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Intensification of Azeotropic Distillation for Ethanol Dehydration using Data-based Optimization, Steady-state Simulation and Sensitivity Analysis

T. Fattahi, E. Salehi^{*}, Z. Hosseini

Department of Chemical Engineering, Faculty of Engineering, Arak University, Arak, 38156-8-8349, Iran

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ABSTRACT

The Ethanol-water separation involves a well-known azeotrope that confines the achievement of the ethanol purity to the values higher than 95 wt% using straightforward distillation. Many attempts have been made to identify how it can be possible to produce ultra-pure ethanol (99.95 wt%) for various valuable applications. In practice, minimizing the total cost of the process is of high importance beside having the finished product with utmost purity. As a consequence, finding the best process conditions imposed to apply the simulation and statistical optimization methods in combination. Numerical optimization provides the best trade-offs to achieve the goals. In this research, the separation of the ethanol/water mixture (87 wt%) was simulated using azeotropic distillation in Aspen plus[©] environment. Indeed, cyclohexane was chosen as an effective azeotrope-former. The UNIQUAC equation was used to describe the phase behavior. The two-column arrangement, in which the first column was used to dehydrate ethanol and the second to recover the entrainer, was applied in this simulation. The effect of important process variables, including the number of the trays in columns and the feed-tray position in each tower on the total capital cost were investigated. Finally, the process variables were optimized via the Response Surface Methodology to minimize the total cost of the process. The results uncovered that the total capital cost would be minimized if the number of the trays in the azeotropic (C1) and recovery (C2)columns were set to 34 and 40, whereas, the feed-tray numbers were adjusted to 19 and 9 respectively.

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1. Introduction

Fossil fuel termination and air pollution are controversial and much-disputed issues within the context of energy concerns. A biomassoriginated fuel such as ethanol, as a renewable energy resource, is a short-term alternative. So, the combination of ethanol in the roll of the octane-booster or fuel-modifier, with other fuels such as gasoline has gradually been developed in some countries[1-3]. The finishing step of the ethanol production process is dehydration [4-6]. As illustrated in Fig. 1, with a positive deviation from the Raoult's law, the ethanol/water mixture can be obtained with the ethanol purity of about 95 % wt via simple distillation, even though the required purity of ethanol for mixing with gasoline must be at least 99.2 % wt.



Figure 1. T-x-y diagram of the Ethanol-water binary mixture (Derived by Aspen plus[©] version 10 ; the T-x-y plot by using the UNIQUAC equation)

A common separation method to dewater the ethanol/water mixture is azeotropic distillation. Two or more columns in various arrangements besides the addition of a third component as an entrainer to the binary mixture are applied to produce high-purity (more than %99) ethanol. The added substance makes a new low-boiling point azeotrope with one of the main components [6], and finally, the desired high-purity product can be achieved. If the deviation from Rault's law is large enough $(1.0 \ll \gamma_i^l)$ the phase separation may occur and a low-boiling heterogenic azeotrope would be formed in which the vapor phase is in equilibrium with two different liquid phases [7].

A common heterogeneous azeotropic distillation process is composed of a recovery

column followed by an azeotropic distillation column. The hydrated ethanol and the entrainer which can be benzene, pentane, isooctane, and cyclohexane [8], are fed to the azeotropic column to obtain the pure ethanol from the bottom. A ternary minimum-boilingpoint azeotrope is formed at the tower overhead that includes water, ethanol, and the applied entrainer (Fig.2). While the top stream of the column is a heterogeneous mixture, the liquid phase can readily be separated into organic and aqueous phases in a decanter. The light organic phase which is rich in entrainer, should be recycled to the azeotropic column by a reflux stream. The aqueous phase containing a new binary azeotrope between water and the third component is fed to the second column to recover the entrainer at the top and the residue

water at the bottom [9]. Some surveys [10-12], have been focused on comparing benzene with cyclohexane in the role of entrainer. They have expressed that the energy consumption is reduced in the case of using cyclohexane beside avoiding the carcinogenic effects.

The interpretation of the demeanor and possibility of separation in distillation towers is deeply conjunct with the Residual Curve Maps (RCMs) analysis. As depicted in Fig. 2, the ternary diagram of ethanol-watercyclohexane includes one minimum-boiling

binary homogeneous azeotrope, two minimum-boiling binary heterogeneous azeotropes, and a minimum-boiling ternary one. heterogeneous Accordingly, three distillation regions can be distinguished within the phase diagram. In this case, it should be noticed that ethanol and water (major separating components) are located in different distillation regions. Accordingly, to obtain pure ethanol, the first the column feed composition needs to fall within the region II [13].



Figure 2. Ethanol-Water-Cyclohexane ternary diagram-Molar basis (Derived by Aspen plus[©] version 10; the residual plot by using the UNIQUAC equation)

Several studies have been done to determine the non-homogeneous azeotropic distillation system sequence [5, 9, 10, 13-16]. Common sequences include three or four columns with various implementations of the recovery section. It has been illustrated that the column sequence and stream injection locations are influencing parameters that greatly affect the reboiler energy consumption, waste of ethanol and ethanol contamination by the entrainer [17]. Mortaheb et al., demonstrated that the number of required trays would be diminished by rising up of the recycle stream flowrate. They found that if the feed tray gets nearer to the bottom of the tower, more trays are required [14]. It is claimed that vapor and liquid flowrates will be significantly increased when the recycle stream flowrate is raised. Luyben's investigations [10] showed that to have the desired economy, the ethanol purity in the first column should be at least 85 mol%. Moreover, the energy consumption will be reduced while the feed tray is upper. Wolf et al. [12], utilized the factorial design and RSM to optimize the energy consumption. Their study focused on the effect of the decanter temperature on the energy consumption. Previous studies have only dealt with the design, control and influence of operating parameters and the ternary diagram description to archive a highpurity product in a case study, as summarized in Table1.

Table 1

Item No.	Methodology	Survey main focus	Ref.
1	Process Simulation by Hysys Applying RSM	Selection of the best configuration regarding energy consumption amount Optimization of process parameters at the selected best configuration by RSM to minimize Energy consumption	[5]
		Entrainer: Benzene 3-Tower arrangement	
2	using rigorous simulation	Effects of design parameters on the energy and capital investment Distillate composition trade-off Entrainer: Benzene, Cyclohexane	[10]
3	Ternary map explanation	Heterogeneous azeotropic distillation Different configurations	[18]
4	process analysis and dynamic simulation	Design and control in industrial-scale Interpretation of heterogeneous azeotropic distillation column systems Isopropyl alcohol and water with cyclohexane system Total annual cost (TAC) analysis Optimum design of the two-column approach	[19]
5	Ternary map explanation	Suggestion of possible column configurations with respect to RCMs for any azeotropic system	[7]
6	Ternary map explanation	Feasible column sequence for the separation Isopropyl alcohol and water with cyclohexane system	[15]

Some of important studies focused on the ethanol dehydration process

	The Aspen Plus steady-state and dynamic simulation	The comparison of all the costs calculated for the three design alternatives	
7	Using a dynamic model by Aspen Dynamics developing a plant-wide control scheme Ternary map explanation	Use of a decanter to cross a distillation boundary production of anhydrous ethanol from an ethanol/water mixture using benzene Process parameters controlling to achievement of 99% wt purity Investigation of effective parameters on higher purity (99.9% wt)	[20]
8	Steady-state simulation and sensitivity analysis Literature-based control scheme using the Aspen Dynamics An intelligent control design replacement	Ternary system ethanol-water-benzene Sensitivity analysis of operating parameters such as the reflux, recycle and feed currents of C1; the flow entering to the heat exchanger-decanter subsystem; and the aqueous current from the decanter, feeding C2.	[21]

The optimal process design involves mapping and the interpretation of RCMs in the particular case. Moreover, little attention has been paid to the ability of data-based approaches to optimize basic design parameters such as the feed-tray number and the number of trays for the production of highpurity ethanol under the minimized Total Annual Cost. When the multivariate and/or multi-objective optimizations are aimed, process simulators are not individually sufficient [18]. The novel approach in this study is combining statistical data-based optimization methods with the process simulation for analyzing the design parameters and optimizing the total capital cost of the ethanol dehydration process. Results lead to a valuable set of design data in which the production of ultra-pure ethanol (99.95 wt%), can be achieved with the lowest fixed investment for the process.

2. Methodology

2.1. Case study and process simulation

In the present study, the azeotropic dehydration of ethanol has been simulated in a steady-state mode by Aspen Plus[®] version 10. two-sequential-column The arrangement equipped with a decanter has been considered for ethanol dehydration using cyclohexane as entrainer via azeotropic distillation [19]. To predict the thermodynamic properties of a seriously non-ideal system of ethanol-watercyclohexane, the UNIQUAC activity model has been applied for the prediction of the liquid phase behavior whereas cyclohexane was considered as an appropriate entrainer [20]. Furthermore, the Redlich–Kwong (RK) equation of state was utilized for the prediction of the vapor phase behavior. It is noted that the maximum separation efficiency has been archived when cyclohexane was used as a carrier [19]. Most of previous studies have been concentrated on the azeotropic column (C1) however, the recovery column (C2) needs more consideration because the overhead product of C2 must be recycled into C1. The base case flowsheet of the two-column azeotropic distillation is displayed in Fig. 3.



Figure 3. Ethanol-Water separation system by Cyclohexane entrainer (Base case, Data is extracted from the present simulation by Aspen plus[©] version 10)

There are three feed inlets and two product outlet streams, so the degree of the freedom of C1 would be 2. The main feed stream enters column C1 at a concentration of 87 mol% of ethanol, near the binary azeotrope point, and a vapor fraction of 0.3. The simulation was handled on the basis of 100 kmol/h of the main feed. The top product stream of C1 contains a mixture in the ternary azeotrope composition (D3), which is separated into organic and aqueous phases under an appropriate condition in the decanter.

As well as the formation of two liquid phases in the decanter after condensation, the generation of pure ethanol of 0.9995 mol % is

desired as the bottom product of C1. This value was adjusted in all the cases studied to reduce the degree of freedom. The number of the required trays of 62 and 100 (including the reboiler) was considered in C1 and C2 respectively, as done in the base case [10]. Tables 2 to 4 illustrate the input data of C1, decanter, and C2. It is worth mentioning that the ranges of the process variables (applied according to values reported in the base case), were considered to evaluate the flexibility of the process parameters via the Aspen optimization simulation, data-based and sensitivity analysis assessment.

	Con	figuration	Strea	Streams Condenser		3-Phase		
Number	of	62	D1	1	pressure	1bar	Starting stage	1
stages								
Condenser		Total Valid	FEED	20			Ending stage	62
Phases		Vapour-Liquid-						
		Liquid	D2	20			Key components	Water
Convergence		Strange non-ideal						
		liquid						
Spec		Bottoms rate=50						
		Reflux						
		Ratio=3.5						

Table 2

Input data of C1

Table 3

Input da	ata of	decante	r
ã			

Specificati	ons	Key components
Pressure	1bar	Water
Temperature	25°C	

The organic phase formed in the decanter was recycled to C1 as the reflux stream and a makeup stream containing cyclohexane was

Table 4

Input data of C2

added to the organic reflux (R1), to compensate the entrainer loss. Also, the aqueous phase was fed to C2 for recovery. The degree of the freedom of C2 with one feed and two products is 2, and so, the run of the flow sheet based on a specification is inevitable. The production of pure water (0.9999 mol%) is expected at the bottom of C2, so, this value was fixed.

Configuration		Streams		Condenser	
Number of stages	100	R2	30	Pressure	1bar
Condenser	Total Valid				
Phases	VLL				
Convergence	Strange non-ideal liquid				
Spec Bottoms rate=8					
	Reflux Ratio=5				

2.2. Design of the experiments

The Response Surface Methodology (RSM) was used to predict the target function i.e., the total capital cost. Therefore, the Box-Behnken algorithm was employed using the Design Expert v.10 software (Stat-Ease, USA). The selected process variables were considered as "the number of trays" and "the feed-tray number" in both C1 and C2 columns.

Box and Behnken have offered some designs for a spherical space considering only three levels for every factor. The balanced incomplete block design structure is considered the basis of the design class. Indeed, all points suggested by the Box– Behnken design (BBD) are put on a spherical area by the radius of $\sqrt{2}$. Moreover, no point at the vertices of the cubic zone created by the upper and lower limits for each factor are included in this design [21, 22]. The total number of the runs in BBD can be obtained via N= 2k (k-1) + cp, where k is the number of factors and (cp) is the number of the central data points [22].

The flexibility of the process simulation was investigated for different parameters via the Aspen plus sensitivity analyzer (SA) module to find out the most effective design parameters with an acceptable range of variation. Attention was paid that as well as the formation of two different liquid phases in the decanter, the aim of the purity of 99.95 wt% of ethanol must be met. So, the experimental design was established considering the identified factors where the tray number of C1 was set to 34 (Causality is explained in the result and discussion section).

Table 5 indicates the levels of the selected variables. The range of variation for each factor was selected based on the values reported in the previous studies.

Table 5

Levels of variables in the Design of Experiments (DOE)

Variables		Levels			
v al lables		-1	0	1	
Feed tray number of C1	FT1	1	12.5	24	
Feed tray number of C2	FT2	8	21.5	35	
Number of trays of C2	N2	40	55	70	

Simulation was done for each design case (based on the Table of Experiments suggestions) and the flow-sheet results were transferred to the Economy Analyzer module in the Aspen Software. So, the estimated total capital cost (target function) for all the runs was extracted from the Economy Analyzer and inserted in the DOE optimization tool.

The quadratic form of the response-surface model was extended to describe the total capital cost as target function [23]:

$$R = \beta_0 + \sum_{i=1}^n \beta_i x_i + \sum_{i=1}^n \beta_{ii} x_i^2 + \sum_{i=1}^n \sum_{j=i+1}^n \beta_{ij} x_i x_j + \varepsilon$$
(1)

where β_0 , β_i , β_{ii} , and β_{ij} are the equation constants. The validation of the predicted model was checked by the compatibility of the simulation results with the model response under the suggested optimal conditions. To identify the significance of the model and parameters, analysis the of variance (ANOVA), was applied. Emphasizing the mentioned data, Fisher's F values and the probability values (P-values), were used. Moreover, the residues, normal distribution, and the curve fitting coefficients of determinations (R^2 , adjusted- R^2 and predicted- \mathbf{R}^2) were utilized to demonstrate the precision of the model [21].

The desirability function approach is one of the nonlinear programming techniques commonly used to solve optimization problems. This approach is followed by transforming the value of each response to a scale-free value between 0 and 1; called individual DFs (di), which are established with respect to the maximum, minimum or average value of the set target related to each response. More details can be found in other references [21, 22, 24].

2.3. Sobol's Sensitivity Analysis

Sobol's method is a variance-based sensitivity analysis which consequently provides useful insight about the contribution of the model inputs to the model outcomes. The method includes the decomposition of the model output variance into the summation of variances of the input parameters. The Sobol sensitivity analysis defines the share of input variables and their interactions of the overall model output variance [25]. Detailed mathematical relations of the Sobol approach are given elsewhere [18]. This approach was applied to clarify the sensitivity of the target function (Total capital cost), approximated by the model to the defined process variables.

3. Results and Discussion

3.1. Evaluation of the purposed model

As mentioned above, a quadratic model was applied for the prediction of the total capital cost of ethanol dehydration via the azeotropic distillation process, in which three variables in three levels were considered. The model was developed under the condition that the tray number of C1 column was adjusted to 34. In backing, the value is selected owing to the investigation of the rangeability of the parameters. Broadly, this value points to the minimum required tray number in which liquid phases can form in the decanter and the required purity is met. Indeed, due to the minimum required trays for minimizing the Total Capital Cost in the base case and the negligible effect of this parameter on the energy consumption (Fig.4), the number of trays in C1 was adjusted to 34. In fact, the reflux flowrate to C1 will decline when the tray number rises, bringing out the lower energy consumption. In contrast, minimizing the number of trays helps to lower the fixed capital cost [10, 11].



Figure 4. Energy consumption of (a) reboiler (b) condenser of C1versus the tray number.

Other three factors were applied in the experimental design and the RSM optimization algorithm was used to minimize the total capital cost. To determine the critical point (maximum, minimum, or saddle) of the predicted model, it is necessary for the polynomial function to contain quadratic terms (Eq. 1) [23]. Therefore, a quadratic form containing BBD as a symmetrical design in three levels was followed. Applying BBD for the design of experiments will prevent any out-

Table 6

ANOVA for the Response Surface Quadratic mode

of-range experiments so; all the cases will be physically acceptable in the case of the ethanol dehydration process.

ANOVA results are presented in Table 6. The Model F-value of 706.23 implies that the model is significant. There is only a 0.01% chance that such an F-value could occur due to noise. The values of probability less than 0.0500 indicate that the model terms are significant.

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Source Model	Sum of Squares	df	Mean Square	F Value	P-value
	1.707E+012	9	1.897E+011	706.23	< 0.0001
FT1	1.097E+011	1	1.097E+011	408.49	< 0.0001
FT2	9.283E+009	1	9.283E+009	34.56	0.0020
N2	1.470E+012	1	1.470E+012	5473.52	< 0.0001
FT1×FT2	6.951E+009	1	6.951E+009	25.88	0.0038
FT1×N2	6.496E+007	1	6.496E+007	0.24	0.6437
FT2×N2	1.541E+009	1	1.541E+009	5.74	0.0620
FT12	1.086E+011	1	1.086E+011	404.32	< 0.0001
$FT2^2$	2.633E+009	1	2.633E+009	9.80	0.0259
$N2^2$	1.764E+009	1	1.764E+009	6.57	0.0505
Residual	1.343E+009	5	2.686E+008		
Cor Total	1.708E+012	14			
NTI NI I C	6.01				

N1: Number of trays/stages of C1

N2: Number of trays/stages of C2

FT1: Feed-tray No of C1

FT2: Feed-tray No of C2

In the current case, FT1, FT2, N2, FT1×FT2, FT1², FT2² are significant model terms. The adequate precision known as the signal-to-noise ratio should be greater than 4 to bring out enough desirability. So, the ratio of 85.024

indicates an adequate signal. The interpretation of Fisher's F values and the probability values (P-values) represents the equation (2), which can define the total capital cost versus the significant model terms:

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Total \ Capital \ Cost \ (USD) = 8.12598 \times 10^{6} - 47089.84982 \times FT1 - 12463.96195 \times FT2 + 16099.44257 \times N2 + 268.50242 \times (FT1 \times FT2) + 1296.74858 \times FT1^{2} + 146.52949 \times FT2^{2} (2)
```

The variables in equation (2) are obtained from the simulation results and are not coded values. Proceeding the probability and residue plots demonstrate a normal distribution pattern (Fig.

5a and 5b). The model and the experimental results show relatively good compatibility. Also, the random spread values come up with the adequacy of the developed model.



Figure 5. (a) Normal probability plot vs. the studentized residuals (i.s. the variance-scaled residuals) (b) Predicted vs. simulation results of the total Capital Cost.

The goodness-of-fit coefficients (\mathbb{R}^2 , adjusted- \mathbb{R}^2 and predicted- \mathbb{R}^2) for the objective function were all close to 1, with the values of 0.9992, 0.9978 and 0.9874 respectively. The results of

the experimental design, simulation results (simulated responses) and predicted responses (by the expert model) are shown in Table 7.

Table 7	
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Designed experiments via Box- Behnken for 3 Factors

EXP	FT1	FT2	N2	Total Capital Cost (USD)	
No.				Simulation	Predicted
				result	result
				(response)	
1	1	21.5	70	9620360	9632961
2	1	35	55	9211160	9197483
3	24	35	55	9051140	9046638
4	12.5	35	70	9419660	9420723
5	12.5	8	40	8496320	8495248
6	1	8	55	9208230	9212723
7	12.5	21.5	55	8889800	8889796
8	24	21.5	40	8554010	8541401
9	12.5	35	40	8507030	8524128
10	24	21.5	70	9387260	9390686
11	12.5	21.5	55	8889800	8889796
12	1	21.5	40	8770990	8767556
13	12.5	21.5	55	8889800	8889796
14	24	8	55	8881470	8895138
15	12.5	8	70	9330450	9313343

3.2. Binary interactions of the process variables

Another attractive finding was observing the significant effect of the binary interactions of parameters through 3D plots, as illustrated in Fig. 6a to 6d. Generally, an interaction term displays the synergetic influence of parameters by which the response is affected. Binary interactions of parameters can be demonstrated

in the corresponding images of the 3D plot of the model. In conformity with ANOVA results, the effect of the Total Capital Cost of the model on the corresponding coordinates depicts the synergic effect of FT1 and FT2 to be considerable (Fig.6). The interpretation of the 3D plot reveals the simultaneous effect of FT1 and FT2 on the total capital cost of the purposed process.



Figure 6. FT1-FT2 Binary interaction plot.

This means that even though the increase in the feed-tray-number of C1 and C2 causes a fall in the Total capital cost, their synergic effect brings out a little effect. In continuation, the sensitivity analysis results will give a better sight of the effectiveness of the parameters.

3.3. Sobol's sensitivity results

The most striking results obtained from the Sobol's sensitivity analysis method is presented in Fig.7. As a consequence, the number of the trays of C2 is the most effective parameter by the impact share of 73% and FT1 ranks the second with 23%. Surprisingly, FT2 with 3% has the minimum influence on the Total Capital Cost (TCC) of the process. In fact, the investigation of the sensitivity of the target function to the changes of its structural terms can make a practical view to provide a better design condition.



Figure 7. Sensitivity analysis results obtained from Sobol's method

As it is clear, the binary interaction versus absolute variables (especially N2 and FT1) is neglected. Moreover, the influence of the variation of total tray number of the recovery column is about 3 times more than the impact of the change in the feed tray number of the azeotropic column. So, it looks that a decrease in the number of the stages of the recovery column can result in achieving a lower capital cost (Fig.8 a). On the other hand, when the number of stages in the recovery column rises, the total Capital Cost is downward at first and then displays a slight rise, as it is clear in Fig.8 (b). It can be found that there is an optimal feed-tray number between stages 18 and 19 in which the Total Capital Cost is minimum. In agreement with the sensitivity analysis results, the feed-tray number of the recoverycolumn represents a low impact on the Total Capital Cost (Fig.8 c).



Figure 8. Effect of the parameters variation on the Total Capital Cost around the optimum point: (a) Tray number of the recovery column (b) Feed-tray No of the Azeotropic column (c) Feed-tray No of the recovery column.

3.4. Optimization

To intensify the Total capital cost of the ethanol dehydration process by cyclohexane,

the optimization of parameters was conducted to meet the minimum possible value of the capital cost. The desirability function approach was utilized to find the optimal condition. Results revealed that the Total Capital cost would be minimized where the number of trays and feed-tray number of the azeotropic column (C1) are set to 34 and 19 respectively. In addition, under the optimal conditions, the number of the trays and the feed-tray number in the recovery column (C2) are 40 and 9 respectively. Accordingly, the minimum value of the total capital cost is obtained as 8.46087×10^6 USD under the optimal conditions. This result was also confirmed by the recheck simulation with more than 97% accuracy.



Figure 9. Operating cost variation versus the number of stags of recovery at FT1=19,FT2=9, N1=34

Fig. 9 presents the operating cost growth with the increase in the stage number of the recovery column. On the other hand, the energy consumption of the proposed process in the present study is also minimum within the investigated range.

4. Conclusion

The main focus of this work was the application of data-based optimization methods in consolidation with the process simulation. The ethanol dehydration process using a two-stage distillation-recovery columns arrangement was aimed. Such design has rarely been studied due to the complicated azeotropic conditions and narrow pocket of safe and processable zone in the ternary phase diagram. Concerning the combined approach,

the impacts of the stage number and the feedtray location of the columns on the total capital cost (as objective function), in the base case model, were evaluated via the response surface methodology (RSM). The predicted model was valid according to the confirmation of the response value via the process simulation under the obtained optimal conditions. Ultimately, the Sobol's sensitivity analysis was employed to investigate the share of the selected parameters influencing the response. The results uncovered that in the tow-column configuration design, TCC would be minimized when the stage number and feedtray location (design parameters) in the azeotropic column are set to 34 and 19 respectively, and also, these values are adjusted to 40 and 9 in the recovery column. In

addition, the most effective parameters on the total capital cost are the number of the trays in the recovery column (with 73% impact) and the feed-tray location in the azeotropic column (with 24% impact), under the condition that the number of the stages in the first column was adjusted to 34. Also, the feed input location in the second column showed a negligible effect (about 3%) on the TCC.

Conflict of interest statement

Authors declare that there is no conflict of interest regarding this manuscript.

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Nomenclature

Symbol	Definition
C1	Azeotropic column, First Column
C2	Recovery Column, second column
B1	The bottom product of C1
B2	The bottom product of C2
D1	Reflux stream of C1 including ethanol-rich phase and Makeup of entrainer
D2	The top product of C2, Recycle stream
D3	Overhead stream of C1
R1	Ethanol-rich stream, Organic reflux
R2	Entrainer-rich stream, Feed of C2
RCM	Residual Curve Map
RK equation	The Redlich–Kwong equation of state
RSM	Response Surface Method
ANOVA	Analysis of variance
DOE	Design of Experiments
N1	Number of trays/stages of C1
N2	Number of trays/stages of C2
FT1	Feed-tray No of C1
FT2	Feed-tray No of C2
EtOH	Ethanol
Cyclo-Hex	Cyclohexane
SA	Sensitivity Analysis
BBD	Box–Behnken design
TCC	Total Capital Cost

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