the data follow the normal distribution (or any particular distribution). It is a statistical test that compares the actual distribution with the theoretical normal distribution [45]. A normal probability plot of the residuals and Anderson-Darling Normality for side stream and the diameter of a prefractionator are shown in Fig. 5. The data points reasonably fall in a straight line, which falls mainly between the 95% confidence interval limits, and so it can be concluded that the data is normally distributed. Also the p-values of

Table 7. RSM results for each of the operational conditions

Std. order	Factor 1	Factor 2	Factor 3	Response 1	Response 2	Response 3	Response 4	Response 5	Response 6	Response 7
	A: RR	B: Rv	C: Rl	D	S	B	Qr (KW)	Dp (Cm)	Dm (Cm)	Dt (Cm)
5	15	0.25	0.2	0.9872	0.9947	0.9352	5.923	4.363	7.825	12.188
15	20	0.25	0.2	0.9897	0.9969	0.9378	7.751	5.018	8.966	13.984
6	15	0.75	0.2	0.9806	0.9548	0.8533	5.908	7.631	4.678	12.309
8	20	0.75	0.2	0.9821	0.9605	0.865	7.73	8.742	5.33	14.072
7	15	0.25	0.7	0.9526	0.916	0.7945	5.853	4.249	7.7	11.949
4	20	0.25	0.7	0.9626	0.9319	0.8201	7.681	4.896	8.852	13.748
3	15	0.75	0.7	0.9905	0.9545	0.8444	5.927	7.629	4.714	12.343
2	20	0.75	0.7	0.991	0.9683	0.874	7.752	8.731	5.395	14.126
11	15	0.5	0.45	0.99	0.9914	0.9254	5.927	6.226	6.459	12.685
1	20	0.5	0.45	0.9907	0.9947	0.9324	7.752	7.128	7.394	14.522
12	17.5	0.25	0.45	0.9682	0.9651	0.8878	6.79	4.578	8.332	12.91
9	17.5	0.75	0.45	0.9904	0.997	0.9373	6.842	8.212	5.039	13.251
14	17.5	0.5	0.2	0.9911	0.9883	0.9177	6.842	6.701	6.943	13.644
13	17.5	0.5	0.7	0.9855	0.9385	0.8139	6.827	6.646	6.937	13.583
10	17.5	0.5	0.45	0.9904	0.9934	0.9295	6.841	6.691	6.944	13.635

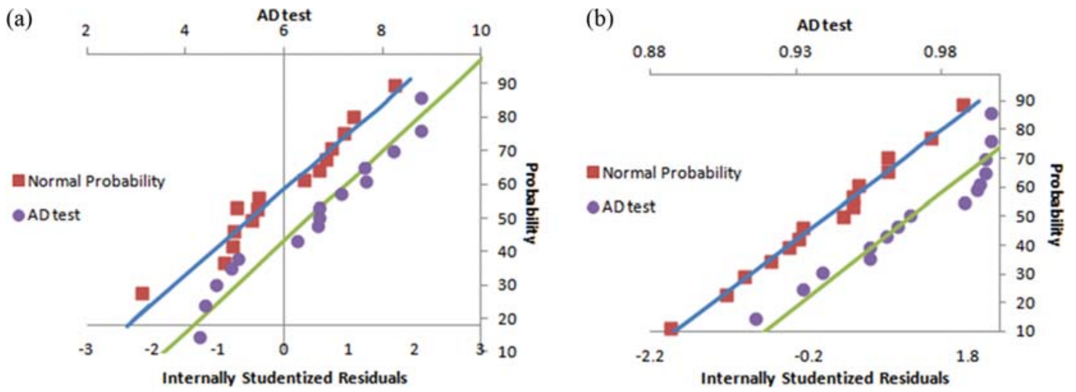

Fig. 5. Normal probability plot residuals and AD test for, (a) diameter of prefractionator (b) side stream.

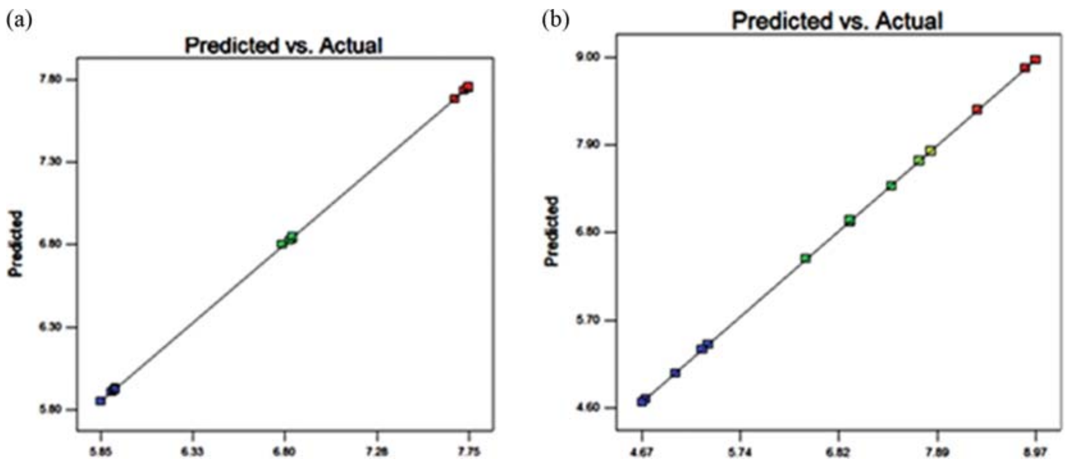

Fig. 6. Scatter diagram of predicted response versus actual response for, (a) Q_R, (b) diameter of main column.

two plots of AD test are more than 0.05, which suggests that the data follow the normal distribution.

Fig. 6 displays the relationship between the actual and predicted values for the diameter of a DWC. These plots help recognize the model satisfactoriness. The residuals are close to the diagonal line, so it is concluded that an adequate agreement between simulated data and predicted values.

In Table 8, P-values of the model and each parameter demonstrate that the model is statistically significant and show the effect of parameters and interaction on the parameters. The ANOVA results represent a relationship between R_v (B), R_l (C), the interaction of them, and distillate purity. Furthermore, according to the

Table 8. ANOVA analysis for optimization process parameters (p-value)

Source	D	S	B	Q_R	D_p	D_m	D_t
Model	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
A-RR	0.1356	0.1869	0.2339	<0.0001	<0.0001	<0.0001	<0.0001
B-Rv	<0.0001	0.3132	0.9816	0.0012	<0.0001	<0.0001	<0.0001
C-Rl	0.0007	0.0002	0.0005	0.0054	0.0133	0.0164	0.0094
AB	0.2359	-	-	0.6957	<0.0001	<0.0001	0.6376
AC	-	-	0.4617	0.8955	0.8239	0.3208	0.8234
BC	<0.0001	0.0003	0.0017	0.0004	0.0276	0.0002	0.0022
A2	-	-	-	0.7095	0.7448	0.2988	0.8678
B2	0.0002	0.2095	0.5348	0.0063	<0.0001	<0.0001	<0.0001
C2	-	0.0001	0.0018	0.5445	0.9053	0.6205	0.7845

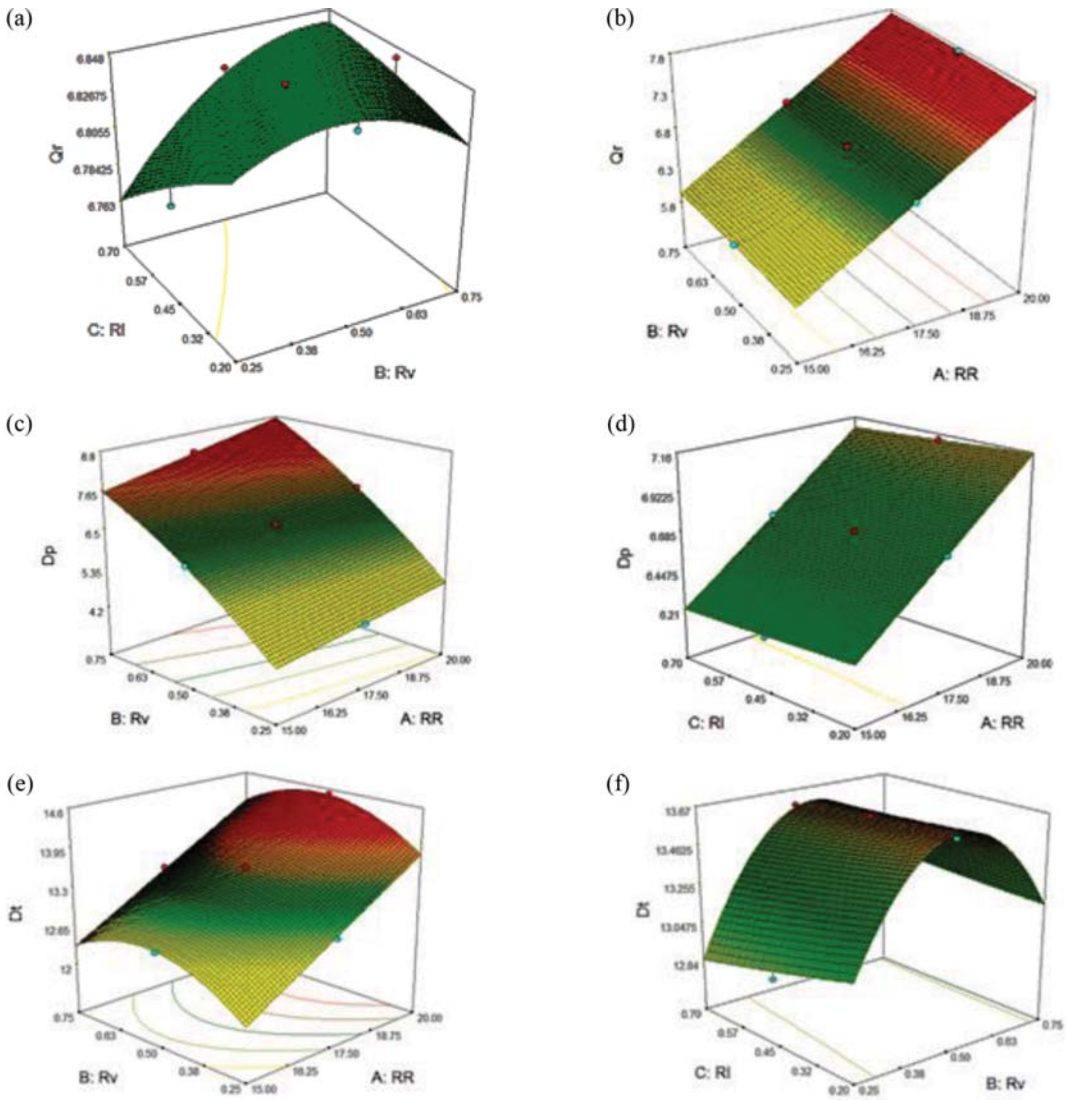

Fig. 7. Three-dimensional response surface plot for the interactive effect of process parameters on (a), (b) reboiler duty; (c), (d) diameter of prefractionator; (e), (g) total diameter.

p-value, significant model terms for side stream were found to be R_v and interaction between R_v and R_l. The response surface diagram of the multi-factors interactions is shown in Fig. 7.

The results indicate that the interaction between R_v and R_l has the most effect on reboiler duty; also, with increasing R_l and decreasing R_v, the energy efficiency of a DWC is decreased. As shown in Fig. 7(b), to have the minimum reboiler duty, the reflux rate should be decreased. As can be seen from Fig. 7(c), while RR was reduced to approximately 17 the D_p was reduced, and around this minimum range, the R_l does not affect the diameter of prefractionator. This trend is similar for interaction of BC. As illustrated in Fig. 7(d), at an optimum range of R_v, parameter R_l has no effect on the optimization of D_p. Fig. 7(e) depicts the effects of R_v and RR on total diameter of a DWC. As clearly illustrated in Fig. 7(g), for decreasing the D_t, R_v and R_l should decrease simultaneously and around point (15.73, 0.32) the diameter is minimized.

Using the point prediction option in the software, the optimum values for RR, R_L and R_V were estimated to be 15, 0.32, and 0.44, respectively. At these values of R, L, V, the product purities are high (D=0.995, S=0.996, B=0.993). Also, the energy requirement in the reboiler after the optimization was found to be 5.93 KW. Thus, the reboiler duty for a DWC was found to be less than that of the initial design. Furthermore, the diameter of the column was (D_p= 6.81 m and D_m=5.84 m). Eventually, our study demonstrates that the optimum location for the dividing wall of this feed is in the center of the column.

CONCLUSION

A practical method is proposed for energy optimization and investment of dividing wall columns (DWCs) based on response surface methodology (RSM). This design technique optimizes the parameters of DWC simultaneously with minimal simulation runs. The effect of factors and their interactions on energy requirement, product quality, and diameter of DWC was studied. Results show that effect of interaction between vapor split ratio and liquid split ratio and also reboiler duty are the important parameters in DWC design. Moreover, the interaction between Rv and RR showed the greatest impact on the diameter of prefractionator. Results demonstrate that for each response, different parameters and interactions were important. Therefore, to optimize a divided wall column, all parameters should be considered simultaneously. The predicted results by the RSM showed a good agreement with the simulated results. Undoubtedly, RSM is a powerful technique to optimize process parameters of a DWC.

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NOMENCLATURE

A, B, C : chemical components
B : bottom product
D : distillate
DWC : divided wall column
Dp : diameter of prefractionator
Dm : diameter of main column
Dt : total diameter of column
E : random error
Nf : feed tray number
Np : number of trays in prefractionator
Ns : side product tray number
Nw : vertical position of divided wall
Nt : total number of trays
QR : reboiler duty
RR : reflux ratio
Rv : vapor split ratio
Rl : liquid split ratio
S : side stream product
X : levels of the independent variables
Y : predicted response

Greek Letters

B : regression coefficients of the independent variables

Indexes

i : linear coefficient
ii : the squared effect
ij : interaction effect
j : quadratic coefficient

Abbreviations

ANOVA : analysis of variance
CCD : central composite design
DWC : divided wall column
RSM : response surface method

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